Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 10:30 AM JST

PDB ID	:	6JLU
EMDB ID	:	EMD-9839
Title	:	Structure of PSII-FCP supercomplex from a centric diatom Chaetoceros gracilis at 3.02 angstrom resolution
Authors	:	Pi, X.; Zhao, S.; Wang, W.; Kuang, T.; Sui, S.; Shen, J.
Deposited on	:	2019-03-06
Resolution	:	3.02 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:

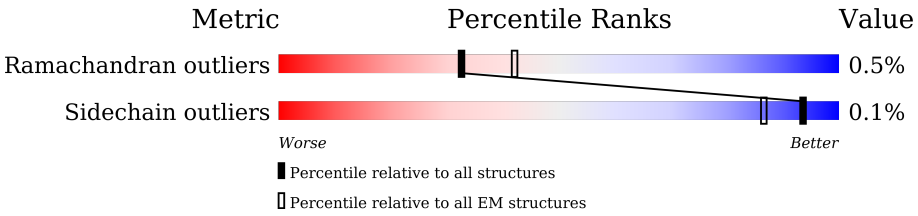
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.02 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)
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	359	92% 7%
1	a	359	92% 7%
2	B	509	5% 98%
2	b	509	5% 98%
3	C	450	99%
3	c	450	99%
4	D	341	99%
4	d	341	99%
5	E	79	13% 100%

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Mol	Chain	Length	Quality of chain
5	e	79	11% 100%
6	F	32	22% 100%
6	f	32	16% 100%
7	G	179	56% 68% 32%
7	g	179	58% 68% 32%
8	H	65	6% 98%
8	h	65	6% 98%
9	I	34	100%
9	i	34	100%
10	J	34	24% 94% 6%
10	j	34	15% 94% 6%
11	K	37	5% 100%
11	k	37	100%
12	L	38	97%
12	l	38	97%
13	M	41	7% 98%
13	m	41	12% 98%
14	N	30	7% 97%
14	n	30	7% 97%
15	O	249	6% 98%
15	o	249	6% 98%
16	P	226	12% 98%
16	p	226	12% 98%
17	Q	211	10% 68% 30%
17	q	211	11% 68% 30%

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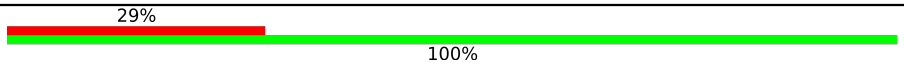
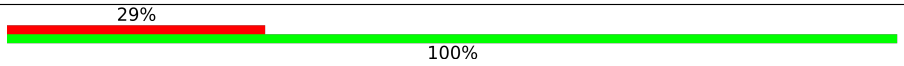
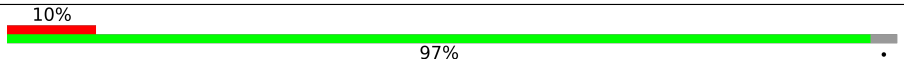
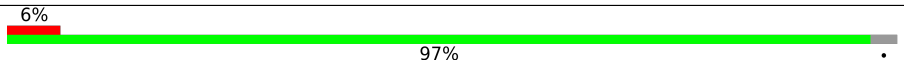
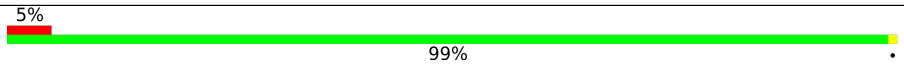
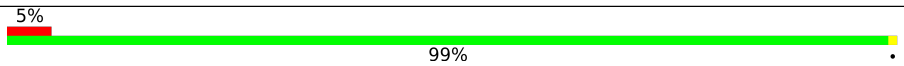
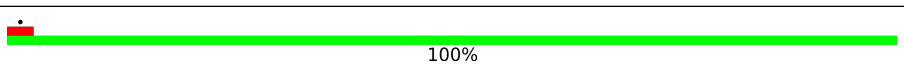
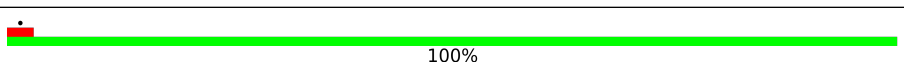
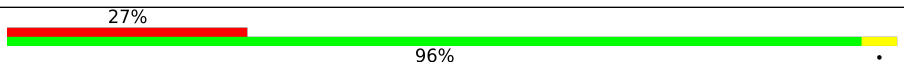
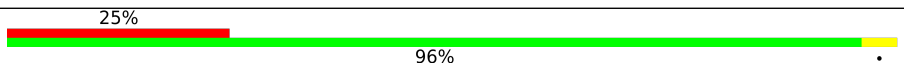
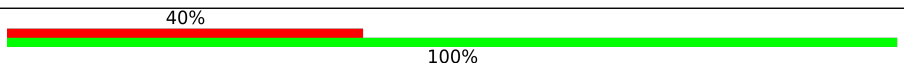
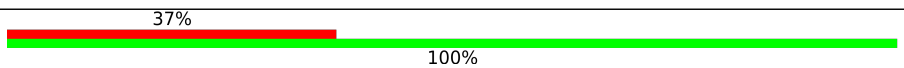
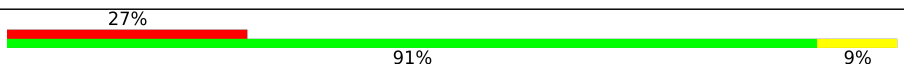
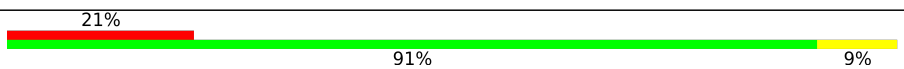
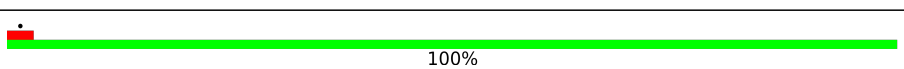
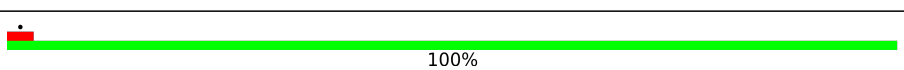
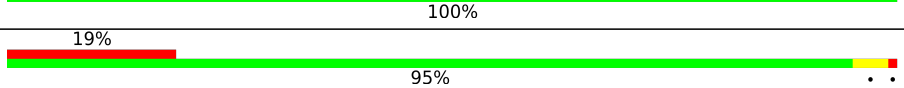
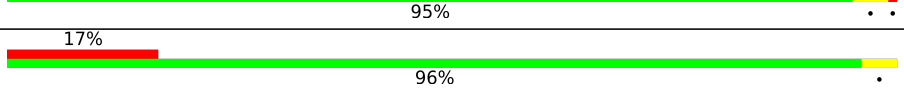
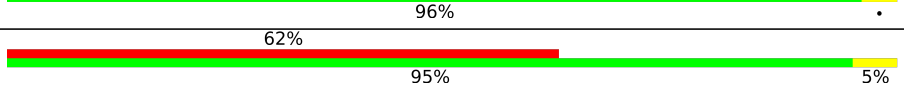
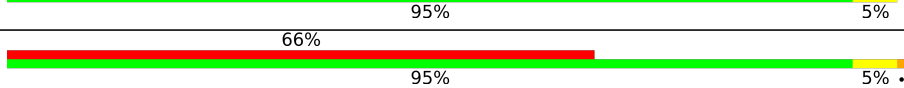
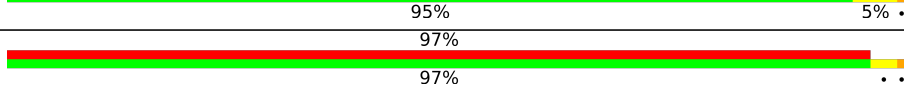
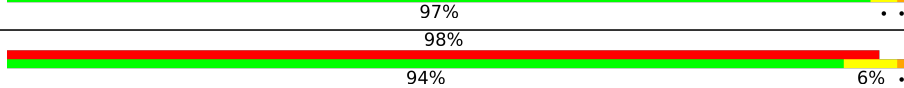
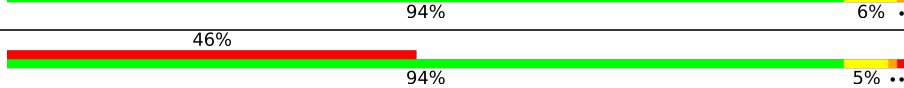
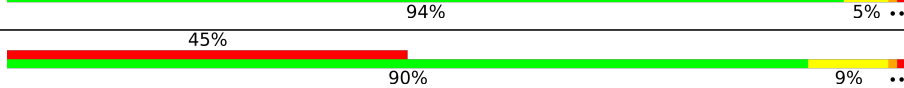
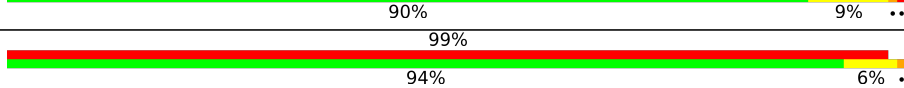
Mol	Chain	Length	Quality of chain
18	R	73	
18	r	73	
19	T	31	
19	t	31	
20	U	93	
20	u	93	
21	V	137	
21	v	137	
22	W	51	
22	w	51	
23	X	35	
23	x	35	
24	Y	33	
24	y	33	
25	Z	61	
25	z	61	
26	0	178	
26	10	178	
27	1	172	
27	11	172	
27	12	172	
27	13	172	
27	14	172	
27	15	172	
27	16	172	

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Mol	Chain	Length	Quality of chain
27	17	172	95% 92% 8%
27	18	172	22% 91% 9%
27	2	172	98% 92% 6%
27	3	172	94% 94% 6%
27	4	172	47% 95% 5%
27	5	172	49% 91% 9%
27	6	172	99% 93% 6%
27	7	172	95% 91% 8%
27	8	172	20% 90% 9%
28	19	166	100% 100%
28	9	166	100% 100%

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
31	CLA	0	307	X	-	-	-
31	CLA	0	308	X	-	-	-
31	CLA	0	311	X	-	-	-
31	CLA	0	312	X	-	-	-
31	CLA	0	313	X	-	-	-
31	CLA	0	316	X	-	-	-
31	CLA	1	307	X	-	-	-
31	CLA	1	310	X	-	-	-
31	CLA	1	312	X	-	-	-
31	CLA	1	313	X	-	-	-
31	CLA	1	316	X	-	-	-
31	CLA	1	321	X	-	-	-
31	CLA	10	307	X	-	-	-
31	CLA	10	308	X	-	-	-
31	CLA	10	311	X	-	-	-
31	CLA	10	312	X	-	-	-
31	CLA	10	313	X	-	-	-
31	CLA	10	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	10	316	X	-	-	-
31	CLA	10	317	X	-	-	-
31	CLA	11	307	X	-	-	-
31	CLA	11	308	X	-	-	-
31	CLA	11	310	X	-	-	-
31	CLA	11	312	X	-	-	-
31	CLA	11	313	X	-	-	-
31	CLA	11	315	X	-	-	-
31	CLA	11	316	X	-	-	-
31	CLA	12	307	X	-	-	-
31	CLA	12	308	X	-	-	-
31	CLA	12	310	X	-	-	-
31	CLA	12	312	X	-	-	-
31	CLA	12	316	X	-	-	-
31	CLA	13	307	X	-	-	-
31	CLA	13	308	X	-	-	-
31	CLA	13	310	X	-	-	-
31	CLA	13	312	X	-	-	-
31	CLA	14	306	X	-	-	-
31	CLA	14	307	X	-	-	-
31	CLA	14	309	X	-	-	-
31	CLA	14	311	X	-	-	-
31	CLA	14	312	X	-	-	-
31	CLA	14	314	X	-	-	-
31	CLA	14	315	X	-	-	-
31	CLA	15	306	X	-	-	-
31	CLA	15	307	X	-	-	-
31	CLA	15	309	X	-	-	-
31	CLA	15	311	X	-	-	-
31	CLA	15	313	X	-	-	-
31	CLA	16	308	X	-	-	-
31	CLA	16	309	X	-	-	-
31	CLA	16	311	X	-	-	-
31	CLA	16	313	X	-	-	-
31	CLA	16	314	X	-	-	-
31	CLA	16	316	X	-	-	-
31	CLA	17	307	X	-	-	-
31	CLA	17	310	X	-	-	-
31	CLA	17	312	X	-	-	-
31	CLA	17	313	X	-	-	-
31	CLA	17	315	X	-	-	-
31	CLA	18	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	18	307	X	-	-	-
31	CLA	18	309	X	-	-	-
31	CLA	18	312	X	-	-	-
31	CLA	18	314	X	-	-	-
31	CLA	19	307	X	-	-	-
31	CLA	19	308	X	-	-	-
31	CLA	19	310	X	-	-	-
31	CLA	19	311	X	-	-	-
31	CLA	19	312	X	-	-	-
31	CLA	19	313	X	-	-	-
31	CLA	19	315	X	-	-	-
31	CLA	2	306	X	-	-	-
31	CLA	2	307	X	-	-	-
31	CLA	2	309	X	-	-	-
31	CLA	3	307	X	-	-	-
31	CLA	3	308	X	-	-	-
31	CLA	3	310	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	315	X	-	-	-
31	CLA	4	307	X	-	-	-
31	CLA	4	309	X	-	-	-
31	CLA	4	311	X	-	-	-
31	CLA	4	312	X	-	-	-
31	CLA	4	314	X	-	-	-
31	CLA	4	315	X	-	-	-
31	CLA	5	306	X	-	-	-
31	CLA	5	307	X	-	-	-
31	CLA	5	309	X	-	-	-
31	CLA	5	311	X	-	-	-
31	CLA	5	314	X	-	-	-
31	CLA	6	308	X	-	-	-
31	CLA	6	309	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	313	X	-	-	-
31	CLA	6	314	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	307	X	-	-	-
31	CLA	7	310	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	8	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	8	307	X	-	-	-
31	CLA	8	309	X	-	-	-
31	CLA	8	312	X	-	-	-
31	CLA	8	314	X	-	-	-
31	CLA	9	307	X	-	-	-
31	CLA	9	308	X	-	-	-
31	CLA	9	310	X	-	-	-
31	CLA	9	311	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	A	403	X	-	-	-
31	CLA	A	404	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C	514	X	-	-	-
31	CLA	D	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	D	404	X	-	-	-
31	CLA	D	405	X	-	-	-
31	CLA	P	601	X	-	-	-
31	CLA	P	602	X	-	-	-
31	CLA	P	603	X	-	-	-
31	CLA	P	604	X	-	-	-
31	CLA	P	605	X	-	-	-
31	CLA	P	606	X	-	-	-
31	CLA	P	607	X	-	-	-
31	CLA	P	608	X	-	-	-
31	CLA	P	610	X	-	-	-
31	CLA	R	101	X	-	-	-
31	CLA	W	202	X	-	-	-
31	CLA	Z	101	X	-	-	-
31	CLA	a	403	X	-	-	-
31	CLA	a	404	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c	513	X	-	-	-
31	CLA	c	514	X	-	-	-
31	CLA	d	401	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	p	601	X	-	-	-
31	CLA	p	602	X	-	-	-
31	CLA	p	603	X	-	-	-
31	CLA	p	604	X	-	-	-
31	CLA	p	605	X	-	-	-
31	CLA	p	606	X	-	-	-
31	CLA	p	607	X	-	-	-
31	CLA	p	608	X	-	-	-
31	CLA	p	610	X	-	-	-
31	CLA	r	101	X	-	-	-
31	CLA	w	203	X	-	-	-
31	CLA	z	101	X	-	-	-
31	CLA	z	103	X	-	-	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 102777 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 PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2617	1711	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2617	1711	429	462	15		

- Molecule 2 is a protein called PsbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3960	2588	669	690	13		
2	b	503	Total	C	N	O	S	0	0
			3960	2588	669	690	13		

- Molecule 3 is a protein called PsbC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3496	2290	583	609	14		
3	c	450	Total	C	N	O	S	0	0
			3496	2290	583	609	14		

- Molecule 4 is a protein called PsbD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2696	1781	441	464	10		
4	d	341	Total	C	N	O	S	0	0
			2696	1781	441	464	10		

- Molecule 5 is a protein called PsbE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total 642	C 415	N 106	O 121	0	0
5	e	79	Total 642	C 415	N 106	O 121	0	0

- Molecule 6 is a protein called PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total 259	C 178	N 43	O 37	S 1	0	0
6	f	32	Total 259	C 178	N 43	O 37	S 1	0	0

- Molecule 7 is a protein called Psb31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	122	Total 922	C 580	N 167	O 174	S 1	0	0
7	g	122	Total 922	C 580	N 167	O 174	S 1	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total 506	C 335	N 82	O 87	S 2	0	0
8	h	65	Total 506	C 335	N 82	O 87	S 2	0	0

- Molecule 9 is a protein called PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total 278	C 188	N 43	O 46	S 1	0	0
9	i	34	Total 278	C 188	N 43	O 46	S 1	0	0

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	34	Total 247	C 167	N 38	O 42	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	34	Total 247	C 167	N 38	O 42	0	0

- Molecule 11 is a protein called PsbK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total 300	C 210	N 44	O 45	S 1	0	0
11	k	37	Total 300	C 210	N 44	O 45	S 1	0	0

- Molecule 12 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total 301	C 203	N 47	O 51	0	0
12	l	37	Total 301	C 203	N 47	O 51	0	0

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	41	Total 308	C 203	N 50	O 55	0	0
13	m	41	Total 308	C 203	N 50	O 55	0	0

- Molecule 14 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	30	Total 150	C 90	N 30	O 30	0	0
14	n	30	Total 150	C 90	N 30	O 30	0	0

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	249	Total 1881	C 1188	N 310	O 375	S 8	0	0
15	o	249	Total 1881	C 1188	N 310	O 375	S 8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	185	SER	ASN	conflict	UNP B6ZHE8
O	336	GLU	ASP	conflict	UNP B6ZHE8
o	185	SER	ASN	conflict	UNP B6ZHE8
o	336	GLU	ASP	conflict	UNP B6ZHE8

- Molecule 16 is a protein called FCP-D.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	226	Total	C	N	O	S	0	0
			1745	1129	290	321	5		
16	p	226	Total	C	N	O	S	0	0
			1745	1129	290	321	5		

- Molecule 17 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	147	Total	C	N	O	S	0	0
			1143	725	188	229	1		
17	q	147	Total	C	N	O	S	0	0
			1143	725	188	229	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	30	VAL	ILE	conflict	UNP B6ZHE9
Q	34	ALA	GLY	conflict	UNP B6ZHE9
Q	70	ILE	VAL	conflict	UNP B6ZHE9
Q	110	SER	ASN	conflict	UNP B6ZHE9
Q	133	GLY	ALA	conflict	UNP B6ZHE9
q	30	VAL	ILE	conflict	UNP B6ZHE9
q	34	ALA	GLY	conflict	UNP B6ZHE9
q	70	ILE	VAL	conflict	UNP B6ZHE9
q	110	SER	ASN	conflict	UNP B6ZHE9
q	133	GLY	ALA	conflict	UNP B6ZHE9

- Molecule 18 is a protein called PsbG.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			365	219	73	73		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	73	Total 365	C 219	N 73	O 73	0	0

- Molecule 19 is a protein called PsbT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total 250	C 174	N 36	O 38	S 2	0	0
19	t	30	Total 250	C 174	N 36	O 38	S 2	0	0

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	93	Total 711	C 454	N 119	O 136	S 2	0	0
20	u	93	Total 711	C 454	N 119	O 136	S 2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	33	ILE	VAL	conflict	UNP B6ZHF0
U	60	SER	ALA	conflict	UNP B6ZHF0
u	33	ILE	VAL	conflict	UNP B6ZHF0
u	60	SER	ALA	conflict	UNP B6ZHF0

- Molecule 21 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	137	Total 1043	C 652	N 182	O 205	S 4	0	0
21	v	137	Total 1043	C 652	N 182	O 205	S 4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	70	ASN	SER	conflict	UNP B6ZHF4
v	70	ASN	SER	conflict	UNP B6ZHF4

- Molecule 22 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	51	Total	C	N	O	S	0	0
			394	247	73	71	3		
22	w	51	Total	C	N	O	S	0	0
			394	247	73	71	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	35	Total	C	N	O	S	0	0
			244	159	40	44	1		
23	x	35	Total	C	N	O	S	0	0
			244	159	40	44	1		

- Molecule 24 is a protein called PsbY.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	33	Total	C	N	O	0	0
			256	168	47	41		
24	y	33	Total	C	N	O	0	0
			256	168	47	41		

- Molecule 25 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	61	Total	C	N	O	S	0	0
			452	301	68	82	1		
25	z	61	Total	C	N	O	S	0	0
			452	301	68	82	1		

- Molecule 26 is a protein called FCP-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	178	Total	C	N	O	S	0	0
			1291	827	219	241	4		
26	10	178	Total	C	N	O	S	0	0
			1291	827	219	241	4		

- Molecule 27 is a protein called FCP-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		

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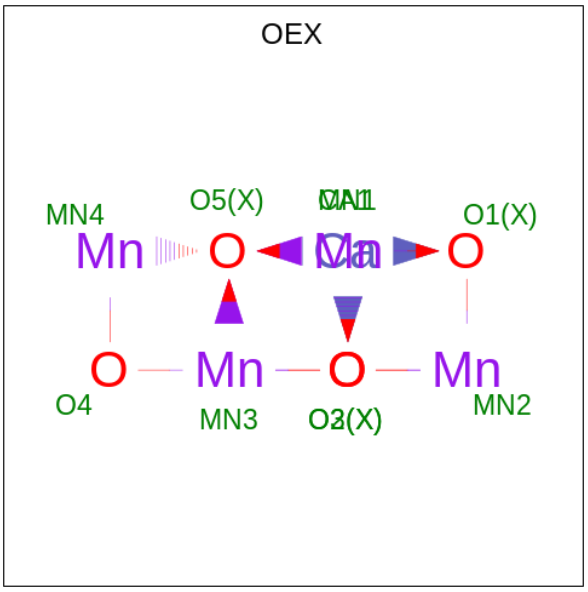
Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	3	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	4	172	Total	C	N	O	S	0	0
			1313	855	212	241	5		
27	5	172	Total	C	N	O	S	0	0
			1280	826	207	242	5		
27	6	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	7	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	8	172	Total	C	N	O	S	0	0
			1291	832	211	243	5		
27	11	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	12	172	Total	C	N	O	S	0	0
			1328	866	215	243	4		
27	13	172	Total	C	N	O	S	0	0
			1332	869	215	243	5		
27	14	172	Total	C	N	O	S	0	0
			1313	855	212	241	5		
27	15	172	Total	C	N	O	S	0	0
			1280	826	207	242	5		
27	16	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	17	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	18	172	Total	C	N	O	S	0	0
			1304	841	215	243	5		

- Molecule 28 is a protein called FCP-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	9	166	Total	C	N	O	S	0	0
			1286	829	212	241	4		
28	19	166	Total	C	N	O	S	0	0
			1286	829	212	241	4		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

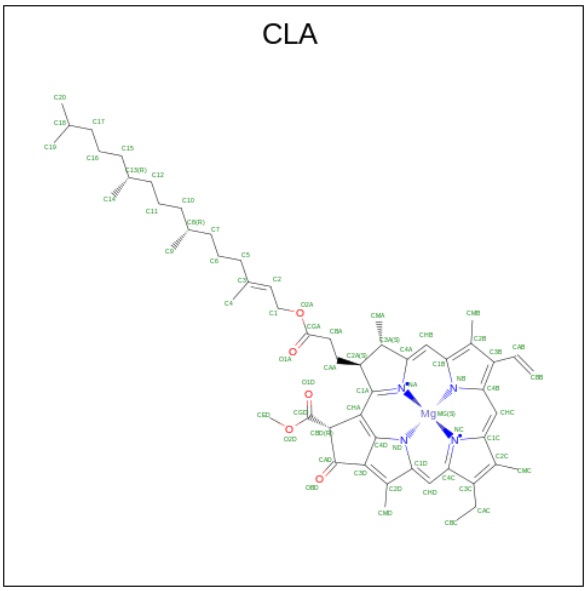


Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	A	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	A	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	D	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
31	D	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
31	D	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

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Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	P	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Z	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	a	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	a	1	Total	C	Mg	N	O	0
			174	144	3	12	15	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
31	d	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
31	d	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
31	d	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	p	1	Total	C	Mg	N	O	0
			447	365	9	36	37	
31	r	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	z	1	Total	C	Mg	N	O	0
			99	79	2	8	10	
31	z	1	Total	C	Mg	N	O	0
			99	79	2	8	10	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	

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Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	0	1	Total	C	Mg	N	O	0
			394	316	8	32	38	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	1	1	Total	C	Mg	N	O	0
			413	339	8	32	34	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	2	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	3	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	4	1	Total	C	Mg	N	O	0
			313	257	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	5	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	

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Mol	Chain	Residues	Atoms					AltConf
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	
31	6	1	Total	C	Mg	N	O	0
			280	228	6	24	22	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	7	1	Total	C	Mg	N	O	0
			265	211	6	24	24	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	8	1	Total	C	Mg	N	O	0
			307	249	6	24	28	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	10	1	Total	C	Mg	N	O	0
			442	354	9	36	43	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	11	1	Total	C	Mg	N	O	0
			351	287	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	

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Mol	Chain	Residues	Atoms					AltConf
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	12	1	Total	C	Mg	N	O	0
			330	266	7	28	29	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	13	1	Total	C	Mg	N	O	0
			345	282	7	28	28	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	14	1	Total	C	Mg	N	O	0
			374	308	7	28	31	
31	15	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	15	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	15	1	Total	C	Mg	N	O	0
			295	239	6	24	26	
31	15	1	Total	C	Mg	N	O	0
			295	239	6	24	26	

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Mol	Chain	Residues	Atoms					AltConf
31	15	1	Total 295	C 239	Mg 6	N 24	O 26	0
31	15	1	Total 295	C 239	Mg 6	N 24	O 26	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	16	1	Total 280	C 228	Mg 6	N 24	O 22	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	17	1	Total 265	C 211	Mg 6	N 24	O 24	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	18	1	Total 307	C 249	Mg 6	N 24	O 28	0
31	19	1	Total 408	C 340	Mg 7	N 28	O 33	0

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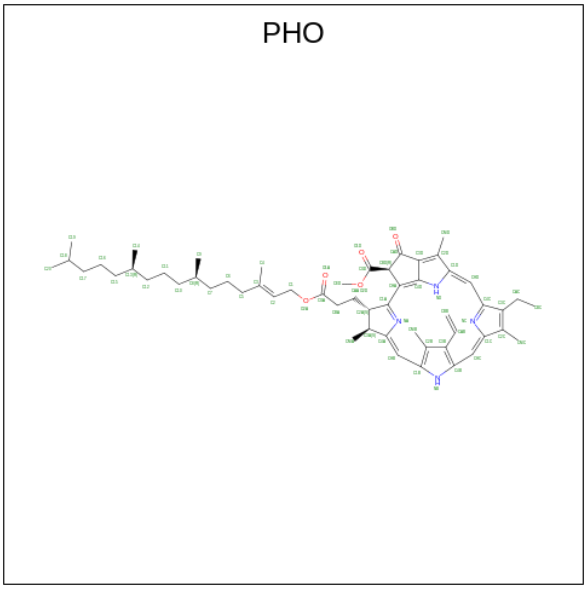
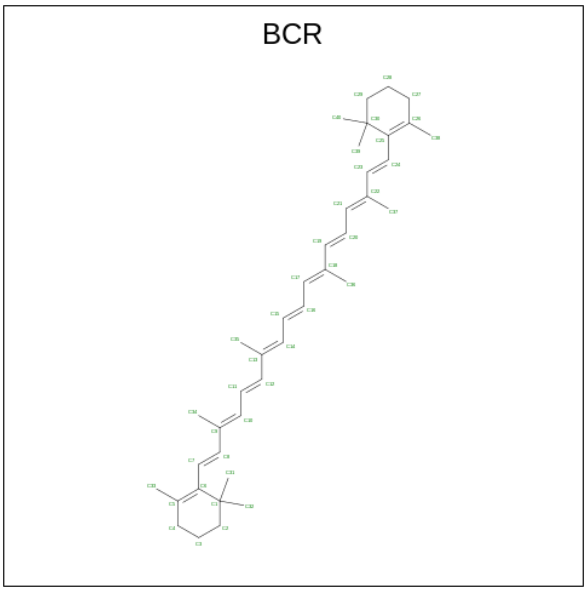
Mol	Chain	Residues	Atoms					AltConf
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
31	19	1	Total	C	Mg	N	O	0
			408	340	7	28	33	

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	D	1	Total	C	N	O	0
			64	55	4	5	
32	a	1	Total	C	N	O	0
			64	55	4	5	
32	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 33 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C 40 40	0
33	B	1	Total C 120 120	0
33	B	1	Total C 120 120	0
33	B	1	Total C 120 120	0
33	C	1	Total C 120 120	0
33	C	1	Total C 120 120	0
33	C	1	Total C 120 120	0
33	F	1	Total C 40 40	0
33	H	1	Total C 40 40	0
33	Y	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 120 120	0
33	b	1	Total C 120 120	0
33	b	1	Total C 120 120	0

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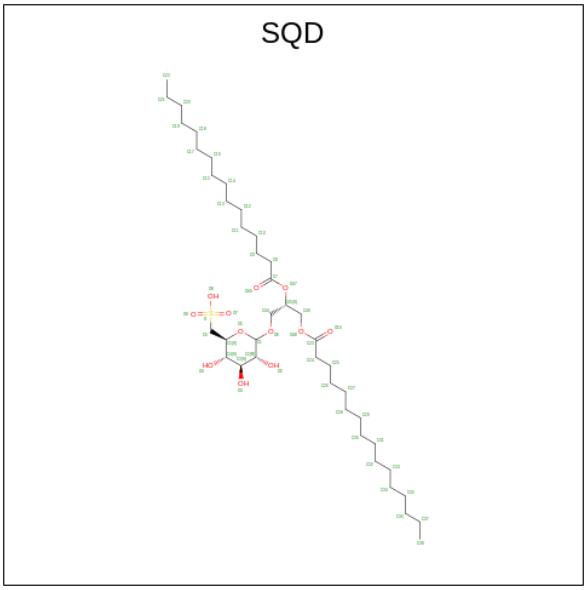
Mol	Chain	Residues	Atoms	AltConf
33	c	1	Total C 120 120	0
33	c	1	Total C 120 120	0
33	c	1	Total C 120 120	0
33	f	1	Total C 40 40	0
33	h	1	Total C 40 40	0
33	y	1	Total C 40 40	0

- Molecule 34 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
34	A	1	Total C O S 94 68 24 2	0
34	A	1	Total C O S 94 68 24 2	0
34	B	1	Total C O S 54 41 12 1	0
34	L	1	Total C O S 54 41 12 1	0
34	a	1	Total C O S 54 41 12 1	0

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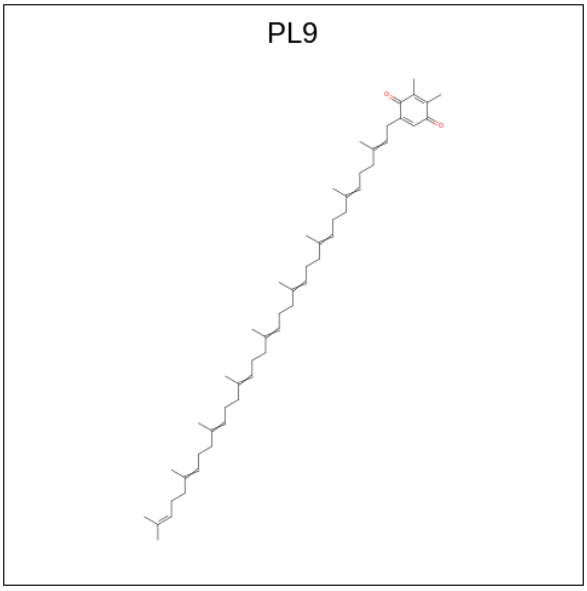
Mol	Chain	Residues	Atoms				AltConf
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	i	1	Total	C	O	S	0
			40	27	12	1	
34	l	1	Total	C	O	S	0
			54	41	12	1	
34	0	1	Total	C	O	S	0
			41	28	12	1	
34	10	1	Total	C	O	S	0
			41	28	12	1	

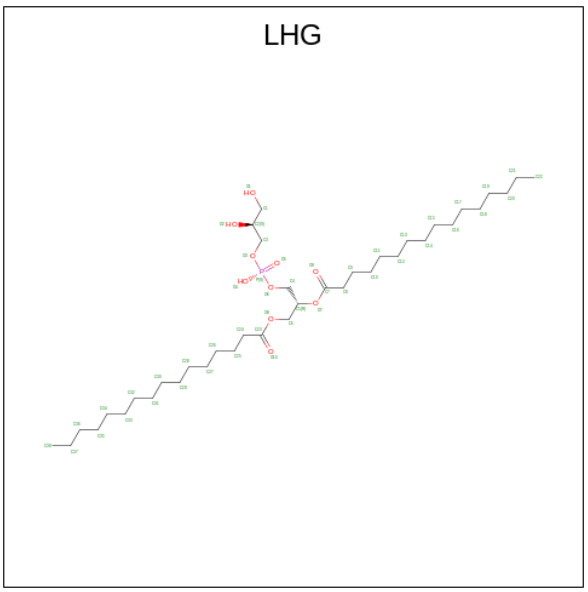
- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			33	31	2	
35	D	1	Total	C	O	0
			55	53	2	
35	a	1	Total	C	O	0
			33	31	2	
35	d	1	Total	C	O	0
			55	53	2	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			37	26	10	1	
36	B	1	Total	C	O	P	0
			43	32	10	1	
36	C	1	Total	C	O	P	0
			40	29	10	1	
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	L	1	Total	C	O	P	0
			49	38	10	1	
36	P	1	Total	C	O	P	0
			27	16	10	1	
36	Z	1	Total	C	O	P	0
			25	14	10	1	
36	a	1	Total	C	O	P	0
			37	26	10	1	
36	b	1	Total	C	O	P	0
			43	32	10	1	
36	d	1	Total	C	O	P	0
			49	38	10	1	
36	l	1	Total	C	O	P	0
			49	38	10	1	
36	p	1	Total	C	O	P	0
			27	16	10	1	
36	w	1	Total	C	O	P	0
			40	29	10	1	

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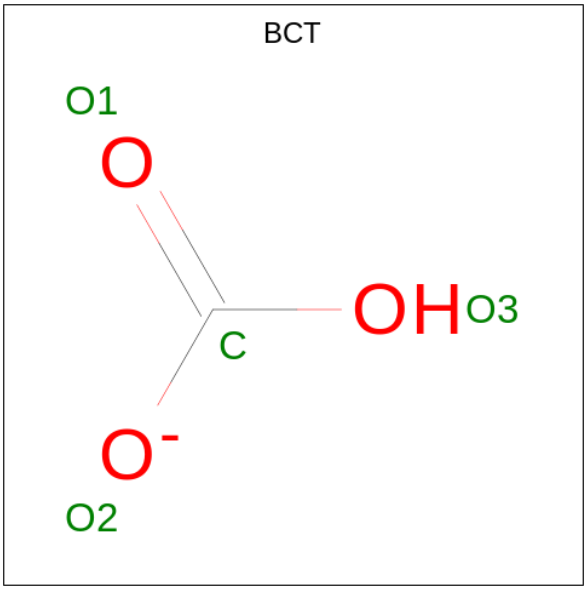
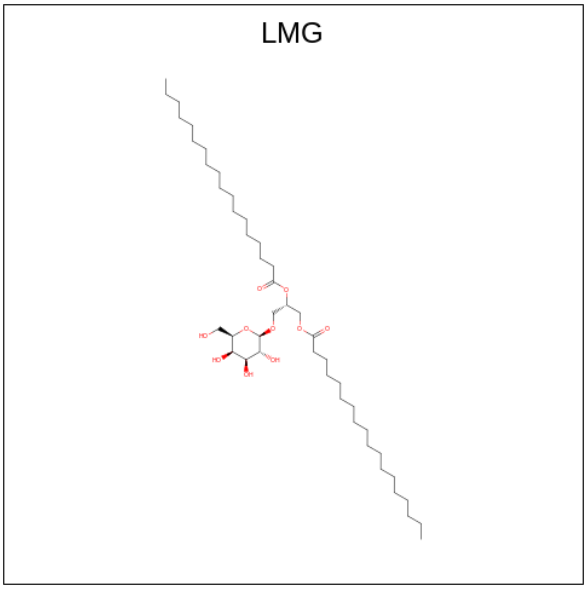
Mol	Chain	Residues	Atoms				AltConf
36	z	1	Total	C	O	P	0
			25	14	10	1	
36	4	1	Total	C	O	P	0
			35	24	10	1	
36	5	1	Total	C	O	P	0
			25	14	10	1	
36	8	1	Total	C	O	P	0
			70	48	20	2	
36	8	1	Total	C	O	P	0
			70	48	20	2	
36	14	1	Total	C	O	P	0
			35	24	10	1	
36	15	1	Total	C	O	P	0
			25	14	10	1	
36	18	1	Total	C	O	P	0
			70	48	20	2	
36	18	1	Total	C	O	P	0
			70	48	20	2	

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
37	A	1	Total	C	O	0
			4	1	3	
37	a	1	Total	C	O	0
			4	1	3	

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



Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			51	41	10	
38	C	1	Total	C	O	0
			51	41	10	
38	D	1	Total	C	O	0
			77	57	20	
38	D	1	Total	C	O	0
			77	57	20	
38	F	1	Total	C	O	0
			46	36	10	
38	J	1	Total	C	O	0
			50	40	10	
38	K	1	Total	C	O	0
			46	36	10	
38	M	1	Total	C	O	0
			40	30	10	
38	N	1	Total	C	O	0
			28	18	10	
38	P	1	Total	C	O	0
			31	21	10	
38	W	1	Total	C	O	0
			48	38	10	
38	Z	1	Total	C	O	0
			31	21	10	

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Mol	Chain	Residues	Atoms			AltConf
38	b	1	Total	C	O	0
			51	41	10	
38	c	1	Total	C	O	0
			82	62	20	
38	c	1	Total	C	O	0
			82	62	20	
38	d	1	Total	C	O	0
			77	57	20	
38	d	1	Total	C	O	0
			77	57	20	
38	f	1	Total	C	O	0
			46	36	10	
38	j	1	Total	C	O	0
			50	40	10	
38	k	1	Total	C	O	0
			46	36	10	
38	m	1	Total	C	O	0
			40	30	10	
38	n	1	Total	C	O	0
			28	18	10	
38	p	1	Total	C	O	0
			31	21	10	
38	w	1	Total	C	O	0
			48	38	10	
38	0	1	Total	C	O	0
			31	21	10	
38	1	1	Total	C	O	0
			81	61	20	
38	1	1	Total	C	O	0
			81	61	20	
38	4	1	Total	C	O	0
			49	39	10	
38	5	1	Total	C	O	0
			73	53	20	
38	5	1	Total	C	O	0
			73	53	20	
38	10	1	Total	C	O	0
			31	21	10	
38	11	1	Total	C	O	0
			81	61	20	
38	11	1	Total	C	O	0
			81	61	20	

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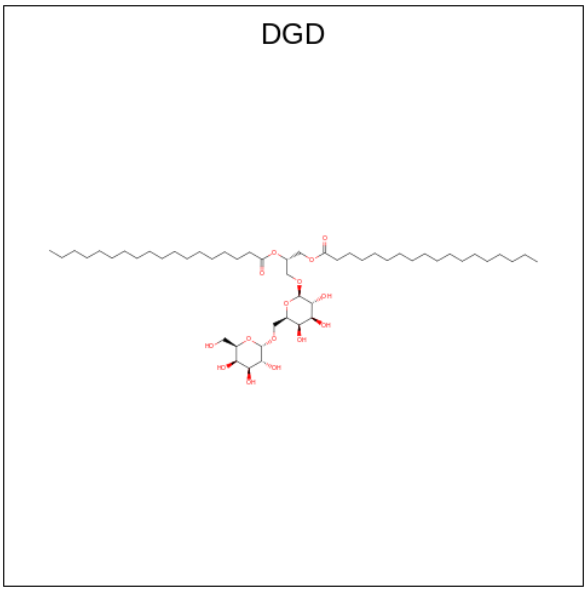
Mol	Chain	Residues	Atoms	AltConf
38	14	1	Total C O 49 39 10	0
38	15	1	Total C O 73 53 20	0
38	15	1	Total C O 73 53 20	0

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
39	B	1	Total C O 54 39 15	0
39	C	1	Total C O 179 134 45	0
39	C	1	Total C O 179 134 45	0
39	C	1	Total C O 179 134 45	0
39	H	1	Total C O 62 47 15	0
39	W	1	Total C O 56 41 15	0
39	b	1	Total C O 55 40 15	0
39	c	1	Total C O 179 134 45	0

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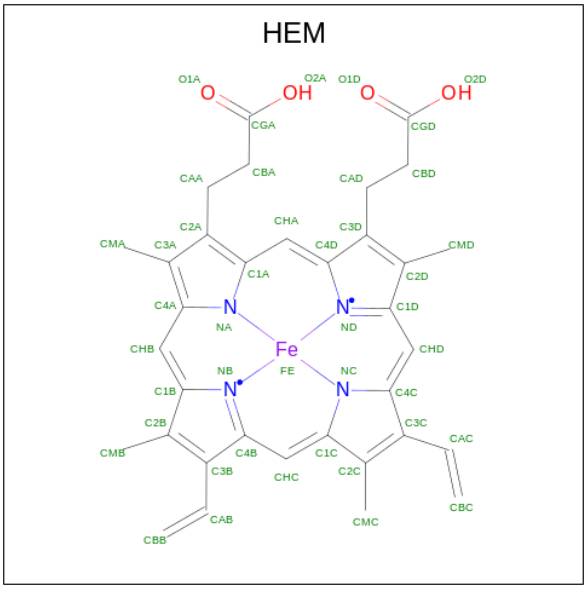
Mol	Chain	Residues	Atoms			AltConf
39	c	1	Total	C	O	0
			179	134	45	
39	c	1	Total	C	O	0
			179	134	45	
39	h	1	Total	C	O	0
			62	47	15	
39	w	1	Total	C	O	0
			56	41	15	
39	1	1	Total	C	O	0
			54	39	15	
39	11	1	Total	C	O	0
			60	45	15	

- Molecule 40 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
40	C	1	Total	Cl	0
			1	1	
40	c	1	Total	Cl	0
			1	1	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
41	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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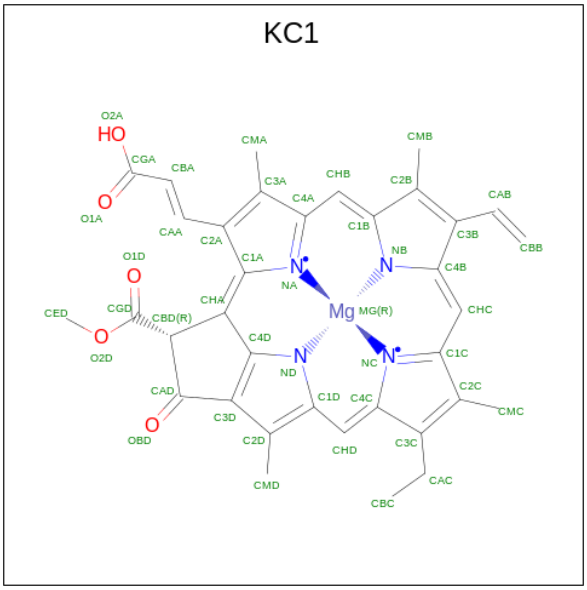
Mol	Chain	Residues	Atoms					AltConf
41	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
42	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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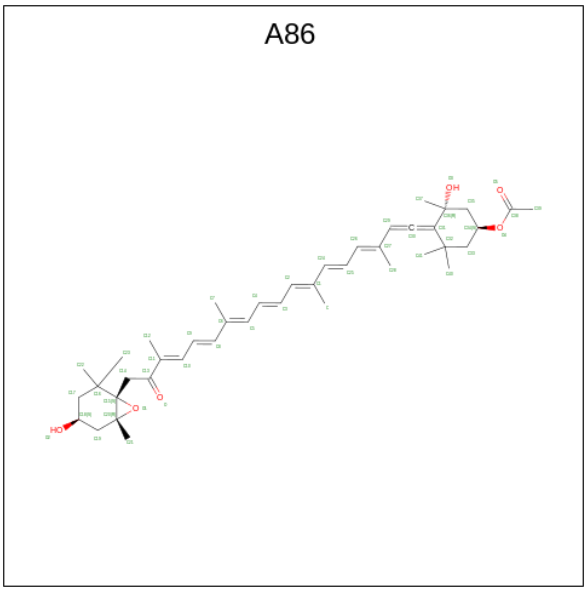
Mol	Chain	Residues	Atoms					AltConf
42	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	16	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
42	16	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
42	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 43 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7 ,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
43	P	1	Total	C	O	0
			96	84	12	
43	P	1	Total	C	O	0
			96	84	12	
43	p	1	Total	C	O	0
			96	84	12	
43	p	1	Total	C	O	0
			96	84	12	
43	0	1	Total	C	O	0
			288	252	36	
43	0	1	Total	C	O	0
			288	252	36	
43	0	1	Total	C	O	0
			288	252	36	
43	0	1	Total	C	O	0
			288	252	36	
43	0	1	Total	C	O	0
			288	252	36	
43	0	1	Total	C	O	0
			288	252	36	
43	1	1	Total	C	O	0
			336	294	42	
43	1	1	Total	C	O	0
			336	294	42	
43	1	1	Total	C	O	0
			336	294	42	
43	1	1	Total	C	O	0
			336	294	42	

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Mol	Chain	Residues	Atoms			AltConf
43	1	1	Total	C	O	0
			336	294	42	
43	1	1	Total	C	O	0
			336	294	42	
43	1	1	Total	C	O	0
			336	294	42	
43	2	1	Total	C	O	0
			240	210	30	
43	2	1	Total	C	O	0
			240	210	30	
43	2	1	Total	C	O	0
			240	210	30	
43	2	1	Total	C	O	0
			240	210	30	
43	2	1	Total	C	O	0
			240	210	30	
43	3	1	Total	C	O	0
			288	252	36	
43	3	1	Total	C	O	0
			288	252	36	
43	3	1	Total	C	O	0
			288	252	36	
43	3	1	Total	C	O	0
			288	252	36	
43	3	1	Total	C	O	0
			288	252	36	
43	3	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	4	1	Total	C	O	0
			288	252	36	
43	5	1	Total	C	O	0
			288	252	36	

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Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			288	252	36	
43	5	1	Total	C	O	0
			288	252	36	
43	5	1	Total	C	O	0
			288	252	36	
43	5	1	Total	C	O	0
			288	252	36	
43	5	1	Total	C	O	0
			288	252	36	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	6	1	Total	C	O	0
			336	294	42	
43	7	1	Total	C	O	0
			288	252	36	
43	7	1	Total	C	O	0
			288	252	36	
43	7	1	Total	C	O	0
			288	252	36	
43	7	1	Total	C	O	0
			288	252	36	
43	7	1	Total	C	O	0
			288	252	36	
43	7	1	Total	C	O	0
			288	252	36	
43	8	1	Total	C	O	0
			240	210	30	
43	8	1	Total	C	O	0
			240	210	30	
43	8	1	Total	C	O	0
			240	210	30	

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Mol	Chain	Residues	Atoms			AltConf
43	8	1	Total	C	O	0
			240	210	30	
43	8	1	Total	C	O	0
			240	210	30	
43	9	1	Total	C	O	0
			288	252	36	
43	9	1	Total	C	O	0
			288	252	36	
43	9	1	Total	C	O	0
			288	252	36	
43	9	1	Total	C	O	0
			288	252	36	
43	9	1	Total	C	O	0
			288	252	36	
43	9	1	Total	C	O	0
			288	252	36	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	10	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	
43	11	1	Total	C	O	0
			336	294	42	

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Mol	Chain	Residues	Atoms			AltConf
43	11	1	Total	C	O	0
			336	294	42	
43	12	1	Total	C	O	0
			288	252	36	
43	12	1	Total	C	O	0
			288	252	36	
43	12	1	Total	C	O	0
			288	252	36	
43	12	1	Total	C	O	0
			288	252	36	
43	12	1	Total	C	O	0
			288	252	36	
43	12	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	13	1	Total	C	O	0
			288	252	36	
43	14	1	Total	C	O	0
			240	210	30	
43	14	1	Total	C	O	0
			240	210	30	
43	14	1	Total	C	O	0
			240	210	30	
43	14	1	Total	C	O	0
			240	210	30	
43	14	1	Total	C	O	0
			240	210	30	
43	15	1	Total	C	O	0
			240	210	30	
43	15	1	Total	C	O	0
			240	210	30	
43	15	1	Total	C	O	0
			240	210	30	

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Mol	Chain	Residues	Atoms			AltConf
43	15	1	Total	C	O	0
			240	210	30	
43	15	1	Total	C	O	0
			240	210	30	
43	16	1	Total	C	O	0
			288	252	36	
43	16	1	Total	C	O	0
			288	252	36	
43	16	1	Total	C	O	0
			288	252	36	
43	16	1	Total	C	O	0
			288	252	36	
43	16	1	Total	C	O	0
			288	252	36	
43	16	1	Total	C	O	0
			288	252	36	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	17	1	Total	C	O	0
			336	294	42	
43	18	1	Total	C	O	0
			240	210	30	
43	18	1	Total	C	O	0
			240	210	30	
43	18	1	Total	C	O	0
			240	210	30	
43	18	1	Total	C	O	0
			240	210	30	
43	18	1	Total	C	O	0
			240	210	30	
43	19	1	Total	C	O	0
			288	252	36	

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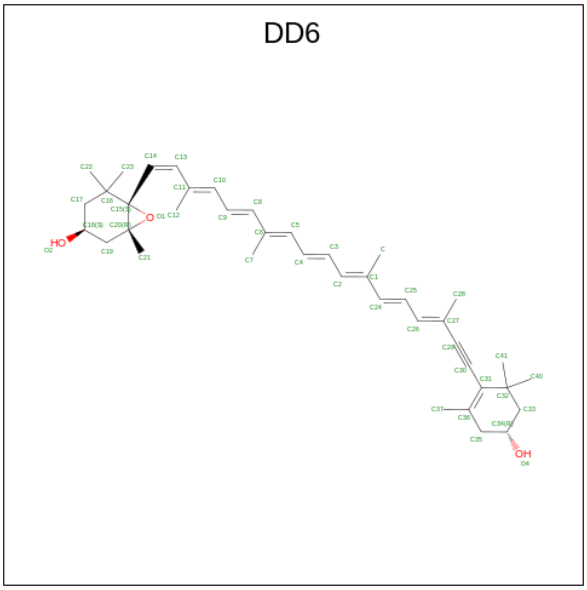
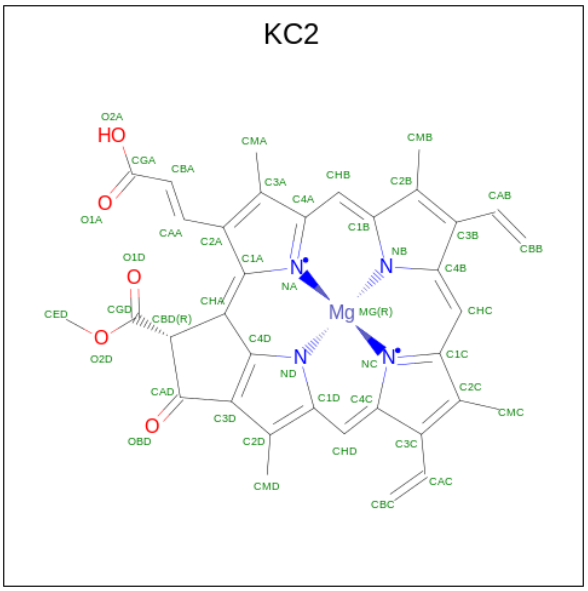
Mol	Chain	Residues	Atoms			AltConf
43	19	1	Total 288	C 252	O 36	0
43	19	1	Total 288	C 252	O 36	0
43	19	1	Total 288	C 252	O 36	0
43	19	1	Total 288	C 252	O 36	0
43	19	1	Total 288	C 252	O 36	0

- Molecule 44 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: $C_{40}H_{54}O_3$).



Mol	Chain	Residues	Atoms			AltConf
44	P	1	Total 43	C 40	O 3	0
44	p	1	Total 43	C 40	O 3	0

- Molecule 45 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
45	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	1	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	1	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	2	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	2	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	3	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	3	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	4	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	4	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	5	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	5	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	6	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	6	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	7	1	Total	C	Mg	N	O	0
			90	70	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
45	7	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	8	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	8	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	11	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	11	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	12	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	12	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	13	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	13	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	14	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	14	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	15	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	15	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	16	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	16	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	17	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	17	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	18	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
45	18	1	Total	C	Mg	N	O	0
			90	70	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
45	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 46 is water.

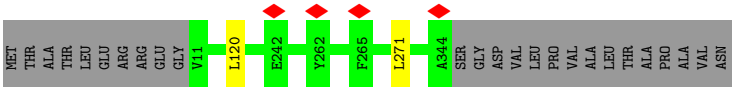
Mol	Chain	Residues	Atoms		AltConf
46	Z	1	Total	O	0
			1	1	

3 Residue-property plots (i)

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

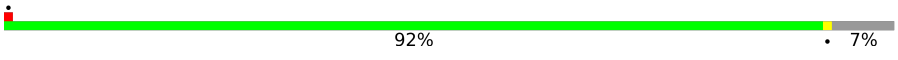
• Molecule 1: PsbA

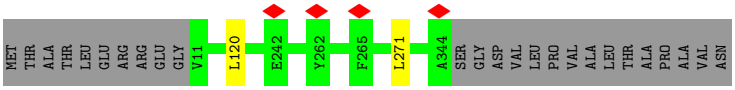
Chain A:



• Molecule 1: PsbA

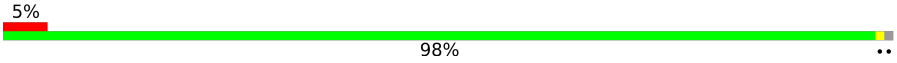
Chain a:

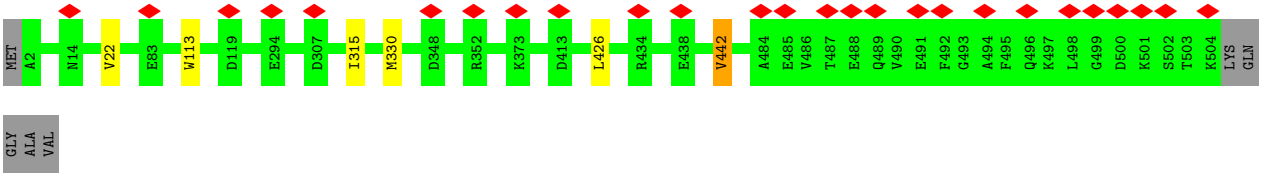




• Molecule 2: PsbB

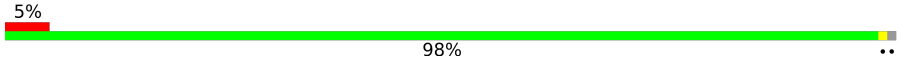
Chain B:

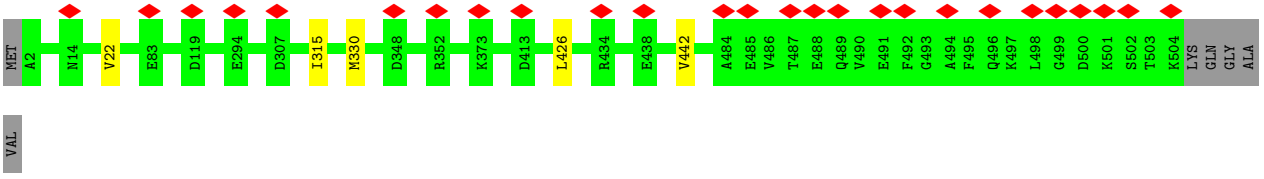




• Molecule 2: PsbB

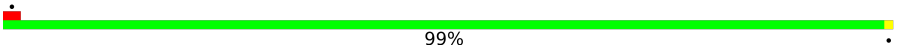
Chain b:

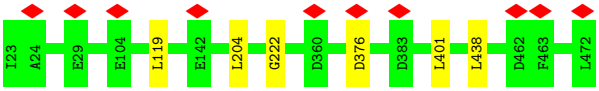




• Molecule 3: PsbC

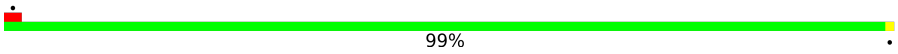
Chain C:

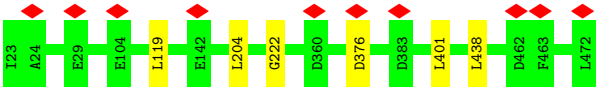




• Molecule 3: PsbC

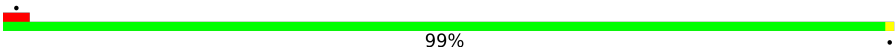
Chain c:

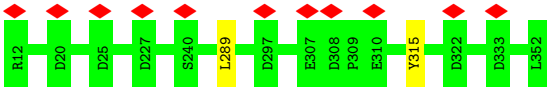




• Molecule 4: PsbD

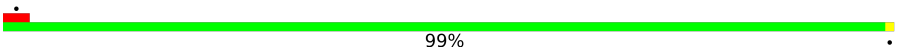
Chain D:

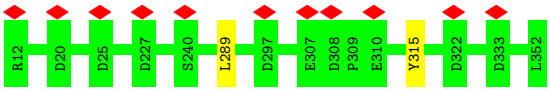




• Molecule 4: PsbD

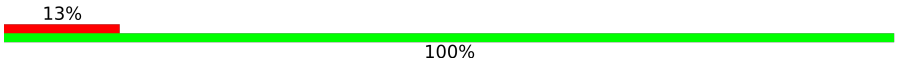
Chain d:

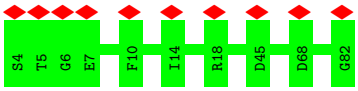




• Molecule 5: PsbE

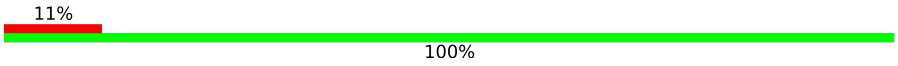
Chain E:

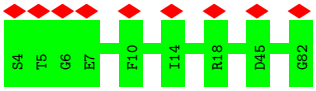




• Molecule 5: PsbE

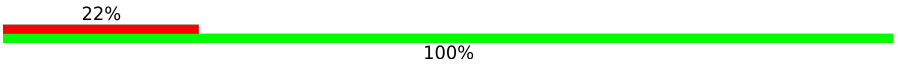
Chain e:

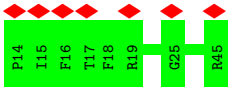




• Molecule 6: PsbF

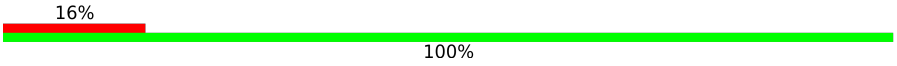
Chain F:

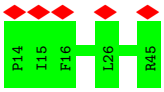




• Molecule 6: PsbF

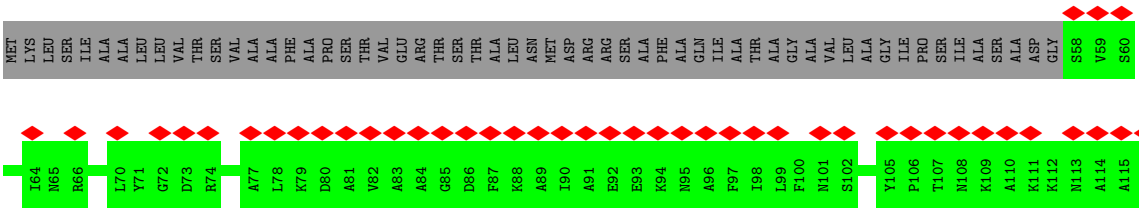
Chain f:





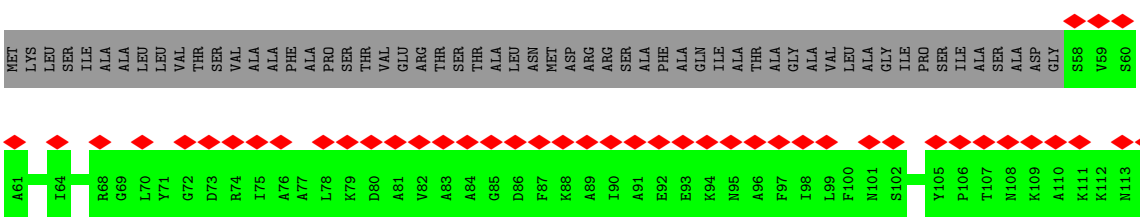
• Molecule 7: Psb31

Chain G:



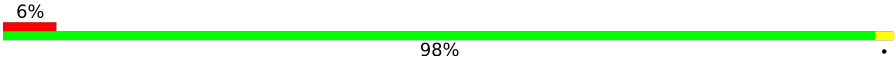
• Molecule 7: Psb31

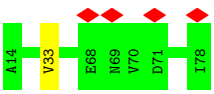
Chain g:



• Molecule 8: Photosystem II reaction center protein H

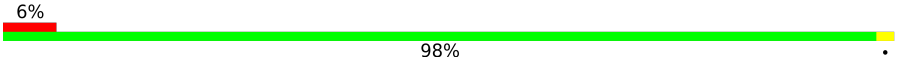
Chain H:

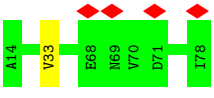




• Molecule 8: Photosystem II reaction center protein H

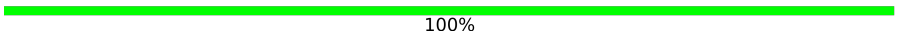
Chain h:





• Molecule 9: PsbI

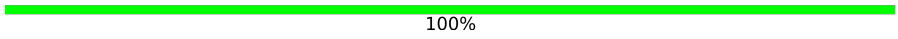
Chain I:



There are no outlier residues recorded for this chain.

• Molecule 9: PsbI

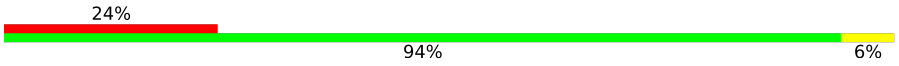
Chain i:

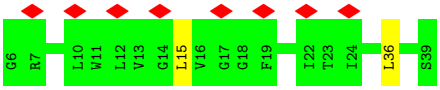


There are no outlier residues recorded for this chain.

• Molecule 10: PsbJ

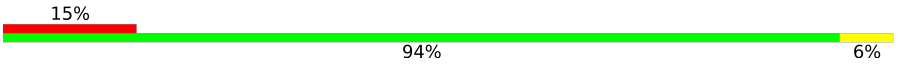
Chain J:

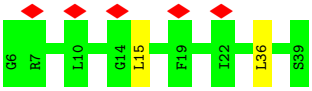




• Molecule 10: PsbJ

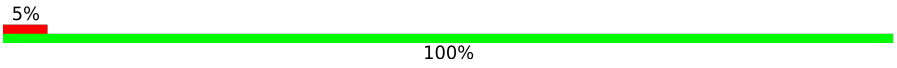
Chain j:

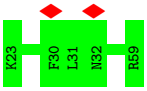




• Molecule 11: PsbK

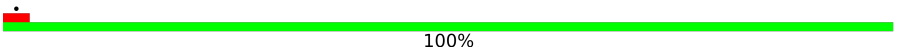
Chain K:

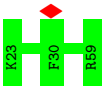




• Molecule 11: PsbK

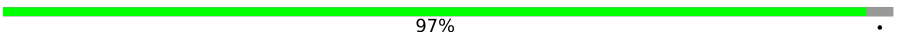
Chain k:





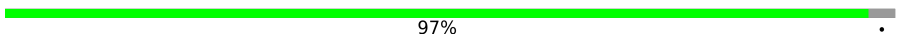
• Molecule 12: PsbL

Chain L:



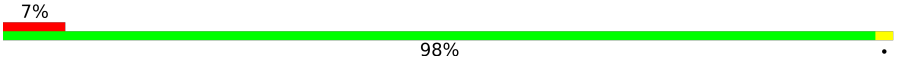
• Molecule 12: PsbL

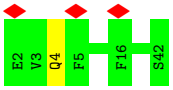
Chain l:



• Molecule 13: PsbM

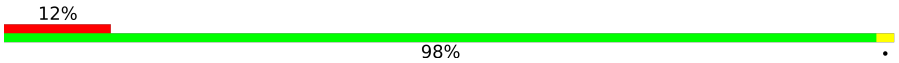
Chain M:

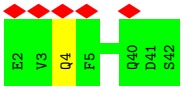




• Molecule 13: PsbM

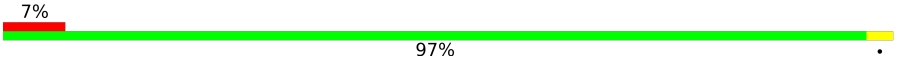
Chain m:

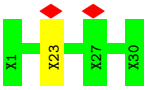




• Molecule 14: Psb34

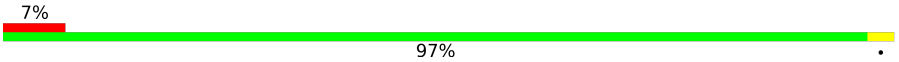
Chain N:

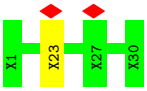




• Molecule 14: Psb34

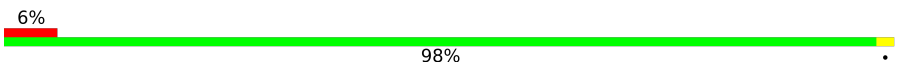
Chain n:

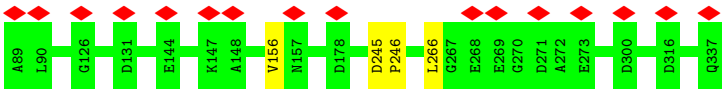




• Molecule 15: Extrinsic protein in photosystem II

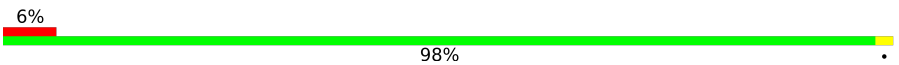
Chain O:

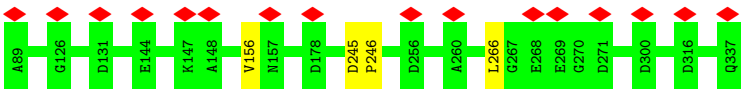




• Molecule 15: Extrinsic protein in photosystem II

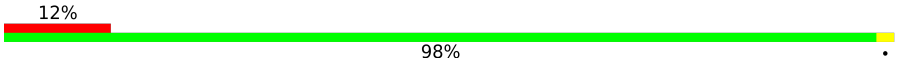
Chain o:

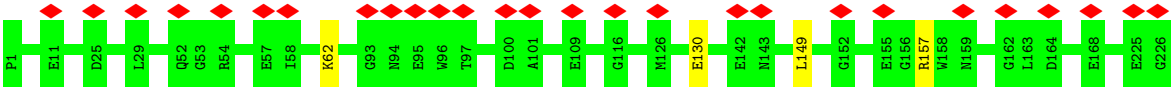




• Molecule 16: FCP-D

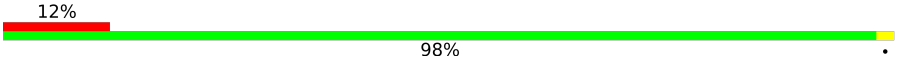
Chain P:

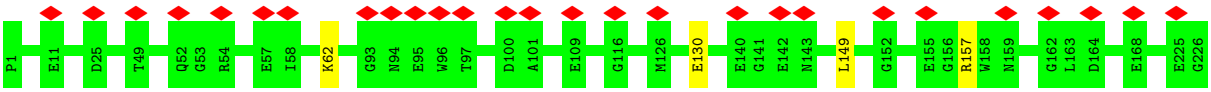




• Molecule 16: FCP-D

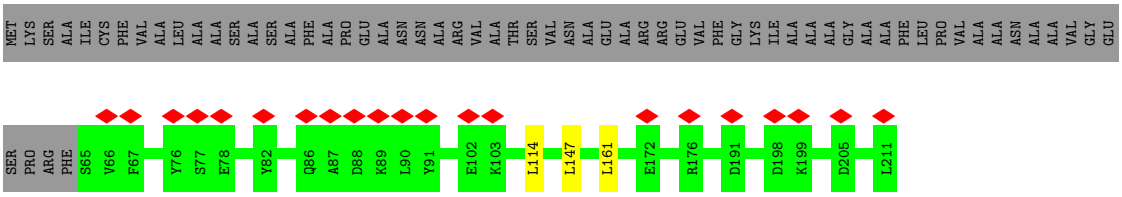
Chain p:





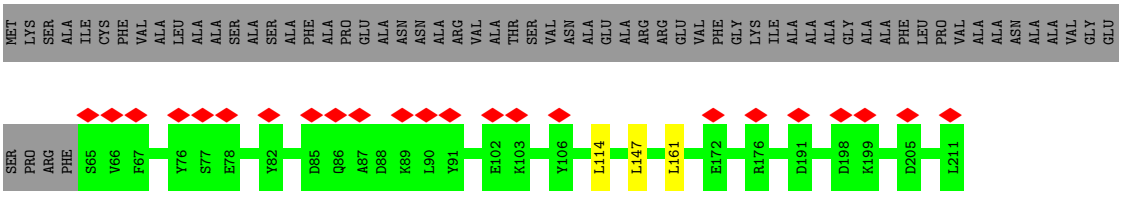
• Molecule 17: Extrinsic protein in photosystem II

Chain Q:



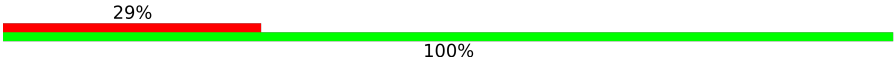
• Molecule 17: Extrinsic protein in photosystem II

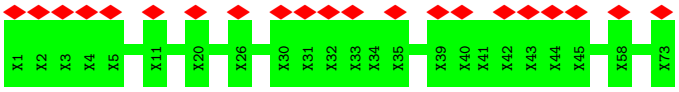
Chain q:



• Molecule 18: PsbG

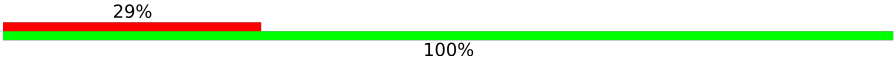
Chain R:

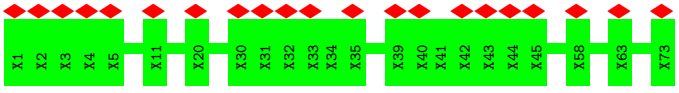




• Molecule 18: PsbG

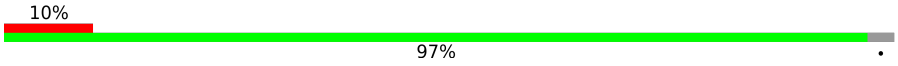
Chain r:

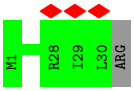




• Molecule 19: PsbT

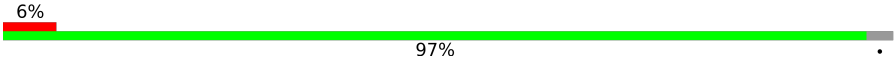
Chain T:

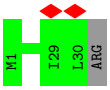




• Molecule 19: PsbT

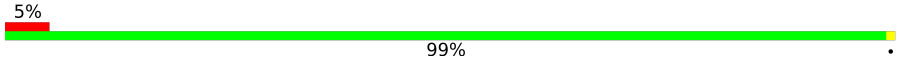
Chain t:

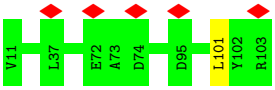




• Molecule 20: Extrinsic protein in photosystem II

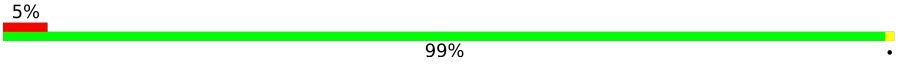
Chain U:

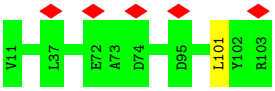




• Molecule 20: Extrinsic protein in photosystem II

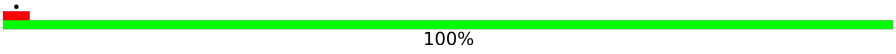
Chain u:

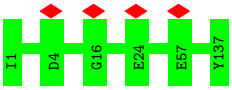




• Molecule 21: Cytochrome c-550

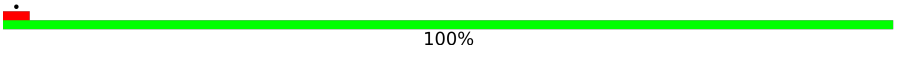
Chain V:

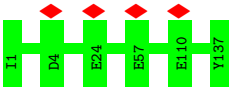




• Molecule 21: Cytochrome c-550

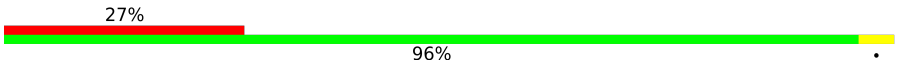
Chain v:

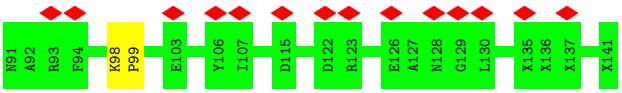




• Molecule 22: PsbW

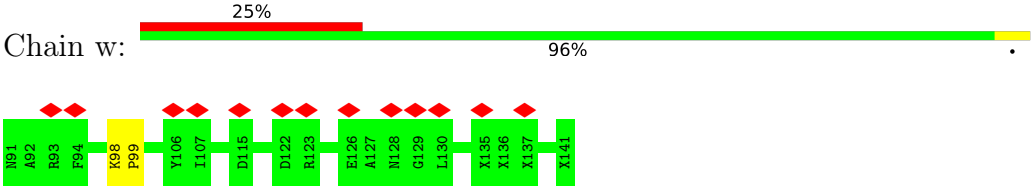
Chain W:





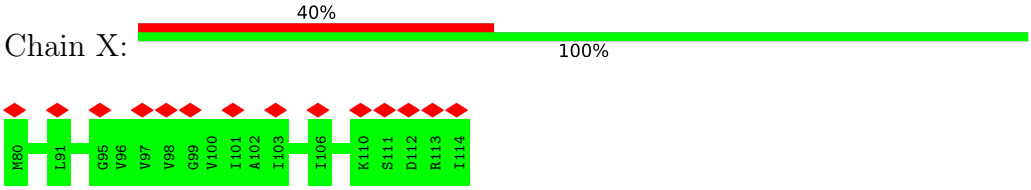
• Molecule 22: PsbW

Chain w:



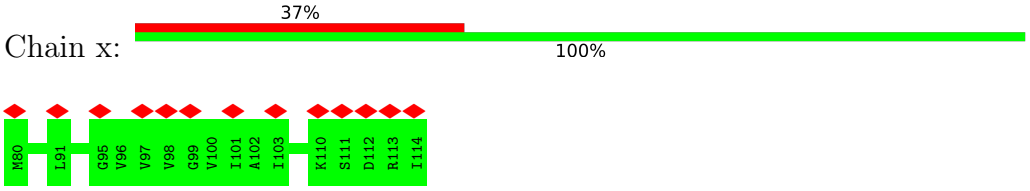
• Molecule 23: Photosystem II reaction center X protein

Chain X:



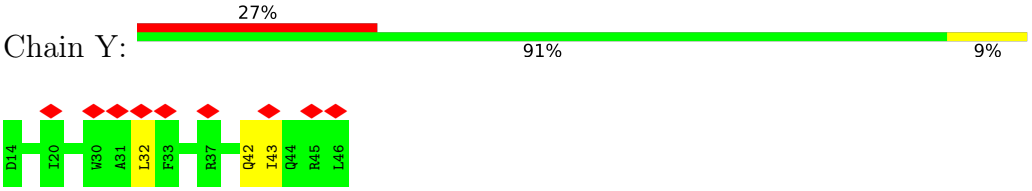
• Molecule 23: Photosystem II reaction center X protein

Chain x:



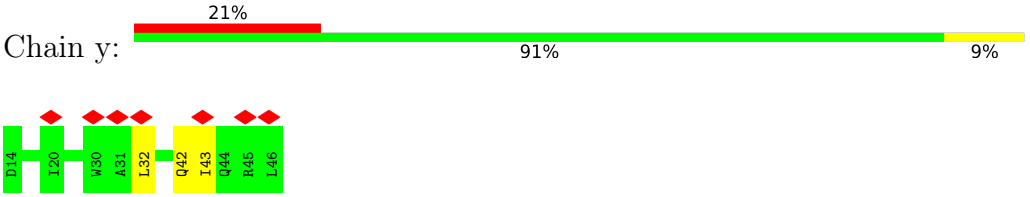
• Molecule 24: PsbY

Chain Y:



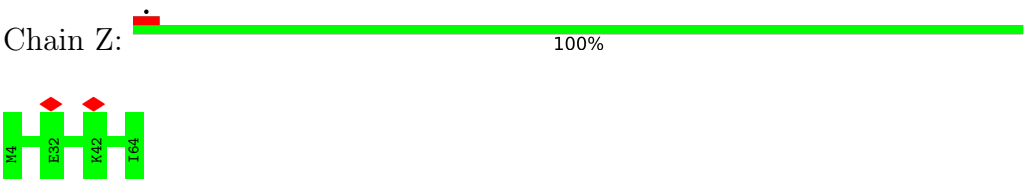
• Molecule 24: PsbY

Chain y:



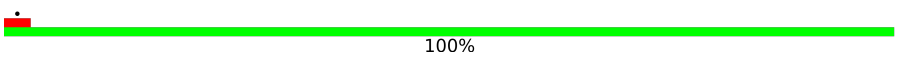
• Molecule 25: PsbZ

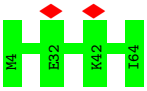
Chain Z:



• Molecule 25: PsbZ

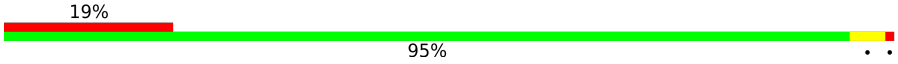
Chain z:

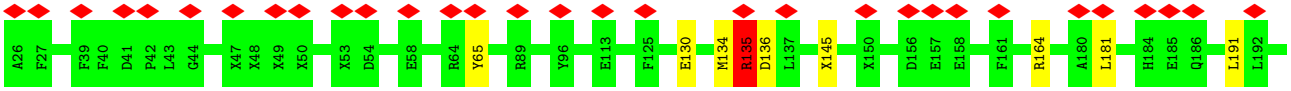




• Molecule 26: FCP-E

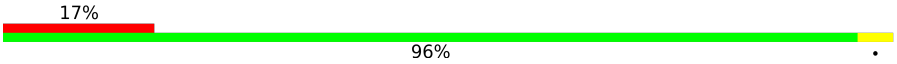
Chain 0:

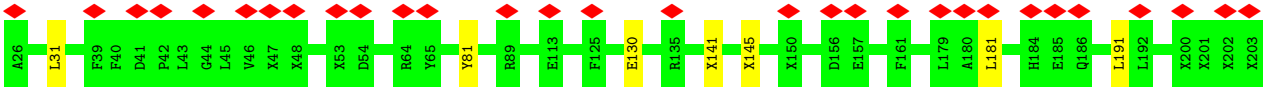




• Molecule 26: FCP-E

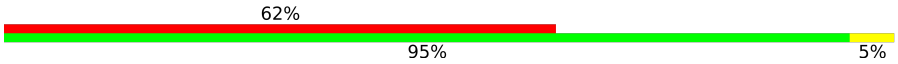
Chain 10:

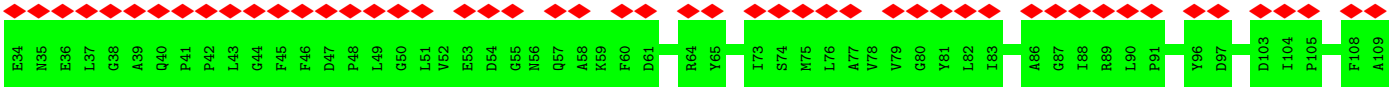


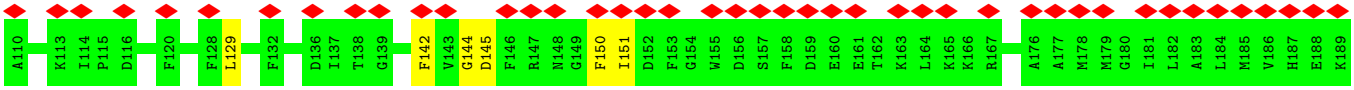


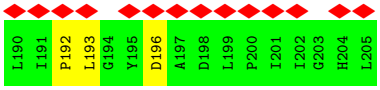
• Molecule 27: FCP-A

Chain 1:



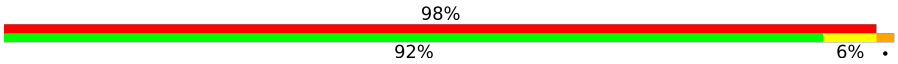


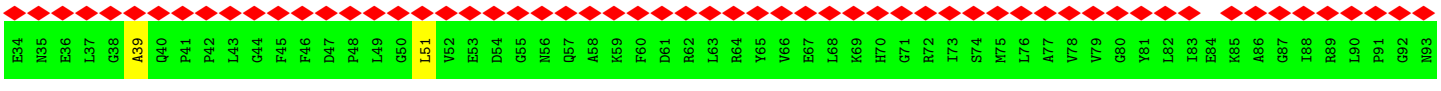


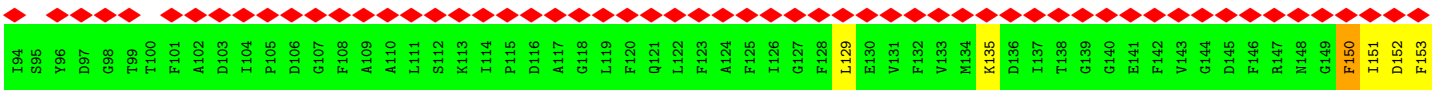


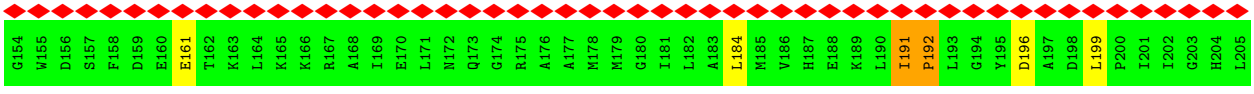
• Molecule 27: FCP-A

Chain 2:



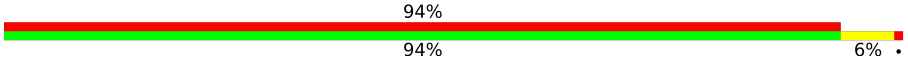


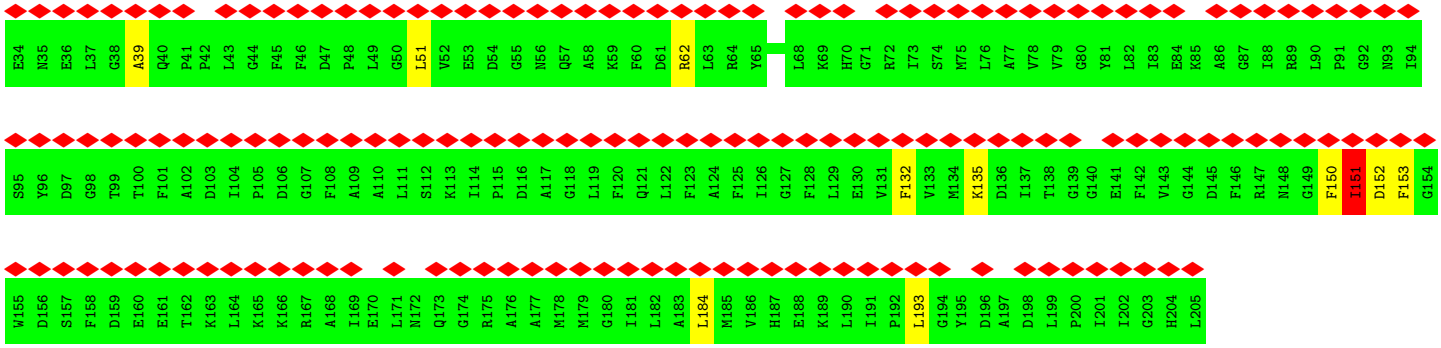




• Molecule 27: FCP-A

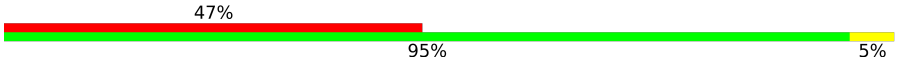
Chain 3:

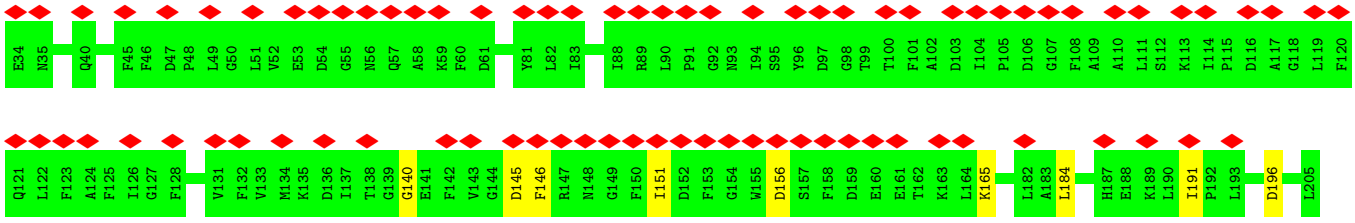




• Molecule 27: FCP-A

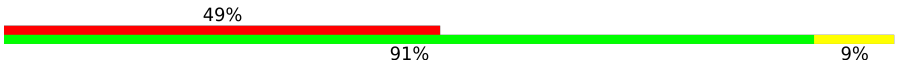
Chain 4:

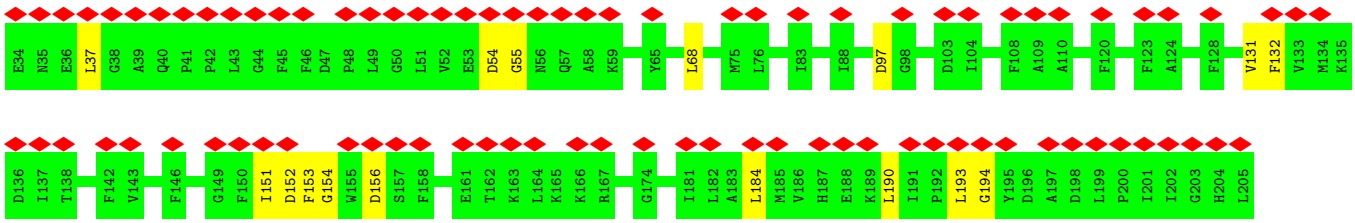




• Molecule 27: FCP-A

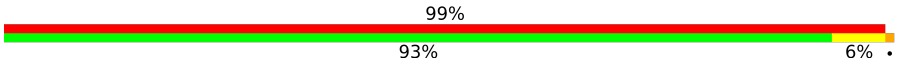
Chain 5:

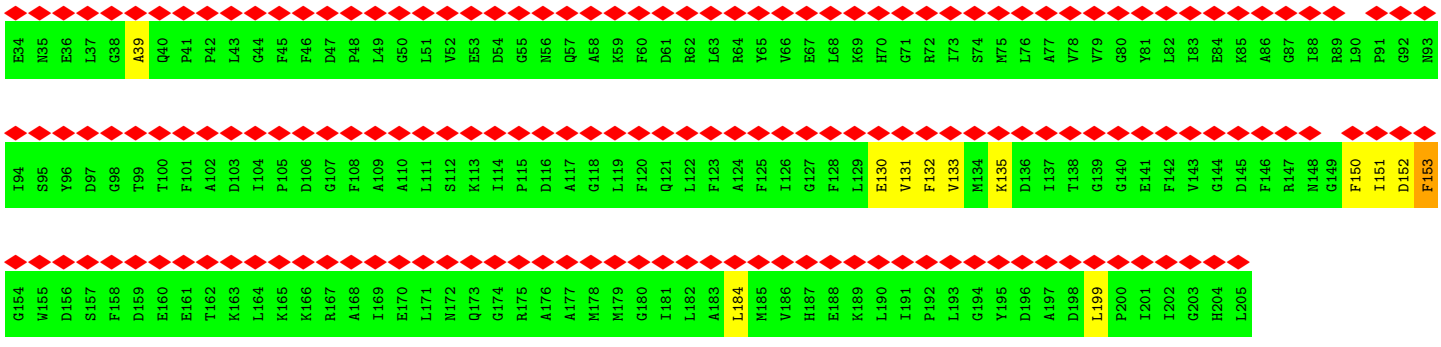




• Molecule 27: FCP-A

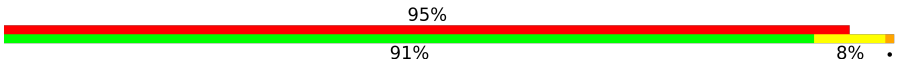
Chain 6:

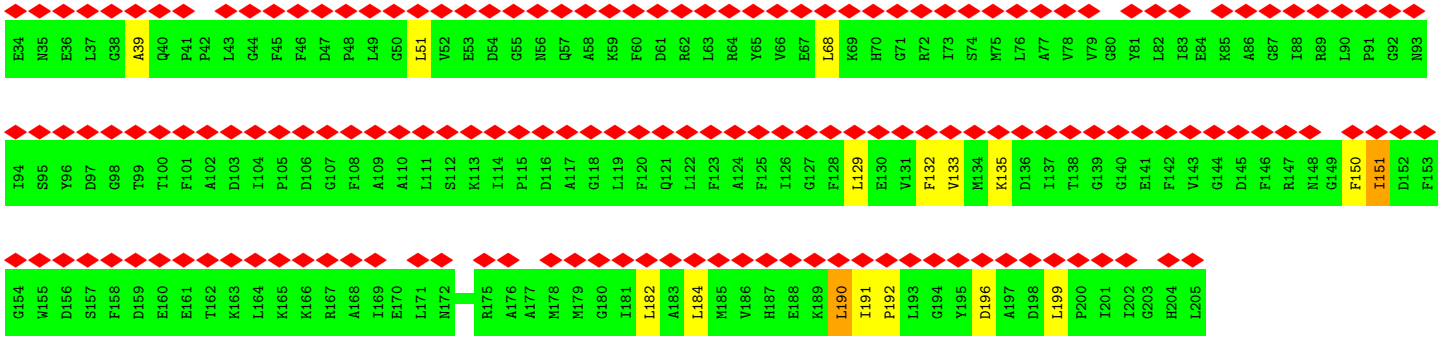




• Molecule 27: FCP-A

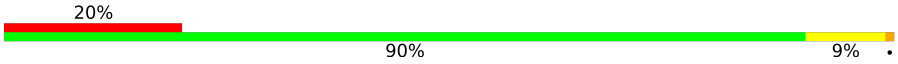
Chain 7:

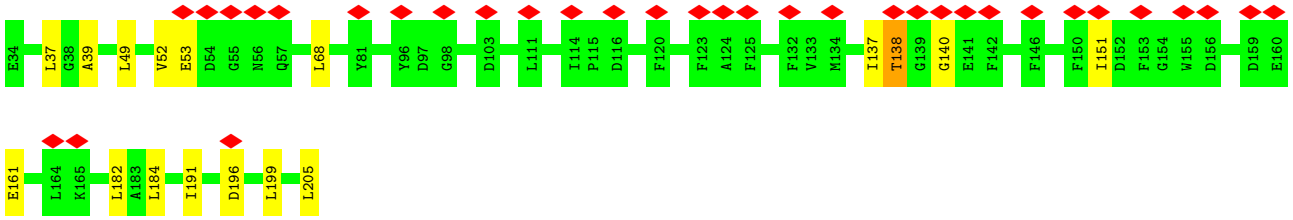




• Molecule 27: FCP-A

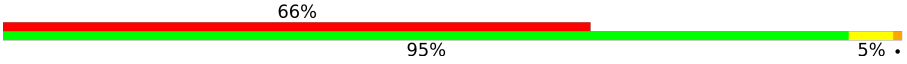
Chain 8:

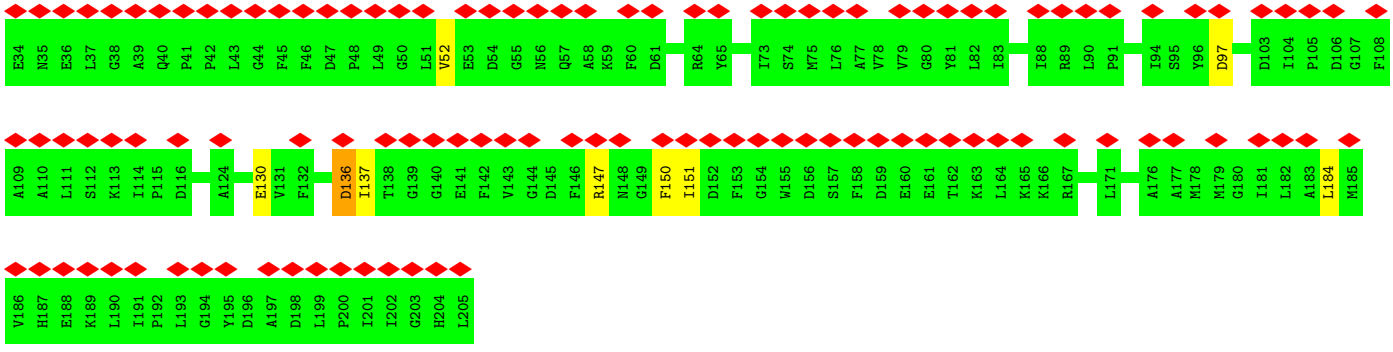




• Molecule 27: FCP-A

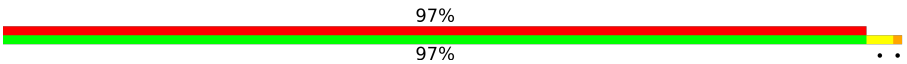
Chain 11:

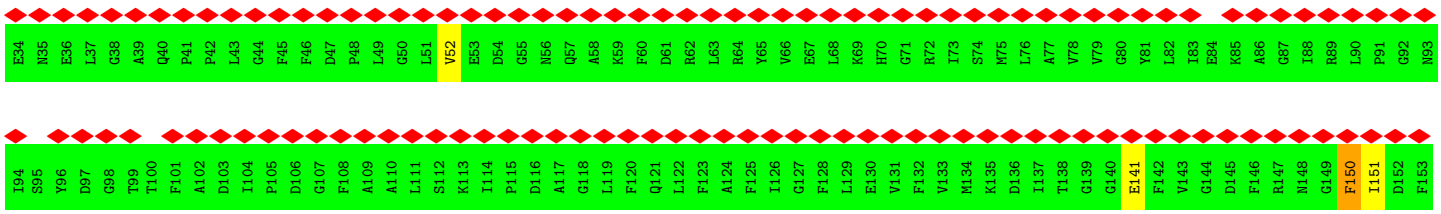


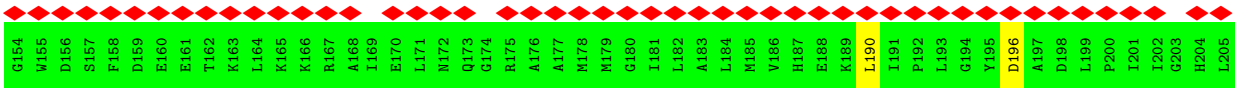


• Molecule 27: FCP-A

Chain 12:

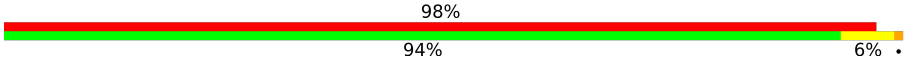


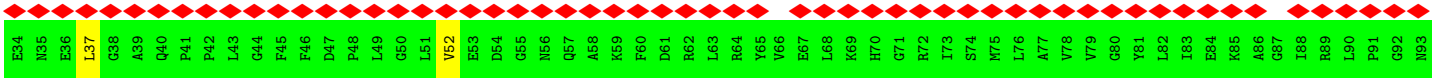


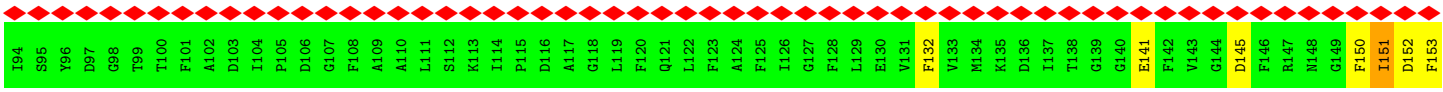


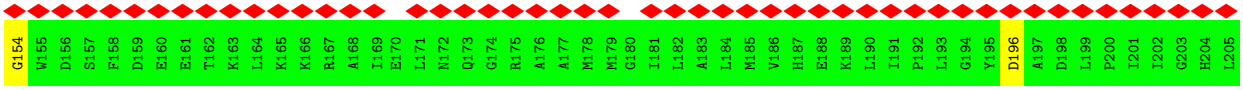
• Molecule 27: FCP-A

Chain 13:



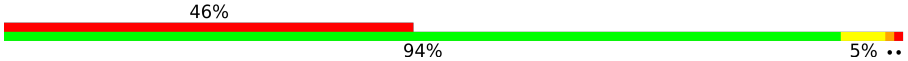


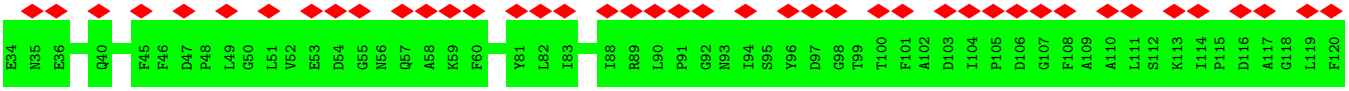


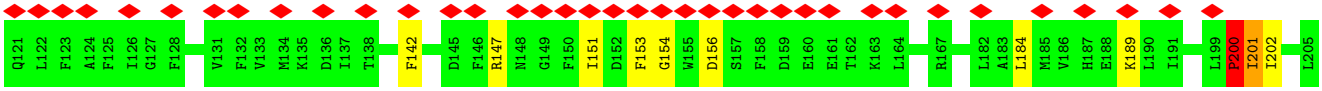


• Molecule 27: FCP-A

Chain 14:

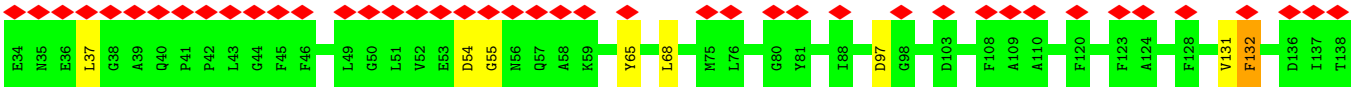


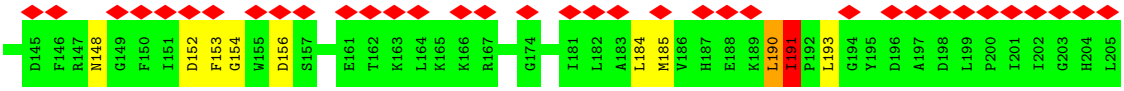




• Molecule 27: FCP-A

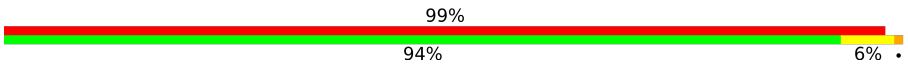
Chain 15:

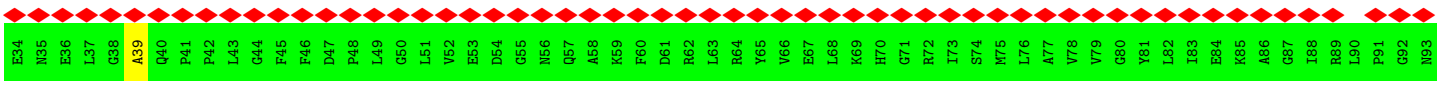


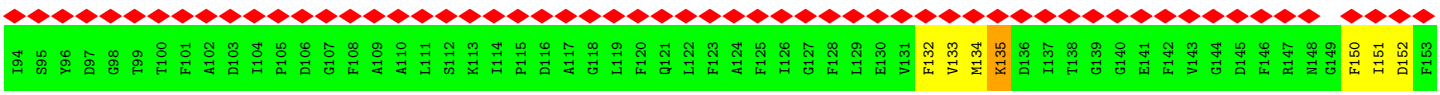


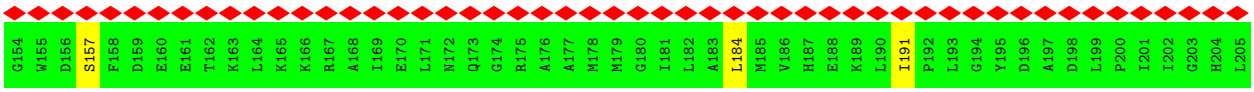
• Molecule 27: FCP-A

Chain 16:



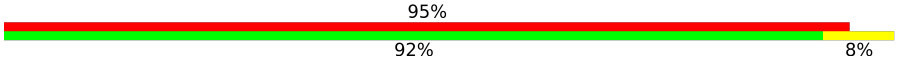


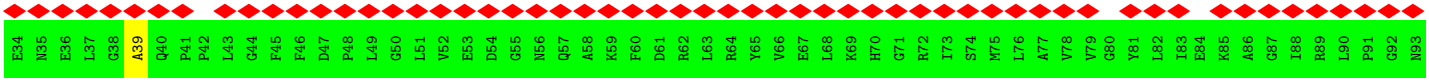


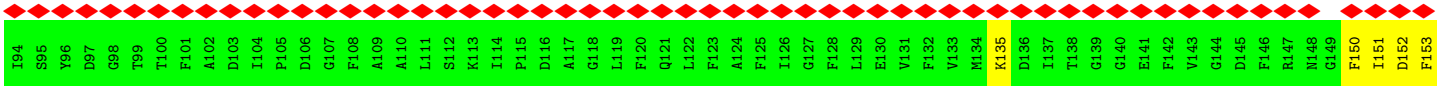


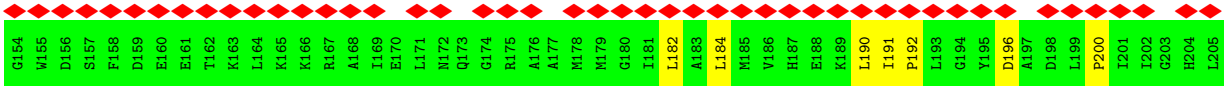
• Molecule 27: FCP-A

Chain 17:



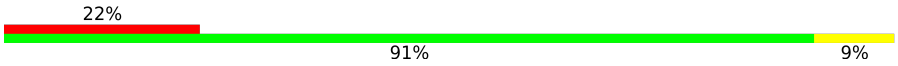


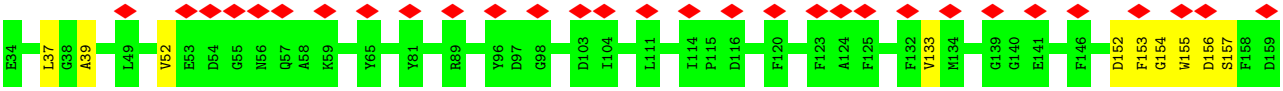


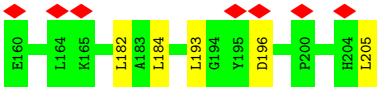


• Molecule 27: FCP-A

Chain 18:

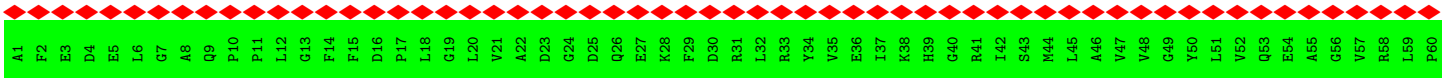


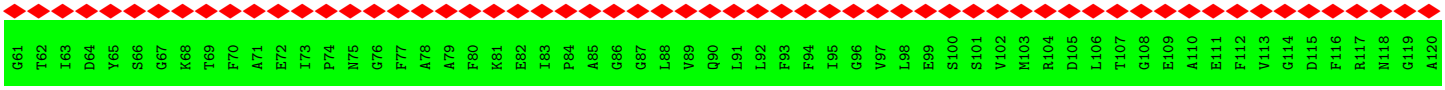


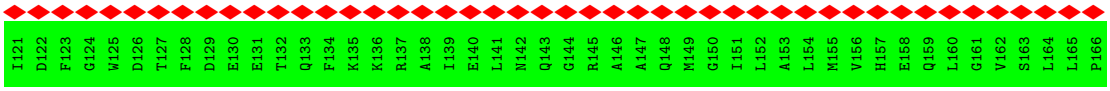


• Molecule 28: FCP-F

Chain 9:

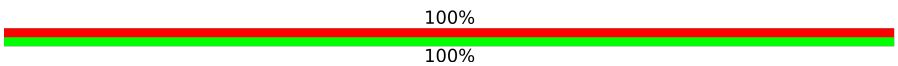


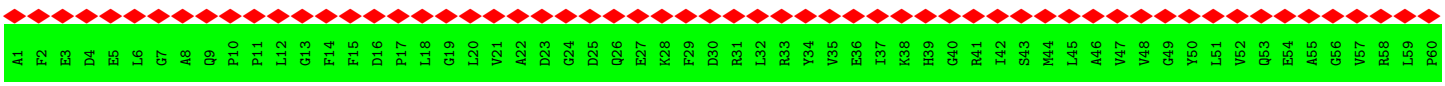


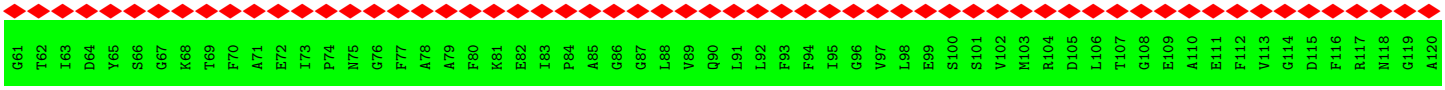


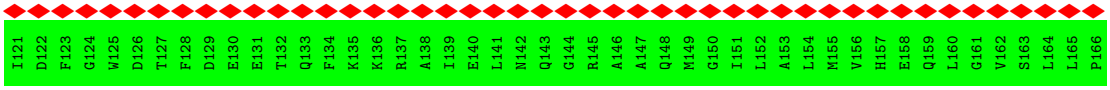
• Molecule 28: FCP-F

Chain 19:






G61 T62 I63 D64 Y65 S66 G67 K68 T69 F70 A71 E72 I73 P74 N75 G76 F77 A78 A79 F80 K81 E82 I83 P84 A85 G86 G87 L88 V89 Q90 L91 L92 F93 F94 I95 G96 V97 L98 E99 S100 S101 V102 M103 R104 D105 L106 T107 G108 E109 A110 E111 F112 V113 G114 D115 F116 R117 N118 G119 A120


I121 D122 F123 G124 W125 D126 T127 F128 D129 E130 E131 T132 Q133 F134 K135 K136 R137 A138 I139 E140 L141 N142 Q143 G144 R145 A146 A147 Q148 M149 G150 I151 L152 A153 L154 M155 V156 H157 E158 Q159 L160 G161 V162 S163 L164 L165 P166

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42033	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	444.2236, 444.2236, 444.2236	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, BCR, KC2, LMG, CLA, DGD, DD6, HEM, CL, PHO, BCT, KC1, A86, OEX, PL9, FE2, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	0/2700	0.70	2/3681 (0.1%)
1	a	0.68	0/2700	0.70	2/3681 (0.1%)
2	B	0.68	2/4092 (0.0%)	0.75	4/5562 (0.1%)
2	b	0.67	1/4092 (0.0%)	0.75	3/5562 (0.1%)
3	C	0.67	0/3613	0.73	5/4926 (0.1%)
3	c	0.67	0/3613	0.73	5/4926 (0.1%)
4	D	0.71	2/2788 (0.1%)	0.73	1/3803 (0.0%)
4	d	0.71	2/2788 (0.1%)	0.73	1/3803 (0.0%)
5	E	0.49	0/660	0.61	0/899
5	e	0.49	0/660	0.61	0/899
6	F	0.47	0/268	0.70	0/363
6	f	0.47	0/268	0.70	0/363
7	G	0.39	0/936	0.60	0/1261
7	g	0.39	0/936	0.60	0/1261
8	H	0.57	1/516 (0.2%)	0.76	0/704
8	h	0.57	1/516 (0.2%)	0.76	0/704
9	I	0.72	0/285	0.74	0/386
9	i	0.72	0/285	0.74	0/386
10	J	0.52	0/253	0.93	1/344 (0.3%)
10	j	0.52	0/253	0.93	1/344 (0.3%)
11	K	0.67	0/311	0.81	0/427
11	k	0.67	0/311	0.80	0/427
12	L	0.69	0/310	0.73	0/423
12	l	0.69	0/310	0.73	0/423
13	M	0.58	0/313	0.70	0/422
13	m	0.58	0/313	0.70	0/422
15	O	0.52	0/1911	0.76	2/2576 (0.1%)
15	o	0.52	0/1911	0.76	2/2576 (0.1%)
16	P	0.54	1/1795 (0.1%)	0.72	1/2441 (0.0%)
16	p	0.54	1/1795 (0.1%)	0.72	1/2441 (0.0%)
17	Q	0.47	0/1164	0.72	4/1569 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	q	0.47	0/1164	0.72	4/1569 (0.3%)
19	T	0.53	0/256	0.71	0/346
19	t	0.52	0/256	0.71	0/346
20	U	0.50	0/726	0.69	1/986 (0.1%)
20	u	0.50	0/726	0.69	1/986 (0.1%)
21	V	0.50	0/1062	0.66	0/1444
21	v	0.51	0/1062	0.66	0/1444
22	W	0.62	0/368	0.93	0/491
22	w	0.62	0/368	0.93	0/491
23	X	0.28	0/244	0.61	0/330
23	x	0.28	0/244	0.61	0/330
24	Y	0.51	0/259	0.97	1/353 (0.3%)
24	y	0.51	0/259	0.97	1/353 (0.3%)
25	Z	0.48	0/460	0.69	0/633
25	z	0.47	0/460	0.69	0/633
26	0	0.73	5/1151 (0.4%)	1.01	7/1550 (0.5%)
26	10	0.66	3/1151 (0.3%)	0.84	3/1550 (0.2%)
27	1	0.63	0/1371	0.90	3/1849 (0.2%)
27	11	0.67	2/1365 (0.1%)	0.95	4/1841 (0.2%)
27	12	0.62	3/1358 (0.2%)	0.88	1/1834 (0.1%)
27	13	0.58	2/1362 (0.1%)	0.89	4/1838 (0.2%)
27	14	0.61	0/1342	0.96	5/1813 (0.3%)
27	15	0.66	0/1306	1.09	15/1769 (0.8%)
27	16	0.54	0/1371	0.97	6/1849 (0.3%)
27	17	0.51	0/1371	0.88	3/1849 (0.2%)
27	18	0.69	0/1330	1.04	10/1797 (0.6%)
27	2	0.62	3/1371 (0.2%)	0.95	6/1849 (0.3%)
27	3	0.53	1/1371 (0.1%)	0.99	8/1849 (0.4%)
27	4	0.60	0/1342	1.02	8/1813 (0.4%)
27	5	0.68	3/1306 (0.2%)	0.96	7/1769 (0.4%)
27	6	0.55	0/1365	0.95	3/1841 (0.2%)
27	7	0.54	0/1365	0.99	9/1841 (0.5%)
27	8	0.68	1/1316 (0.1%)	1.08	11/1781 (0.6%)
28	19	0.39	0/1313	0.57	0/1771
28	9	0.40	0/1313	0.57	0/1771
All	All	0.61	34/77120 (0.0%)	0.81	156/104564 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
3	C	0	2
3	c	0	2
13	M	0	1
13	m	0	1
14	N	0	1
14	n	0	1
16	P	0	1
16	p	0	1
22	W	0	2
22	w	0	2
24	Y	0	1
24	y	0	1
26	0	0	2
26	10	0	2
27	1	0	4
27	11	0	2
27	12	0	2
27	13	0	4
27	14	0	6
27	15	0	9
27	16	0	5
27	17	0	4
27	18	0	3
27	2	0	4
27	3	0	5
27	4	0	2
27	5	0	7
27	6	0	8
27	7	0	5
27	8	0	5
All	All	0	97

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	132	PHE	CD1-CE1	-9.58	1.20	1.39
26	10	130	GLU	CB-CG	-7.27	1.38	1.52
26	0	130	GLU	CB-CG	-7.07	1.38	1.52
26	0	130	GLU	CG-CD	-6.83	1.41	1.51
2	B	22	VAL	CB-CG1	-6.78	1.38	1.52
27	12	150	PHE	CB-CG	-6.77	1.39	1.51

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG1	-6.76	1.38	1.52
27	5	132	PHE	CB-CG	-6.64	1.40	1.51
26	10	130	GLU	CG-CD	-6.52	1.42	1.51
27	12	52	VAL	CB-CG1	-6.50	1.39	1.52
26	0	65	TYR	CD1-CE1	-6.45	1.29	1.39
16	p	130	GLU	CB-CG	-6.40	1.40	1.52
27	13	52	VAL	CB-CG1	-6.36	1.39	1.52
16	P	130	GLU	CB-CG	-6.33	1.40	1.52
26	0	65	TYR	CD2-CE2	-6.20	1.30	1.39
27	11	130	GLU	CB-CG	-6.17	1.40	1.52
27	11	52	VAL	CB-CG1	-6.17	1.40	1.52
4	D	315	TYR	CD1-CE1	-6.05	1.30	1.39
4	d	315	TYR	CD1-CE1	-6.05	1.30	1.39
26	10	81	TYR	CD2-CE2	-5.81	1.30	1.39
27	8	161	GLU	CG-CD	-5.80	1.43	1.51
27	13	141	GLU	CB-CG	-5.79	1.41	1.52
8	h	33	VAL	CB-CG1	-5.77	1.40	1.52
8	H	33	VAL	CB-CG1	-5.73	1.40	1.52
27	2	161	GLU	CB-CG	-5.64	1.41	1.52
26	0	65	TYR	CB-CG	-5.64	1.43	1.51
4	D	315	TYR	CB-CG	-5.54	1.43	1.51
27	2	191	ILE	C-N	5.47	1.44	1.34
4	d	315	TYR	CB-CG	-5.46	1.43	1.51
27	5	132	PHE	CD2-CE2	-5.40	1.28	1.39
27	3	153	PHE	CB-CG	-5.33	1.42	1.51
2	B	113	TRP	CB-CG	-5.15	1.41	1.50
27	12	141	GLU	CG-CD	-5.05	1.44	1.51
27	2	150	PHE	CB-CG	-5.01	1.42	1.51

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	191	ILE	CG1-CB-CG2	-12.36	84.22	111.40
27	3	193	LEU	CB-CG-CD1	-11.57	91.33	111.00
26	0	181	LEU	CB-CG-CD2	-9.61	94.67	111.00
27	7	51	LEU	CA-CB-CG	9.39	136.90	115.30
26	10	181	LEU	CB-CG-CD2	-9.29	95.21	111.00
27	16	135	LYS	CD-CE-NZ	-9.27	90.38	111.70
27	14	184	LEU	CB-CG-CD1	-9.24	95.29	111.00
27	3	193	LEU	CA-CB-CG	9.15	136.35	115.30
27	4	165	LYS	CD-CE-NZ	-9.06	90.86	111.70
27	5	193	LEU	CA-CB-CG	9.02	136.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	0	191	LEU	CA-CB-CG	8.96	135.90	115.30
27	18	184	LEU	CA-CB-CG	8.95	135.88	115.30
27	16	134	MET	CG-SD-CE	-8.88	85.99	100.20
27	15	191	ILE	CG1-CB-CG2	-8.78	92.08	111.40
27	3	51	LEU	CA-CB-CG	8.70	135.31	115.30
27	2	51	LEU	CA-CB-CG	8.50	134.85	115.30
27	4	184	LEU	CB-CG-CD1	-8.31	96.88	111.00
27	6	184	LEU	CA-CB-CG	8.25	134.27	115.30
27	16	184	LEU	CA-CB-CG	8.19	134.14	115.30
27	17	184	LEU	CA-CB-CG	7.90	133.48	115.30
27	7	184	LEU	CA-CB-CG	7.79	133.21	115.30
27	8	184	LEU	CA-CB-CG	7.54	132.65	115.30
26	0	164	ARG	NE-CZ-NH1	-7.42	116.59	120.30
26	10	191	LEU	CA-CB-CG	7.32	132.13	115.30
27	13	37	LEU	CB-CG-CD2	-7.30	98.59	111.00
10	J	15	LEU	CB-CG-CD1	-7.24	98.69	111.00
27	18	37	LEU	CB-CG-CD1	-7.24	98.69	111.00
10	j	15	LEU	CB-CG-CD1	-7.24	98.70	111.00
27	3	184	LEU	CA-CB-CG	7.23	131.93	115.30
27	3	62	ARG	NE-CZ-NH1	-7.17	116.71	120.30
4	d	289	LEU	CB-CG-CD1	-7.16	98.83	111.00
4	D	289	LEU	CB-CG-CD1	-7.16	98.84	111.00
27	14	151	ILE	CG1-CB-CG2	-7.07	95.85	111.40
27	11	147	ARG	CG-CD-NE	-7.06	96.98	111.80
27	2	184	LEU	CA-CB-CG	7.05	131.53	115.30
27	8	191	ILE	CG1-CB-CG2	-7.03	95.94	111.40
27	4	145	ASP	CB-CG-OD1	6.96	124.56	118.30
26	0	135	ARG	NE-CZ-NH2	-6.86	116.87	120.30
27	3	151	ILE	CG1-CB-CG2	-6.83	96.38	111.40
26	0	65	TYR	CA-CB-CG	-6.82	100.44	113.40
27	6	199	LEU	CA-CB-CG	6.72	130.75	115.30
26	0	65	TYR	CB-CG-CD1	-6.63	117.02	121.00
27	7	199	LEU	CA-CB-CG	6.57	130.41	115.30
3	C	438	LEU	CB-CG-CD2	-6.52	99.92	111.00
27	2	199	LEU	CA-CB-CG	6.50	130.26	115.30
27	8	68	LEU	CB-CG-CD1	-6.47	99.99	111.00
3	c	438	LEU	CB-CG-CD2	-6.47	100.00	111.00
27	8	184	LEU	CB-CG-CD1	-6.47	100.00	111.00
27	15	37	LEU	CB-CG-CD2	-6.45	100.04	111.00
16	P	149	LEU	CA-CB-CG	6.42	130.06	115.30
16	p	149	LEU	CA-CB-CG	6.39	130.00	115.30
27	15	193	LEU	CA-CB-CG	6.39	130.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	199	LEU	CA-CB-CG	6.37	129.94	115.30
15	o	245	ASP	CB-CG-OD1	6.35	124.02	118.30
15	O	245	ASP	CB-CG-OD1	6.35	124.01	118.30
17	Q	147	LEU	CA-CB-CG	6.32	129.83	115.30
17	q	147	LEU	CA-CB-CG	6.31	129.82	115.30
27	15	132	PHE	N-CA-CB	-6.27	99.32	110.60
27	14	189	LYS	CD-CE-NZ	-6.27	97.29	111.70
2	b	426	LEU	CA-CB-CG	6.18	129.52	115.30
2	B	426	LEU	CA-CB-CG	6.18	129.51	115.30
27	17	196	ASP	CB-CG-OD1	6.17	123.85	118.30
27	11	136	ASP	CB-CG-OD1	6.15	123.83	118.30
27	8	182	LEU	CA-CB-CG	6.14	129.43	115.30
27	8	37	LEU	CB-CG-CD1	-6.13	100.57	111.00
27	15	68	LEU	CB-CG-CD1	-6.11	100.62	111.00
27	8	49	LEU	CA-CB-CG	6.03	129.17	115.30
27	18	52	VAL	CG1-CB-CG2	-6.01	101.28	110.90
27	2	196	ASP	CB-CG-OD1	5.96	123.66	118.30
27	16	191	ILE	CG1-CB-CG2	-5.95	98.31	111.40
27	5	152	ASP	CB-CG-OD1	5.93	123.64	118.30
27	7	133	VAL	CA-CB-CG2	-5.93	102.00	110.90
27	14	200	PRO	C-N-CA	5.88	136.40	121.70
27	7	151	ILE	CG1-CB-CG2	-5.88	98.48	111.40
27	8	205	LEU	CA-CB-CG	5.80	128.64	115.30
27	13	196	ASP	CB-CG-OD1	5.79	123.51	118.30
27	18	193	LEU	CA-CB-CG	5.78	128.58	115.30
27	15	37	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	271	LEU	CB-CG-CD1	-5.77	101.20	111.00
1	a	271	LEU	CB-CG-CD1	-5.76	101.21	111.00
27	8	52	VAL	CG1-CB-CG2	-5.75	101.70	110.90
27	15	185	MET	CG-SD-CE	5.74	109.38	100.20
15	O	266	LEU	CA-CB-CG	-5.74	102.10	115.30
15	o	266	LEU	CA-CB-CG	-5.74	102.10	115.30
27	18	205	LEU	CA-CB-CG	5.73	128.47	115.30
17	Q	161	LEU	CA-CB-CG	5.69	128.40	115.30
27	18	182	LEU	CA-CB-CG	5.69	128.39	115.30
27	12	196	ASP	CB-CG-OD1	5.69	123.42	118.30
17	q	161	LEU	CA-CB-CG	5.68	128.36	115.30
26	0	164	ARG	NE-CZ-NH2	5.68	123.14	120.30
27	16	184	LEU	CB-CG-CD1	-5.65	101.39	111.00
2	B	330	MET	CG-SD-CE	-5.64	91.17	100.20
3	C	119	LEU	CB-CG-CD1	-5.63	101.42	111.00
3	c	119	LEU	CB-CG-CD1	-5.63	101.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	156	ASP	CB-CG-OD1	5.63	123.36	118.30
2	b	330	MET	CG-SD-CE	-5.61	91.23	100.20
27	6	184	LEU	CB-CG-CD1	-5.60	101.47	111.00
27	15	184	LEU	CB-CG-CD1	-5.60	101.48	111.00
27	15	156	ASP	CB-CG-OD1	5.58	123.33	118.30
27	4	151	ILE	CG1-CB-CG2	-5.57	99.14	111.40
27	7	129	LEU	CA-CB-CG	5.57	128.11	115.30
27	1	129	LEU	CA-CB-CG	5.53	128.02	115.30
27	7	196	ASP	CB-CG-OD1	5.51	123.26	118.30
27	4	156	ASP	CB-CG-OD1	5.50	123.25	118.30
26	10	31	LEU	CB-CG-CD2	-5.50	101.65	111.00
27	13	145	ASP	CB-CG-OD2	5.43	123.19	118.30
27	5	97	ASP	CB-CG-OD1	5.43	123.19	118.30
27	2	184	LEU	CB-CG-CD1	-5.42	101.79	111.00
27	15	68	LEU	CA-CB-CG	5.40	127.73	115.30
27	14	156	ASP	CB-CG-OD1	5.39	123.15	118.30
2	b	315	ILE	CG1-CB-CG2	-5.38	99.57	111.40
17	Q	147	LEU	CB-CG-CD2	-5.37	101.87	111.00
17	q	147	LEU	CB-CG-CD2	-5.37	101.88	111.00
2	B	315	ILE	CG1-CB-CG2	-5.37	99.60	111.40
27	4	145	ASP	CB-CG-OD2	-5.35	113.49	118.30
27	3	184	LEU	CB-CG-CD1	-5.34	101.93	111.00
27	4	196	ASP	CB-CG-OD1	5.32	123.09	118.30
27	11	184	LEU	CA-CB-CG	5.32	127.53	115.30
27	7	182	LEU	CA-CB-CG	5.32	127.52	115.30
27	5	184	LEU	CB-CG-CD1	-5.28	102.03	111.00
24	y	32	LEU	CB-CG-CD2	5.27	119.95	111.00
3	C	204	LEU	CA-CB-CG	5.26	127.40	115.30
27	16	134	MET	CB-CG-SD	5.25	128.16	112.40
27	15	97	ASP	CB-CG-OD1	5.25	123.03	118.30
20	u	101	LEU	CA-CB-CG	5.25	127.37	115.30
3	C	401	LEU	CA-CB-CG	5.25	127.37	115.30
27	11	97	ASP	CB-CG-OD1	5.25	123.02	118.30
3	c	204	LEU	CA-CB-CG	5.23	127.33	115.30
27	15	148	ASN	N-CA-C	5.23	125.11	111.00
24	Y	32	LEU	CB-CG-CD2	5.23	119.88	111.00
20	U	101	LEU	CA-CB-CG	5.22	127.30	115.30
3	c	401	LEU	CA-CB-CG	5.21	127.28	115.30
27	3	62	ARG	NE-CZ-NH2	5.19	122.90	120.30
27	18	182	LEU	CB-CG-CD1	-5.19	102.17	111.00
27	17	182	LEU	CA-CB-CG	5.19	127.23	115.30
1	a	120	LEU	CA-CB-CG	-5.18	103.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	37	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	120	LEU	CA-CB-CG	-5.17	103.40	115.30
27	18	153	PHE	N-CA-CB	-5.17	101.29	110.60
27	15	152	ASP	CB-CG-OD1	5.16	122.95	118.30
27	15	191	ILE	CA-CB-CG2	5.15	121.21	110.90
27	1	196	ASP	CB-CG-OD1	5.15	122.94	118.30
27	15	190	LEU	C-N-CA	5.15	134.57	121.70
2	B	442	VAL	CG1-CB-CG2	5.14	119.12	110.90
27	5	68	LEU	CB-CG-CD1	-5.11	102.31	111.00
3	c	438	LEU	CA-CB-CG	5.11	127.05	115.30
3	C	438	LEU	CA-CB-CG	5.10	127.04	115.30
27	8	196	ASP	CB-CG-OD1	5.09	122.88	118.30
27	1	145	ASP	CB-CG-OD1	-5.08	113.72	118.30
17	q	114	LEU	CA-CB-CG	5.08	126.97	115.30
27	7	68	LEU	CB-CG-CD1	-5.07	102.38	111.00
27	2	129	LEU	CA-CB-CG	5.06	126.95	115.30
17	Q	114	LEU	CA-CB-CG	5.05	126.92	115.30
27	18	196	ASP	CB-CG-OD1	5.05	122.84	118.30
27	13	151	ILE	CG1-CB-CG2	-5.00	100.40	111.40
27	18	133	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

All (97) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	0	134	MET	Peptide
26	0	145	UNK	Peptide
27	1	142	PHE	Peptide
27	1	144	GLY	Peptide
27	1	150	PHE	Peptide
27	1	192	PRO	Peptide
26	10	141	UNK	Peptide
26	10	145	UNK	Peptide
27	11	136	ASP	Peptide
27	11	150	PHE	Peptide
27	12	150	PHE	Peptide
27	12	190	LEU	Peptide
27	13	132	PHE	Peptide
27	13	150	PHE	Peptide
27	13	153	PHE	Peptide
27	13	154	GLY	Peptide
27	14	142	PHE	Peptide

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Mol	Chain	Res	Type	Group
27	14	147	ARG	Peptide
27	14	153	PHE	Peptide
27	14	154	GLY	Peptide
27	14	200	PRO	Peptide
27	14	201	ILE	Peptide
27	15	131	VAL	Peptide
27	15	132	PHE	Mainchain
27	15	153	PHE	Peptide
27	15	154	GLY	Peptide
27	15	190	LEU	Peptide
27	15	191	ILE	Mainchain
27	15	54	ASP	Peptide
27	15	55	GLY	Peptide
27	15	65	TYR	Peptide
27	16	132	PHE	Peptide
27	16	135	LYS	Peptide
27	16	150	PHE	Peptide
27	16	157	SER	Peptide
27	16	39	ALA	Peptide
27	17	135	LYS	Peptide
27	17	150	PHE	Peptide
27	17	153	PHE	Peptide
27	17	39	ALA	Peptide
27	18	152	ASP	Peptide
27	18	154	GLY	Peptide
27	18	39	ALA	Peptide
27	2	135	LYS	Peptide
27	2	150	PHE	Peptide
27	2	153	PHE	Peptide
27	2	39	ALA	Peptide
27	3	132	PHE	Peptide
27	3	135	LYS	Peptide
27	3	150	PHE	Peptide
27	3	151	ILE	Peptide
27	3	39	ALA	Peptide
27	4	140	GLY	Peptide
27	4	146	PHE	Peptide
27	5	131	VAL	Peptide
27	5	151	ILE	Peptide
27	5	153	PHE	Peptide
27	5	154	GLY	Peptide
27	5	190	LEU	Peptide

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Mol	Chain	Res	Type	Group
27	5	54	ASP	Peptide
27	5	55	GLY	Peptide
27	6	130	GLU	Peptide
27	6	131	VAL	Peptide
27	6	132	PHE	Peptide
27	6	135	LYS	Peptide
27	6	150	PHE	Peptide
27	6	152	ASP	Peptide
27	6	153	PHE	Peptide
27	6	39	ALA	Peptide
27	7	132	PHE	Peptide
27	7	135	LYS	Peptide
27	7	150	PHE	Peptide
27	7	190	LEU	Peptide
27	7	39	ALA	Peptide
27	8	137	ILE	Peptide
27	8	138	THR	Peptide
27	8	140	GLY	Peptide
27	8	151	ILE	Peptide
27	8	39	ALA	Peptide
2	B	442	VAL	Peptide
3	C	222	GLY	Peptide
3	C	376	ASP	Peptide
13	M	4	GLN	Peptide
14	N	23	UNK	Peptide
16	P	157	ARG	Peptide
22	W	98	LYS	Peptide
22	W	99	PRO	Peptide
24	Y	42	GLN	Peptide
2	b	442	VAL	Peptide
3	c	222	GLY	Peptide
3	c	376	ASP	Peptide
13	m	4	GLN	Peptide
14	n	23	UNK	Peptide
16	p	157	ARG	Peptide
22	w	98	LYS	Peptide
22	w	99	PRO	Peptide
24	y	42	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	332/359 (92%)	321 (97%)	11 (3%)	0	100	100
1	a	332/359 (92%)	321 (97%)	11 (3%)	0	100	100
2	B	501/509 (98%)	479 (96%)	22 (4%)	0	100	100
2	b	501/509 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	448/450 (100%)	420 (94%)	28 (6%)	0	100	100
3	c	448/450 (100%)	420 (94%)	28 (6%)	0	100	100
4	D	339/341 (99%)	322 (95%)	17 (5%)	0	100	100
4	d	339/341 (99%)	321 (95%)	18 (5%)	0	100	100
5	E	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
5	e	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
6	F	30/32 (94%)	27 (90%)	3 (10%)	0	100	100
6	f	30/32 (94%)	27 (90%)	3 (10%)	0	100	100
7	G	120/179 (67%)	114 (95%)	6 (5%)	0	100	100
7	g	120/179 (67%)	114 (95%)	6 (5%)	0	100	100
8	H	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
9	i	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
10	j	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	35/38 (92%)	31 (89%)	4 (11%)	0	100	100
12	l	35/38 (92%)	31 (89%)	4 (11%)	0	100	100
13	M	39/41 (95%)	36 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
15	O	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	34	71
15	o	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	34	71
16	P	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	34	71
16	p	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	34	71
17	Q	145/211 (69%)	127 (88%)	18 (12%)	0	100	100
17	q	145/211 (69%)	127 (88%)	18 (12%)	0	100	100
19	T	28/31 (90%)	28 (100%)	0	0	100	100
19	t	28/31 (90%)	28 (100%)	0	0	100	100
20	U	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
20	u	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
21	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
21	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
22	W	43/51 (84%)	36 (84%)	7 (16%)	0	100	100
22	w	43/51 (84%)	36 (84%)	7 (16%)	0	100	100
23	X	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
23	x	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
24	Y	31/33 (94%)	27 (87%)	3 (10%)	1 (3%)	4	21
24	y	31/33 (94%)	27 (87%)	3 (10%)	1 (3%)	4	21
25	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
25	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
26	0	145/178 (82%)	128 (88%)	15 (10%)	2 (1%)	11	41
26	10	145/178 (82%)	130 (90%)	15 (10%)	0	100	100
27	1	170/172 (99%)	141 (83%)	27 (16%)	2 (1%)	13	46
27	11	170/172 (99%)	146 (86%)	22 (13%)	2 (1%)	13	46
27	12	170/172 (99%)	146 (86%)	23 (14%)	1 (1%)	25	62
27	13	170/172 (99%)	150 (88%)	18 (11%)	2 (1%)	13	46
27	14	170/172 (99%)	148 (87%)	19 (11%)	3 (2%)	8	35
27	15	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	25	62
27	16	170/172 (99%)	146 (86%)	21 (12%)	3 (2%)	8	35
27	17	170/172 (99%)	146 (86%)	18 (11%)	6 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	18	170/172 (99%)	142 (84%)	25 (15%)	3 (2%)	8 35
27	2	170/172 (99%)	147 (86%)	19 (11%)	4 (2%)	6 28
27	3	170/172 (99%)	145 (85%)	23 (14%)	2 (1%)	13 46
27	4	170/172 (99%)	149 (88%)	21 (12%)	0	100 100
27	5	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	25 62
27	6	170/172 (99%)	143 (84%)	24 (14%)	3 (2%)	8 35
27	7	170/172 (99%)	142 (84%)	24 (14%)	4 (2%)	6 28
27	8	170/172 (99%)	136 (80%)	32 (19%)	2 (1%)	13 46
28	19	164/166 (99%)	162 (99%)	2 (1%)	0	100 100
28	9	164/166 (99%)	162 (99%)	2 (1%)	0	100 100
All	All	9576/10090 (95%)	8700 (91%)	829 (9%)	47 (0%)	32 66

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	1	151	ILE
27	1	193	LEU
27	2	151	ILE
27	3	151	ILE
27	6	151	ILE
27	7	151	ILE
27	8	138	THR
27	11	137	ILE
27	11	151	ILE
27	12	151	ILE
27	13	151	ILE
27	14	201	ILE
27	14	202	ILE
27	15	191	ILE
27	16	151	ILE
27	17	151	ILE
27	17	152	ASP
27	18	155	TRP
27	18	156	ASP
27	3	152	ASP
27	6	133	VAL
27	8	53	GLU
27	16	133	VAL

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Mol	Chain	Res	Type
24	Y	43	ILE
24	y	43	ILE
26	0	135	ARG
27	2	191	ILE
27	7	191	ILE
27	13	152	ASP
27	14	200	PRO
16	P	62	LYS
16	p	62	LYS
26	0	136	ASP
27	2	152	ASP
27	6	153	PHE
27	7	190	LEU
27	17	190	LEU
27	17	191	ILE
27	18	157	SER
27	2	192	PRO
27	16	152	ASP
27	17	192	PRO
27	5	194	GLY
27	7	192	PRO
15	O	246	PRO
15	o	246	PRO
27	17	200	PRO

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	272/291 (94%)	272 (100%)	0	100	100
1	a	272/291 (94%)	272 (100%)	0	100	100
2	B	401/405 (99%)	401 (100%)	0	100	100
2	b	401/405 (99%)	401 (100%)	0	100	100
3	C	355/355 (100%)	355 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	355/355 (100%)	355 (100%)	0	100	100
4	D	273/273 (100%)	273 (100%)	0	100	100
4	d	273/273 (100%)	273 (100%)	0	100	100
5	E	72/72 (100%)	72 (100%)	0	100	100
5	e	72/72 (100%)	72 (100%)	0	100	100
6	F	26/26 (100%)	26 (100%)	0	100	100
6	f	26/26 (100%)	26 (100%)	0	100	100
7	G	88/128 (69%)	88 (100%)	0	100	100
7	g	88/128 (69%)	88 (100%)	0	100	100
8	H	54/54 (100%)	54 (100%)	0	100	100
8	h	54/54 (100%)	54 (100%)	0	100	100
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	J	26/26 (100%)	25 (96%)	1 (4%)	33	68
10	j	26/26 (100%)	25 (96%)	1 (4%)	33	68
11	K	32/32 (100%)	32 (100%)	0	100	100
11	k	32/32 (100%)	32 (100%)	0	100	100
12	L	33/34 (97%)	33 (100%)	0	100	100
12	l	33/34 (97%)	33 (100%)	0	100	100
13	M	30/30 (100%)	30 (100%)	0	100	100
13	m	30/30 (100%)	30 (100%)	0	100	100
15	O	201/201 (100%)	200 (100%)	1 (0%)	88	96
15	o	201/201 (100%)	200 (100%)	1 (0%)	88	96
16	P	174/174 (100%)	174 (100%)	0	100	100
16	p	174/174 (100%)	174 (100%)	0	100	100
17	Q	118/158 (75%)	118 (100%)	0	100	100
17	q	118/158 (75%)	118 (100%)	0	100	100
19	T	27/28 (96%)	27 (100%)	0	100	100
19	t	27/28 (96%)	27 (100%)	0	100	100
20	U	77/78 (99%)	77 (100%)	0	100	100
20	u	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	V	114/115 (99%)	114 (100%)	0	100	100
21	v	114/115 (99%)	114 (100%)	0	100	100
22	W	35/35 (100%)	35 (100%)	0	100	100
22	w	35/35 (100%)	35 (100%)	0	100	100
23	X	27/27 (100%)	27 (100%)	0	100	100
23	x	27/27 (100%)	27 (100%)	0	100	100
24	Y	26/26 (100%)	26 (100%)	0	100	100
24	y	26/26 (100%)	26 (100%)	0	100	100
25	Z	49/49 (100%)	49 (100%)	0	100	100
25	z	49/49 (100%)	49 (100%)	0	100	100
26	0	118/118 (100%)	117 (99%)	1 (1%)	81	93
26	10	118/118 (100%)	118 (100%)	0	100	100
27	1	137/137 (100%)	137 (100%)	0	100	100
27	11	136/137 (99%)	136 (100%)	0	100	100
27	12	134/137 (98%)	134 (100%)	0	100	100
27	13	135/137 (98%)	135 (100%)	0	100	100
27	14	132/137 (96%)	132 (100%)	0	100	100
27	15	124/137 (90%)	124 (100%)	0	100	100
27	16	137/137 (100%)	137 (100%)	0	100	100
27	17	137/137 (100%)	137 (100%)	0	100	100
27	18	131/137 (96%)	131 (100%)	0	100	100
27	2	137/137 (100%)	136 (99%)	1 (1%)	84	94
27	3	137/137 (100%)	137 (100%)	0	100	100
27	4	132/137 (96%)	132 (100%)	0	100	100
27	5	124/137 (90%)	124 (100%)	0	100	100
27	6	136/137 (99%)	136 (100%)	0	100	100
27	7	136/137 (99%)	136 (100%)	0	100	100
27	8	128/137 (93%)	128 (100%)	0	100	100
28	19	131/131 (100%)	131 (100%)	0	100	100
28	9	131/131 (100%)	131 (100%)	0	100	100
All	All	7717/7990 (97%)	7711 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	36	LEU
15	O	156	VAL
10	j	36	LEU
15	o	156	VAL
26	0	135	ARG
27	2	192	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	230	ASN
1	A	322	ASN
1	A	338	ASN
2	B	179	GLN
2	B	318	ASN
3	C	294	ASN
3	C	311	GLN
3	C	313	GLN
3	C	322	GLN
3	C	385	GLN
3	C	415	ASN
4	D	72	ASN
4	D	87	HIS
4	D	142	ASN
4	D	189	HIS
4	D	292	ASN
4	D	338	ASN
6	F	44	GLN
7	G	65	ASN
9	I	33	ASN
11	K	32	ASN
12	L	5	ASN
12	L	14	ASN
13	M	40	GLN
15	O	102	GLN
15	O	286	GLN
15	O	311	GLN
16	P	60	ASN
16	P	205	GLN
20	U	30	ASN

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Mol	Chain	Res	Type
20	U	53	HIS
21	V	17	ASN
21	V	70	ASN
21	V	118	HIS
25	Z	45	GLN
1	a	181	ASN
1	a	230	ASN
1	a	322	ASN
1	a	338	ASN
2	b	179	GLN
2	b	318	ASN
3	c	294	ASN
3	c	311	GLN
3	c	313	GLN
3	c	322	GLN
3	c	415	ASN
4	d	72	ASN
4	d	87	HIS
4	d	142	ASN
4	d	189	HIS
4	d	292	ASN
4	d	338	ASN
6	f	44	GLN
9	i	33	ASN
11	k	32	ASN
12	l	5	ASN
12	l	14	ASN
12	l	38	ASN
13	m	28	GLN
13	m	40	GLN
15	o	102	GLN
15	o	110	ASN
15	o	164	GLN
15	o	286	GLN
15	o	311	GLN
16	p	205	GLN
20	u	30	ASN
20	u	53	HIS
21	v	17	ASN
21	v	70	ASN
21	v	118	HIS
25	z	45	GLN

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Mol	Chain	Res	Type
26	0	169	ASN
26	0	170	GLN
27	1	70	HIS
27	1	187	HIS
27	2	35	ASN
27	2	70	HIS
27	2	173	GLN
27	3	70	HIS
27	4	56	ASN
27	4	172	ASN
27	4	173	GLN
27	5	173	GLN
27	6	70	HIS
27	6	173	GLN
27	7	35	ASN
27	7	70	HIS
27	7	173	GLN
27	8	70	HIS
27	8	173	GLN
27	8	187	HIS
28	9	9	GLN
28	9	143	GLN
28	9	157	HIS
26	10	160	GLN
26	10	169	ASN
26	10	170	GLN
27	11	187	HIS
27	14	173	GLN
27	15	187	HIS
27	16	70	HIS
27	16	173	GLN
27	17	35	ASN
27	17	70	HIS
27	17	187	HIS
27	18	70	HIS
27	18	173	GLN
27	18	187	HIS
28	19	9	GLN
28	19	157	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)

Of 536 ligands modelled in this entry, 4 are monoatomic - leaving 532 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	LMG	N	101	14	28,28,55	1.12	4 (14%)	36,36,63	1.31	6 (16%)
31	CLA	b	617	-	65,73,73	1.49	10 (15%)	76,113,113	1.62	14 (18%)
31	CLA	8	314	-	43,51,73	1.75	9 (20%)	49,86,113	1.71	8 (16%)
31	CLA	15	307	-	65,73,73	1.42	8 (12%)	76,113,113	1.41	9 (11%)
36	LHG	15	316	-	24,24,48	0.79	0	27,30,54	1.25	2 (7%)
33	BCR	b	620	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	9 (16%)
43	A86	8	302	-	44,50,50	1.50	5 (11%)	51,76,76	3.64	27 (52%)
43	A86	2	301	-	44,50,50	1.35	5 (11%)	51,76,76	3.44	24 (47%)
31	CLA	4	314	-	43,51,73	1.81	9 (20%)	49,86,113	1.72	8 (16%)
36	LHG	w	202	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	4 (9%)
43	A86	13	306	43	44,50,50	1.37	3 (6%)	51,76,76	4.62	23 (45%)
43	A86	p	611	-	44,50,50	1.88	10 (22%)	51,76,76	6.01	30 (58%)
43	A86	10	303	-	44,50,50	1.47	7 (15%)	51,76,76	3.57	25 (49%)
31	CLA	11	310	-	50,58,73	1.60	8 (16%)	58,95,113	1.71	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	6	316	-	43,51,73	1.79	6 (13%)	49,86,113	1.70	9 (18%)
35	PL9	D	406	-	55,55,55	2.03	15 (27%)	68,69,69	1.42	12 (17%)
31	CLA	2	306	-	42,50,73	1.74	5 (11%)	48,85,113	2.33	15 (31%)
38	LMG	k	101	-	46,46,55	1.06	4 (8%)	54,54,63	1.45	8 (14%)
31	CLA	15	306	-	42,50,73	1.85	7 (16%)	48,85,113	2.04	12 (25%)
31	CLA	C	512	3	65,73,73	1.47	9 (13%)	76,113,113	1.60	10 (13%)
33	BCR	C	516	-	41,41,41	1.24	5 (12%)	56,56,56	1.35	9 (16%)
31	CLA	P	606	-	43,51,73	2.35	14 (32%)	49,86,113	4.31	26 (53%)
31	CLA	18	309	-	52,60,73	1.54	8 (15%)	60,97,113	1.87	8 (13%)
31	CLA	10	317	-	48,56,73	1.73	9 (18%)	55,92,113	1.68	9 (16%)
45	KC2	12	311	-	48,53,53	3.12	21 (43%)	54,89,89	5.42	34 (62%)
43	A86	13	302	-	44,50,50	1.51	4 (9%)	51,76,76	4.78	27 (52%)
31	CLA	6	308	-	42,50,73	1.73	5 (11%)	48,85,113	2.17	13 (27%)
43	A86	19	302	-	44,50,50	1.43	4 (9%)	51,76,76	5.35	23 (45%)
31	CLA	6	311	-	41,49,73	1.73	6 (14%)	47,84,113	1.92	8 (17%)
45	KC2	18	308	-	48,53,53	3.04	22 (45%)	54,89,89	4.67	31 (57%)
31	CLA	R	101	-	47,55,73	1.69	8 (17%)	54,91,113	1.60	7 (12%)
31	CLA	1	313	-	65,73,73	1.58	9 (13%)	76,113,113	1.47	12 (15%)
33	BCR	a	407	-	41,41,41	1.25	3 (7%)	56,56,56	1.22	6 (10%)
31	CLA	B	611	-	65,73,73	1.63	11 (16%)	76,113,113	1.93	12 (15%)
36	LHG	4	317	-	34,34,48	0.76	1 (2%)	37,40,54	1.25	3 (8%)
31	CLA	c	504	31	65,73,73	1.45	8 (12%)	76,113,113	1.62	14 (18%)
45	KC2	6	310	-	48,53,53	3.15	22 (45%)	54,89,89	4.36	26 (48%)
31	CLA	3	307	-	42,50,73	1.77	6 (14%)	48,85,113	2.16	16 (33%)
31	CLA	15	311	27	45,53,73	1.99	10 (22%)	52,89,113	2.00	15 (28%)
31	CLA	C	502	-	65,73,73	1.42	8 (12%)	76,113,113	1.57	10 (13%)
43	A86	12	302	-	44,50,50	1.48	5 (11%)	51,76,76	4.72	30 (58%)
43	A86	14	301	-	44,50,50	1.37	4 (9%)	51,76,76	2.76	22 (43%)
31	CLA	18	306	42	50,58,73	1.63	9 (18%)	58,95,113	1.87	15 (25%)
42	KC1	3	314	27	48,53,53	3.11	20 (41%)	55,89,89	6.59	32 (58%)
38	LMG	F	102	-	46,46,55	0.96	4 (8%)	54,54,63	1.49	9 (16%)
43	A86	18	302	-	44,50,50	1.34	4 (9%)	51,76,76	2.48	18 (35%)
31	CLA	B	604	-	65,73,73	1.63	11 (16%)	76,113,113	2.35	17 (22%)
31	CLA	0	311	-	55,63,73	1.52	8 (14%)	64,101,113	1.67	9 (14%)
34	SQD	l	101	-	53,54,54	0.94	5 (9%)	62,65,65	1.51	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	14	314	-	43,51,73	1.83	9 (20%)	49,86,113	1.74	7 (14%)
31	CLA	b	614	-	65,73,73	1.43	8 (12%)	76,113,113	1.41	7 (9%)
31	CLA	11	312	27	46,54,73	1.81	9 (19%)	53,90,113	1.72	10 (18%)
31	CLA	13	312	-	45,53,73	1.79	6 (13%)	52,89,113	1.75	10 (19%)
31	CLA	12	307	-	42,50,73	1.80	7 (16%)	48,85,113	2.25	17 (35%)
31	CLA	19	307	-	61,69,73	1.50	6 (9%)	71,108,113	1.63	9 (12%)
43	A86	5	304	-	44,50,50	1.33	5 (11%)	51,76,76	3.90	29 (56%)
43	A86	6	303	-	44,50,50	1.42	5 (11%)	51,76,76	4.20	26 (50%)
31	CLA	C	506	-	65,73,73	1.39	8 (12%)	76,113,113	1.66	8 (10%)
29	OEX	A	401	1,3	0,15,15	-	-	-		
43	A86	3	306	-	44,50,50	1.30	3 (6%)	51,76,76	4.65	24 (47%)
43	A86	19	301	-	44,50,50	1.32	4 (9%)	51,76,76	4.46	29 (56%)
31	CLA	5	309	-	55,63,73	1.51	8 (14%)	64,101,113	1.77	12 (18%)
34	SQD	L	102	-	53,54,54	0.94	5 (9%)	62,65,65	1.52	11 (17%)
31	CLA	15	313	-	41,49,73	1.86	6 (14%)	47,84,113	1.79	12 (25%)
43	A86	9	304	-	44,50,50	1.27	4 (9%)	51,76,76	4.19	18 (35%)
31	CLA	D	405	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	7 (9%)
36	LHG	l	102	-	48,48,48	0.79	3 (6%)	51,54,54	1.29	7 (13%)
43	A86	15	305	27	44,50,50	1.45	5 (11%)	51,76,76	4.12	23 (45%)
31	CLA	p	602	-	65,73,73	1.47	9 (13%)	76,113,113	1.46	8 (10%)
31	CLA	C	504	31	65,73,73	1.45	8 (12%)	76,113,113	1.62	14 (18%)
33	BCR	A	407	-	41,41,41	1.25	3 (7%)	56,56,56	1.21	6 (10%)
31	CLA	B	602	-	65,73,73	1.46	11 (16%)	76,113,113	1.66	13 (17%)
38	LMG	K	101	-	46,46,55	1.06	4 (8%)	54,54,63	1.45	8 (14%)
45	KC2	7	309	-	48,53,53	3.20	22 (45%)	54,89,89	4.48	27 (50%)
31	CLA	P	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.45	8 (10%)
32	PHO	D	402	-	51,69,69	1.07	6 (11%)	47,99,99	1.47	8 (17%)
43	A86	p	613	31	44,50,50	1.42	4 (9%)	51,76,76	3.70	29 (56%)
33	BCR	h	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.36	8 (14%)
38	LMG	15	315	-	36,36,55	1.20	4 (11%)	44,44,63	1.74	9 (20%)
31	CLA	8	307	-	61,69,73	1.53	11 (18%)	71,108,113	1.69	12 (16%)
36	LHG	8	316	-	30,30,48	0.78	1 (3%)	33,36,54	1.26	2 (6%)
43	A86	4	304	-	44,50,50	1.30	4 (9%)	51,76,76	3.07	20 (39%)
42	KC1	17	314	27	48,53,53	3.02	19 (39%)	55,89,89	6.05	33 (60%)
38	LMG	1	301	-	36,36,55	1.17	4 (11%)	44,44,63	1.44	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	18	311	27	46,54,73	1.78	10 (21%)	53,90,113	1.77	10 (18%)
45	KC2	7	311	27	48,53,53	3.14	22 (45%)	54,89,89	5.66	36 (66%)
31	CLA	C	507	-	65,73,73	1.50	11 (16%)	76,113,113	1.56	7 (9%)
36	LHG	a	410	1	36,36,48	0.76	1 (2%)	39,42,54	1.24	4 (10%)
43	A86	4	302	-	44,50,50	1.56	5 (11%)	51,76,76	4.11	28 (54%)
36	LHG	d	407	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
43	A86	5	318	42	44,50,50	1.29	4 (9%)	51,76,76	3.52	22 (43%)
38	LMG	W	201	-	48,48,55	0.97	6 (12%)	56,56,63	1.40	9 (16%)
43	A86	12	304	-	44,50,50	1.39	5 (11%)	51,76,76	3.94	18 (35%)
43	A86	13	304	-	44,50,50	1.66	8 (18%)	51,76,76	5.39	27 (52%)
31	CLA	A	406	-	60,68,73	1.42	9 (15%)	70,107,113	1.54	7 (10%)
31	CLA	17	310	-	45,53,73	1.72	5 (11%)	52,89,113	1.85	8 (15%)
39	DGD	w	204	-	57,57,67	1.15	7 (12%)	71,71,81	1.48	10 (14%)
31	CLA	7	308	-	41,49,73	1.85	9 (21%)	47,84,113	1.75	10 (21%)
31	CLA	9	311	43	46,54,73	1.76	4 (8%)	53,90,113	2.02	10 (18%)
31	CLA	B	609	-	65,73,73	1.43	9 (13%)	76,113,113	1.49	8 (10%)
43	A86	0	303	-	44,50,50	1.51	7 (15%)	51,76,76	3.57	25 (49%)
31	CLA	3	316	-	65,73,73	1.50	7 (10%)	76,113,113	2.21	21 (27%)
43	A86	12	305	-	44,50,50	1.33	4 (9%)	51,76,76	3.04	21 (41%)
45	KC2	5	308	-	48,53,53	3.14	23 (47%)	54,89,89	5.09	34 (62%)
39	DGD	C	519	-	63,63,67	1.12	9 (14%)	77,77,81	1.52	15 (19%)
31	CLA	C	503	31	65,73,73	1.53	11 (16%)	76,113,113	2.38	19 (25%)
42	KC1	8	313	31,43	48,53,53	2.91	19 (39%)	55,89,89	7.05	33 (60%)
31	CLA	3	313	-	65,73,73	1.66	8 (12%)	76,113,113	1.64	9 (11%)
31	CLA	4	309	-	65,73,73	1.38	7 (10%)	76,113,113	1.62	8 (10%)
33	BCR	H	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	8 (14%)
31	CLA	0	309	-	59,67,73	1.47	8 (13%)	68,105,113	1.64	9 (13%)
31	CLA	0	307	-	48,56,73	1.74	9 (18%)	55,92,113	1.78	9 (16%)
31	CLA	Z	101	-	51,59,73	1.63	10 (19%)	59,96,113	1.56	8 (13%)
39	DGD	c	518	-	56,56,67	1.22	10 (17%)	70,70,81	1.68	16 (22%)
42	KC1	13	314	-	48,53,53	3.07	19 (39%)	55,89,89	4.99	36 (65%)
43	A86	4	306	-	44,50,50	1.38	5 (11%)	51,76,76	3.99	25 (49%)
43	A86	7	304	-	44,50,50	1.53	6 (13%)	51,76,76	5.71	31 (60%)
31	CLA	3	308	-	43,51,73	1.79	10 (23%)	49,86,113	1.79	9 (18%)
31	CLA	12	312	-	45,53,73	1.74	8 (17%)	52,89,113	1.85	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	SQD	A	408	39	53,54,54	0.96	6 (11%)	62,65,65	1.56	13 (20%)
39	DGD	B	621	-	55,55,67	1.34	7 (12%)	69,69,81	1.74	15 (21%)
42	KC1	P	609	-	48,53,53	2.90	19 (39%)	55,89,89	4.84	34 (61%)
31	CLA	17	308	-	41,49,73	1.84	10 (24%)	47,84,113	1.71	10 (21%)
39	DGD	b	622	34	56,56,67	1.30	9 (16%)	70,70,81	1.62	14 (20%)
39	DGD	C	518	-	56,56,67	1.23	10 (17%)	70,70,81	1.68	17 (24%)
31	CLA	9	315	-	41,49,73	1.82	6 (14%)	47,84,113	1.77	7 (14%)
39	DGD	1	318	-	55,55,67	1.04	3 (5%)	69,69,81	1.36	8 (11%)
31	CLA	b	615	-	65,73,73	1.41	8 (12%)	76,113,113	1.64	12 (15%)
43	A86	6	301	43	44,50,50	1.30	4 (9%)	51,76,76	4.04	28 (54%)
43	A86	17	306	-	44,50,50	1.44	4 (9%)	51,76,76	3.70	22 (43%)
43	A86	5	305	-	44,50,50	1.51	7 (15%)	51,76,76	3.49	23 (45%)
31	CLA	19	315	-	41,49,73	1.83	6 (14%)	47,84,113	1.78	7 (14%)
31	CLA	10	314	-	47,55,73	1.77	9 (19%)	54,91,113	1.83	13 (24%)
31	CLA	C	511	-	65,73,73	1.45	9 (13%)	76,113,113	1.55	9 (11%)
31	CLA	12	316	-	46,54,73	1.82	5 (10%)	53,90,113	1.66	9 (16%)
43	A86	7	306	-	44,50,50	1.31	5 (11%)	51,76,76	3.95	23 (45%)
31	CLA	a	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.58	10 (13%)
31	CLA	11	316	43	41,49,73	1.92	7 (17%)	47,84,113	1.69	9 (19%)
34	SQD	b	601	39	53,54,54	0.90	5 (9%)	62,65,65	1.74	12 (19%)
31	CLA	15	312	-	47,55,73	1.94	12 (25%)	54,91,113	1.88	14 (25%)
31	CLA	12	308	-	65,73,73	1.44	8 (12%)	76,113,113	1.65	11 (14%)
31	CLA	P	610	-	41,49,73	1.75	8 (19%)	47,84,113	1.91	9 (19%)
31	CLA	16	309	-	65,73,73	1.45	10 (15%)	76,113,113	1.58	11 (14%)
43	A86	16	302	43	44,50,50	1.36	4 (9%)	51,76,76	4.05	26 (50%)
44	DD6	P	612	-	39,45,45	2.10	4 (10%)	52,67,67	2.33	17 (32%)
33	BCR	c	515	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	8 (14%)
31	CLA	b	606	-	65,73,73	1.51	12 (18%)	76,113,113	1.54	8 (10%)
32	PHO	a	405	-	51,69,69	1.12	6 (11%)	47,99,99	1.34	8 (17%)
33	BCR	b	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.38	10 (17%)
43	A86	18	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.66	19 (37%)
36	LHG	z	102	-	24,24,48	0.95	0	27,30,54	1.30	3 (11%)
42	KC1	7	314	27	48,53,53	3.14	20 (41%)	55,89,89	4.75	31 (56%)
45	KC2	5	310	27	48,53,53	3.02	22 (45%)	54,89,89	4.67	32 (59%)
42	KC1	9	314	-	48,53,53	3.14	22 (45%)	55,89,89	5.04	36 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	3	303	-	44,50,50	1.47	4 (9%)	51,76,76	4.77	28 (54%)
31	CLA	10	316	-	46,54,73	1.67	8 (17%)	53,90,113	1.67	7 (13%)
43	A86	0	304	-	44,50,50	1.27	5 (11%)	51,76,76	4.49	25 (49%)
31	CLA	P	601	16	65,73,73	1.44	10 (15%)	76,113,113	1.39	7 (9%)
38	LMG	0	317	-	31,31,55	1.35	3 (9%)	39,39,63	1.39	6 (15%)
33	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.42	8 (14%)
38	LMG	P	614	-	31,31,55	0.93	1 (3%)	39,39,63	1.70	9 (23%)
31	CLA	p	603	-	50,58,73	1.61	9 (18%)	58,95,113	1.67	11 (18%)
33	BCR	c	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	7 (12%)
43	A86	12	303	-	44,50,50	1.36	4 (9%)	51,76,76	3.21	21 (41%)
45	KC2	14	310	-	48,53,53	3.10	20 (41%)	54,89,89	5.09	33 (61%)
31	CLA	c	502	-	65,73,73	1.42	8 (12%)	76,113,113	1.58	10 (13%)
43	A86	4	305	-	44,50,50	1.52	9 (20%)	51,76,76	4.09	23 (45%)
38	LMG	c	522	-	31,31,55	1.16	3 (9%)	39,39,63	1.20	3 (7%)
42	KC1	4	313	-	48,53,53	2.89	20 (41%)	55,89,89	5.69	36 (65%)
38	LMG	w	201	-	48,48,55	0.97	6 (12%)	56,56,63	1.41	9 (16%)
38	LMG	Z	102	-	31,31,55	1.16	3 (9%)	39,39,63	1.20	3 (7%)
31	CLA	3	310	-	41,49,73	1.77	5 (12%)	47,84,113	1.92	9 (19%)
31	CLA	z	103	-	48,56,73	1.74	9 (18%)	55,92,113	1.69	10 (18%)
31	CLA	A	404	-	49,57,73	1.64	10 (20%)	55,93,113	1.78	10 (18%)
36	LHG	A	410	1	36,36,48	0.76	1 (2%)	39,42,54	1.24	4 (10%)
31	CLA	19	313	-	65,73,73	1.36	7 (10%)	76,113,113	2.14	15 (19%)
31	CLA	6	314	-	42,50,73	2.03	10 (23%)	48,85,113	2.12	11 (22%)
43	A86	15	301	31	44,50,50	1.61	7 (15%)	51,76,76	4.24	23 (45%)
31	CLA	C	509	-	65,73,73	1.55	9 (13%)	76,113,113	1.93	13 (17%)
36	LHG	5	317	-	24,24,48	0.77	0	27,30,54	1.27	2 (7%)
31	CLA	p	604	-	48,56,73	1.66	8 (16%)	55,92,113	1.77	10 (18%)
33	BCR	C	515	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	8 (14%)
43	A86	13	301	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	26 (50%)
31	CLA	B	606	-	65,73,73	1.48	12 (18%)	76,113,113	2.09	20 (26%)
43	A86	12	306	-	44,50,50	1.49	9 (20%)	51,76,76	3.91	27 (52%)
31	CLA	4	315	-	43,51,73	1.83	9 (20%)	49,86,113	1.99	10 (20%)
31	CLA	b	604	-	65,73,73	1.46	10 (15%)	76,113,113	1.65	15 (19%)
43	A86	5	303	-	44,50,50	1.33	5 (11%)	51,76,76	4.15	24 (47%)
43	A86	3	302	-	44,50,50	1.38	5 (11%)	51,76,76	3.58	27 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	DGD	H	102	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	8 (10%)
45	KC2	13	309	-	48,53,53	3.14	20 (41%)	54,89,89	4.64	27 (50%)
43	A86	6	302	-	44,50,50	1.43	5 (11%)	51,76,76	3.58	23 (45%)
31	CLA	b	610	-	65,73,73	1.43	9 (13%)	76,113,113	1.50	8 (10%)
31	CLA	19	311	43	46,54,73	1.76	6 (13%)	53,90,113	1.97	9 (16%)
45	KC2	19	309	-	48,53,53	3.11	20 (41%)	54,89,89	5.45	34 (62%)
43	A86	10	302	-	44,50,50	1.45	5 (11%)	51,76,76	3.12	20 (39%)
43	A86	1	319	-	44,50,50	1.40	4 (9%)	51,76,76	4.70	27 (52%)
31	CLA	8	309	-	52,60,73	1.56	8 (15%)	60,97,113	1.83	9 (15%)
31	CLA	c	513	-	65,73,73	1.37	8 (12%)	76,113,113	1.55	7 (9%)
31	CLA	p	607	43	43,51,73	1.75	10 (23%)	49,86,113	1.81	12 (24%)
36	LHG	b	623	-	42,42,48	0.73	1 (2%)	45,48,54	1.21	4 (8%)
31	CLA	13	316	-	65,73,73	1.46	6 (9%)	76,113,113	1.54	12 (15%)
38	LMG	B	620	-	51,51,55	0.90	4 (7%)	59,59,63	1.50	11 (18%)
31	CLA	13	315	-	44,52,73	1.86	7 (15%)	49,87,113	1.55	8 (16%)
31	CLA	4	311	-	46,54,73	1.69	7 (15%)	53,90,113	1.78	9 (16%)
43	A86	11	303	-	44,50,50	1.49	4 (9%)	51,76,76	4.52	28 (54%)
43	A86	2	304	-	44,50,50	1.59	7 (15%)	51,76,76	5.40	26 (50%)
45	KC2	16	312	-	48,53,53	3.19	21 (43%)	54,89,89	5.59	35 (64%)
36	LHG	P	615	-	26,26,48	0.87	1 (3%)	29,32,54	1.35	3 (10%)
45	KC2	17	309	-	48,53,53	3.20	21 (43%)	54,89,89	4.47	26 (48%)
31	CLA	4	307	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	8 (10%)
33	BCR	C	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	7 (12%)
31	CLA	2	309	-	43,51,73	1.73	6 (13%)	49,86,113	1.84	8 (16%)
41	HEM	E	101	5,6	41,50,50	1.53	4 (9%)	45,82,82	1.31	6 (13%)
43	A86	2	302	-	44,50,50	1.44	5 (11%)	51,76,76	4.73	27 (52%)
31	CLA	B	603	-	65,73,73	1.46	10 (15%)	76,113,113	1.65	15 (19%)
38	LMG	C	522	-	51,51,55	0.89	2 (3%)	59,59,63	1.24	4 (6%)
39	DGD	11	318	-	61,61,67	0.93	3 (4%)	75,75,81	1.32	10 (13%)
45	KC2	1	309	-	48,53,53	3.12	21 (43%)	54,89,89	4.69	32 (59%)
43	A86	8	303	-	44,50,50	1.57	8 (18%)	51,76,76	3.32	24 (47%)
31	CLA	c	506	-	65,73,73	1.40	8 (12%)	76,113,113	1.66	8 (10%)
31	CLA	17	312	-	47,55,73	1.80	9 (19%)	54,91,113	1.51	8 (14%)
38	LMG	5	316	-	36,36,55	1.22	4 (11%)	44,44,63	1.76	8 (18%)
43	A86	16	306	43	44,50,50	1.70	7 (15%)	51,76,76	5.47	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	D	404	-	65,73,73	1.57	11 (16%)	76,113,113	1.65	12 (15%)
43	A86	18	303	-	44,50,50	1.51	5 (11%)	51,76,76	2.80	19 (37%)
36	LHG	8	315	-	38,38,48	0.69	1 (2%)	41,44,54	1.28	4 (9%)
31	CLA	p	605	16	41,49,73	1.81	7 (17%)	47,84,113	1.82	12 (25%)
42	KC1	16	301	27	48,53,53	3.04	20 (41%)	55,89,89	5.16	35 (63%)
31	CLA	c	507	-	65,73,73	1.50	11 (16%)	76,113,113	1.57	7 (9%)
36	LHG	18	316	-	30,30,48	0.83	1 (3%)	33,36,54	1.22	2 (6%)
31	CLA	13	310	-	41,49,73	1.79	6 (14%)	47,84,113	1.79	8 (17%)
36	LHG	Z	103	-	24,24,48	0.95	0	27,30,54	1.30	3 (11%)
45	KC2	1	311	-	48,53,53	3.03	19 (39%)	54,89,89	5.01	34 (62%)
45	KC2	15	308	-	48,53,53	3.16	22 (45%)	54,89,89	5.30	34 (62%)
43	A86	7	303	-	44,50,50	1.30	4 (9%)	51,76,76	3.07	13 (25%)
41	HEM	v	201	21	41,50,50	1.49	4 (9%)	45,82,82	1.79	10 (22%)
31	CLA	a	404	-	49,57,73	1.64	10 (20%)	55,93,113	1.80	10 (18%)
43	A86	16	307	31	44,50,50	1.45	5 (11%)	51,76,76	3.81	24 (47%)
43	A86	13	303	-	44,50,50	1.32	3 (6%)	51,76,76	2.92	18 (35%)
31	CLA	10	311	-	55,63,73	1.53	8 (14%)	64,101,113	1.68	8 (12%)
43	A86	19	303	-	44,50,50	1.30	5 (11%)	51,76,76	3.32	22 (43%)
43	A86	11	304	31	44,50,50	1.42	6 (13%)	51,76,76	2.96	22 (43%)
39	DGD	c	519	-	63,63,67	1.12	10 (15%)	77,77,81	1.52	15 (19%)
31	CLA	D	401	-	65,73,73	1.41	11 (16%)	76,113,113	1.67	11 (14%)
31	CLA	c	511	-	65,73,73	1.45	9 (13%)	76,113,113	1.56	9 (11%)
43	A86	19	304	-	44,50,50	1.29	4 (9%)	51,76,76	4.23	20 (39%)
38	LMG	b	621	-	51,51,55	0.89	4 (7%)	59,59,63	1.50	11 (18%)
31	CLA	3	312	-	45,53,73	1.85	6 (13%)	52,89,113	1.68	9 (17%)
31	CLA	C	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.72	11 (14%)
31	CLA	0	313	-	42,50,73	1.90	9 (21%)	48,85,113	2.25	11 (22%)
43	A86	10	304	-	44,50,50	1.28	4 (9%)	51,76,76	4.45	25 (49%)
42	KC1	18	313	31,27	48,53,53	2.98	21 (43%)	55,89,89	6.79	33 (60%)
31	CLA	10	313	26	42,50,73	1.92	10 (23%)	48,85,113	2.02	10 (20%)
31	CLA	1	310	-	50,58,73	1.58	8 (16%)	58,95,113	1.75	9 (15%)
31	CLA	2	315	43	46,54,73	1.94	9 (19%)	53,90,113	2.70	21 (39%)
43	A86	1	320	-	44,50,50	1.39	5 (11%)	51,76,76	3.60	26 (50%)
35	PL9	a	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.46	6 (14%)
43	A86	0	305	-	44,50,50	1.31	4 (9%)	51,76,76	3.36	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	0	302	26	44,50,50	1.55	6 (13%)	51,76,76	3.58	23 (45%)
31	CLA	5	306	-	42,50,73	1.79	6 (14%)	48,85,113	1.97	17 (35%)
43	A86	3	305	-	44,50,50	1.72	9 (20%)	51,76,76	5.48	28 (54%)
45	KC2	2	310	-	48,53,53	3.14	22 (45%)	54,89,89	5.79	35 (64%)
43	A86	19	306	-	44,50,50	1.36	4 (9%)	51,76,76	2.97	14 (27%)
38	LMG	1	317	-	45,45,55	0.99	3 (6%)	53,53,63	1.21	5 (9%)
43	A86	7	302	-	44,50,50	1.60	8 (18%)	51,76,76	4.10	25 (49%)
43	A86	10	305	-	44,50,50	1.30	4 (9%)	51,76,76	3.34	25 (49%)
34	SQD	0	318	31	40,41,54	1.11	5 (12%)	49,52,65	1.79	12 (24%)
38	LMG	c	521	-	51,51,55	0.90	2 (3%)	59,59,63	1.24	4 (6%)
45	KC2	8	308	-	48,53,53	3.03	22 (45%)	54,89,89	4.73	31 (57%)
43	A86	8	304	-	44,50,50	1.56	6 (13%)	51,76,76	4.36	25 (49%)
31	CLA	1	308	-	65,73,73	1.48	7 (10%)	76,113,113	1.61	8 (10%)
43	A86	P	613	31	44,50,50	1.42	4 (9%)	51,76,76	3.70	29 (56%)
43	A86	9	306	-	44,50,50	1.61	8 (18%)	51,76,76	3.12	19 (37%)
43	A86	6	307	-	44,50,50	1.65	9 (20%)	51,76,76	4.37	25 (49%)
31	CLA	0	316	-	46,54,73	1.67	8 (17%)	53,90,113	1.67	8 (15%)
33	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	8 (14%)
43	A86	17	302	-	44,50,50	1.79	9 (20%)	51,76,76	3.62	25 (49%)
31	CLA	8	306	42	50,58,73	1.66	9 (18%)	58,95,113	1.97	12 (20%)
42	KC1	2	313	27	48,53,53	3.07	20 (41%)	55,89,89	5.55	33 (60%)
31	CLA	7	310	-	45,53,73	1.70	5 (11%)	52,89,113	1.84	8 (15%)
42	KC1	1	314	-	48,53,53	3.06	19 (39%)	55,89,89	4.48	32 (58%)
31	CLA	16	314	-	42,50,73	2.09	12 (28%)	48,85,113	2.55	17 (35%)
45	KC2	11	309	-	48,53,53	3.00	19 (39%)	54,89,89	5.25	33 (61%)
31	CLA	d	405	-	65,73,73	1.42	10 (15%)	76,113,113	1.48	7 (9%)
38	LMG	p	614	-	31,31,55	0.94	1 (3%)	39,39,63	1.69	9 (23%)
31	CLA	7	307	-	41,49,73	1.82	6 (14%)	47,84,113	2.26	18 (38%)
31	CLA	c	509	-	65,73,73	1.54	9 (13%)	76,113,113	1.92	13 (17%)
31	CLA	r	101	-	47,55,73	1.70	8 (17%)	54,91,113	1.61	8 (14%)
29	OEX	a	401	1,3	0,15,15	-	-	-		
31	CLA	9	307	-	61,69,73	1.48	6 (9%)	71,108,113	1.64	9 (12%)
43	A86	6	304	-	44,50,50	1.36	6 (13%)	51,76,76	3.40	22 (43%)
31	CLA	0	308	-	50,58,73	1.65	7 (14%)	58,95,113	1.73	12 (20%)
31	CLA	10	308	-	50,58,73	1.66	7 (14%)	58,95,113	1.76	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	1	304	31	44,50,50	1.43	5 (11%)	51,76,76	2.85	18 (35%)
43	A86	5	302	-	44,50,50	1.50	5 (11%)	51,76,76	3.24	26 (50%)
31	CLA	B	613	-	65,73,73	1.44	8 (12%)	76,113,113	1.40	7 (9%)
43	A86	15	303	-	44,50,50	1.42	5 (11%)	51,76,76	4.15	23 (45%)
31	CLA	W	202	-	65,73,73	1.47	9 (13%)	76,113,113	1.63	13 (17%)
31	CLA	8	311	-	46,54,73	1.78	10 (21%)	53,90,113	1.71	11 (20%)
43	A86	0	306	-	44,50,50	1.65	8 (18%)	51,76,76	3.10	18 (35%)
31	CLA	16	316	-	43,51,73	1.78	6 (13%)	49,86,113	1.70	9 (18%)
45	KC2	15	310	27	48,53,53	3.01	23 (47%)	54,89,89	4.88	32 (59%)
31	CLA	17	307	-	41,49,73	1.82	5 (12%)	47,84,113	2.25	18 (38%)
31	CLA	9	313	-	65,73,73	1.36	8 (12%)	76,113,113	2.11	13 (17%)
33	BCR	Y	101	-	41,41,41	1.34	4 (9%)	56,56,56	1.59	14 (25%)
31	CLA	b	607	-	65,73,73	1.49	12 (18%)	76,113,113	2.08	21 (27%)
43	A86	17	301	-	44,50,50	1.48	8 (18%)	51,76,76	4.54	24 (47%)
31	CLA	B	607	-	65,73,73	1.52	11 (16%)	76,113,113	1.50	7 (9%)
31	CLA	p	608	16	51,59,73	1.66	8 (15%)	59,96,113	1.67	9 (15%)
31	CLA	2	311	-	45,53,73	1.82	9 (20%)	52,89,113	1.63	8 (15%)
38	LMG	10	319	-	31,31,55	1.41	4 (12%)	39,39,63	1.32	4 (10%)
36	LHG	L	101	-	48,48,48	0.78	3 (6%)	51,54,54	1.29	7 (13%)
38	LMG	11	301	-	36,36,55	1.16	4 (11%)	44,44,63	1.44	6 (13%)
31	CLA	18	312	27	55,63,73	1.81	11 (20%)	64,101,113	1.81	15 (23%)
33	BCR	y	101	-	41,41,41	1.33	4 (9%)	56,56,56	1.59	12 (21%)
43	A86	14	302	43	44,50,50	1.44	5 (11%)	51,76,76	2.43	17 (33%)
31	CLA	p	601	16	65,73,73	1.44	10 (15%)	76,113,113	1.39	7 (9%)
43	A86	11	319	-	44,50,50	1.29	4 (9%)	51,76,76	3.28	18 (35%)
31	CLA	5	312	-	47,55,73	1.80	11 (23%)	54,91,113	1.70	10 (18%)
31	CLA	2	312	-	48,56,73	2.05	9 (18%)	55,92,113	2.02	13 (23%)
42	KC1	0	315	-	48,53,53	2.87	20 (41%)	55,89,89	6.23	34 (61%)
31	CLA	B	601	-	65,73,73	1.48	10 (15%)	76,113,113	1.47	10 (13%)
31	CLA	P	608	16	51,59,73	1.65	8 (15%)	59,96,113	1.66	8 (13%)
36	LHG	D	407	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	7 (13%)
45	KC2	17	311	27	48,53,53	3.15	21 (43%)	54,89,89	5.28	35 (64%)
31	CLA	b	616	-	65,73,73	1.50	11 (16%)	76,113,113	1.63	11 (14%)
39	DGD	h	102	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	8 (10%)
34	SQD	B	623	-	53,54,54	0.91	5 (9%)	62,65,65	1.74	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LMG	d	403	-	40,40,55	1.07	4 (10%)	48,48,63	1.55	7 (14%)
31	CLA	16	311	-	41,49,73	1.75	6 (14%)	47,84,113	1.93	8 (17%)
31	CLA	B	614	-	65,73,73	1.41	8 (12%)	76,113,113	1.63	11 (14%)
34	SQD	i	101	-	39,40,54	1.10	5 (12%)	48,51,65	2.00	12 (25%)
31	CLA	10	309	-	59,67,73	1.47	7 (11%)	68,105,113	1.63	10 (14%)
31	CLA	b	612	-	65,73,73	1.63	11 (16%)	76,113,113	1.93	12 (15%)
31	CLA	c	508	-	65,73,73	1.46	10 (15%)	76,113,113	1.56	11 (14%)
32	PHO	A	405	-	51,69,69	1.12	6 (11%)	47,99,99	1.35	8 (17%)
43	A86	2	303	-	44,50,50	1.35	5 (11%)	51,76,76	3.33	25 (49%)
45	KC2	16	310	-	48,53,53	3.16	22 (45%)	54,89,89	4.38	27 (50%)
32	PHO	d	402	-	51,69,69	1.06	6 (11%)	47,99,99	1.47	7 (14%)
31	CLA	7	315	-	41,49,73	1.81	6 (14%)	47,84,113	1.74	8 (17%)
31	CLA	p	606	-	43,51,73	2.35	14 (32%)	49,86,113	4.31	26 (53%)
36	LHG	B	622	-	42,42,48	0.74	1 (2%)	45,48,54	1.21	4 (8%)
43	A86	10	306	-	44,50,50	1.44	4 (9%)	51,76,76	3.10	19 (37%)
41	HEM	V	201	21	41,50,50	1.48	4 (9%)	45,82,82	1.79	10 (22%)
31	CLA	13	307	-	42,50,73	1.83	5 (11%)	48,85,113	2.02	13 (27%)
31	CLA	18	314	27	43,51,73	1.73	8 (18%)	49,86,113	1.81	9 (18%)
43	A86	7	305	-	44,50,50	1.44	5 (11%)	51,76,76	3.74	23 (45%)
43	A86	14	304	-	44,50,50	1.31	5 (11%)	51,76,76	3.18	23 (45%)
31	CLA	b	609	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	7 (9%)
43	A86	9	305	-	44,50,50	1.58	6 (13%)	51,76,76	5.12	24 (47%)
38	LMG	11	317	-	45,45,55	0.96	2 (4%)	53,53,63	1.25	5 (9%)
43	A86	9	302	-	44,50,50	1.31	4 (9%)	51,76,76	3.02	19 (37%)
43	A86	11	320	-	44,50,50	1.37	3 (6%)	51,76,76	3.74	22 (43%)
43	A86	13	305	-	44,50,50	1.34	4 (9%)	51,76,76	3.10	19 (37%)
45	KC2	18	310	27	48,53,53	3.06	21 (43%)	54,89,89	6.03	35 (64%)
31	CLA	9	308	-	65,73,73	1.42	7 (10%)	76,113,113	1.55	10 (13%)
31	CLA	14	309	-	65,73,73	1.37	7 (10%)	76,113,113	1.61	8 (10%)
31	CLA	A	403	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	10 (13%)
37	BCT	A	412	30	2,3,3	1.38	0	2,3,3	3.94	1 (50%)
43	A86	16	303	-	44,50,50	1.56	6 (13%)	51,76,76	3.53	24 (47%)
31	CLA	7	312	-	47,55,73	1.82	7 (14%)	54,91,113	1.52	8 (14%)
31	CLA	d	401	-	65,73,73	1.41	11 (16%)	76,113,113	1.67	10 (13%)
31	CLA	9	312	43	65,73,73	1.46	7 (10%)	76,113,113	1.54	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	17	315	-	41,49,73	1.78	6 (14%)	47,84,113	1.73	8 (17%)
45	KC2	4	310	-	48,53,53	3.11	20 (41%)	54,89,89	5.09	33 (61%)
43	A86	8	305	-	44,50,50	1.43	6 (13%)	51,76,76	3.66	22 (43%)
39	DGD	c	520	34	63,63,67	1.18	10 (15%)	77,77,81	1.58	14 (18%)
31	CLA	B	616	-	65,73,73	1.49	10 (15%)	76,113,113	1.61	13 (17%)
31	CLA	18	307	-	61,69,73	1.55	10 (16%)	71,108,113	1.73	14 (19%)
31	CLA	b	613	-	65,73,73	1.38	8 (12%)	76,113,113	1.73	11 (14%)
31	CLA	14	315	-	43,51,73	1.82	8 (18%)	49,86,113	2.15	11 (22%)
42	KC1	11	314	-	48,53,53	2.95	22 (45%)	55,89,89	5.27	33 (60%)
31	CLA	C	513	-	65,73,73	1.37	8 (12%)	76,113,113	1.56	8 (10%)
43	A86	18	301	-	44,50,50	1.47	5 (11%)	51,76,76	4.91	26 (50%)
43	A86	1	303	-	44,50,50	1.54	7 (15%)	51,76,76	4.68	27 (52%)
43	A86	3	301	-	44,50,50	1.62	9 (20%)	51,76,76	4.06	26 (50%)
43	A86	15	304	-	44,50,50	1.38	5 (11%)	51,76,76	4.51	29 (56%)
31	CLA	14	306	-	61,69,73	1.59	9 (14%)	71,108,113	2.35	19 (26%)
31	CLA	c	514	-	49,57,73	1.59	7 (14%)	55,93,113	1.73	8 (14%)
45	KC2	11	311	-	48,53,53	3.05	20 (41%)	54,89,89	5.04	33 (61%)
31	CLA	w	203	-	65,73,73	1.47	9 (13%)	76,113,113	1.63	13 (17%)
31	CLA	C	508	-	65,73,73	1.45	10 (15%)	76,113,113	1.55	10 (13%)
31	CLA	12	315	-	41,49,73	1.82	6 (14%)	47,84,113	1.71	7 (14%)
38	LMG	D	408	4	37,37,55	0.90	1 (2%)	45,45,63	1.36	6 (13%)
45	KC2	8	310	-	48,53,53	3.06	21 (43%)	54,89,89	6.00	34 (62%)
31	CLA	3	315	-	44,52,73	1.78	6 (13%)	49,87,113	1.66	8 (16%)
31	CLA	10	312	34,26	46,54,73	1.75	6 (13%)	53,90,113	2.00	11 (20%)
42	KC1	19	314	-	48,53,53	3.13	22 (45%)	55,89,89	5.05	36 (65%)
33	BCR	B	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.38	10 (17%)
43	A86	19	305	-	44,50,50	1.54	6 (13%)	51,76,76	5.10	23 (45%)
42	KC1	10	315	-	48,53,53	2.80	17 (35%)	55,89,89	6.30	37 (67%)
43	A86	18	304	-	44,50,50	1.44	6 (13%)	51,76,76	4.00	22 (43%)
43	A86	3	304	-	44,50,50	1.58	7 (15%)	51,76,76	2.99	21 (41%)
43	A86	17	304	-	44,50,50	1.33	4 (9%)	51,76,76	3.13	13 (25%)
31	CLA	14	307	-	65,73,73	1.42	8 (12%)	76,113,113	1.44	8 (10%)
31	CLA	P	603	-	50,58,73	1.61	9 (18%)	58,95,113	1.67	11 (18%)
39	DGD	C	520	34	63,63,67	1.18	10 (15%)	77,77,81	1.58	13 (16%)
45	KC2	2	308	-	48,53,53	3.22	21 (43%)	54,89,89	4.44	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	9	303	-	44,50,50	1.29	4 (9%)	51,76,76	3.20	21 (41%)
31	CLA	12	310	-	43,51,73	1.74	6 (13%)	49,86,113	1.76	7 (14%)
31	CLA	19	310	-	65,73,73	1.46	5 (7%)	76,113,113	1.54	7 (9%)
34	SQD	10	320	31	40,41,54	1.12	6 (15%)	49,52,65	1.73	10 (20%)
38	LMG	m	101	-	40,40,55	0.95	1 (2%)	48,48,63	1.34	3 (6%)
43	A86	4	303	-	44,50,50	1.40	7 (15%)	51,76,76	2.98	18 (35%)
31	CLA	17	313	27	50,58,73	1.97	9 (18%)	58,95,113	1.92	15 (25%)
43	A86	1	302	-	44,50,50	1.29	3 (6%)	51,76,76	4.93	31 (60%)
31	CLA	10	307	-	48,56,73	1.76	9 (18%)	55,92,113	1.92	13 (23%)
31	CLA	C	514	-	49,57,73	1.59	7 (14%)	55,93,113	1.74	8 (14%)
45	KC2	13	311	-	48,53,53	3.23	21 (43%)	54,89,89	4.39	28 (51%)
31	CLA	b	603	-	65,73,73	1.45	11 (16%)	76,113,113	1.65	13 (17%)
34	SQD	A	411	-	39,40,54	1.10	5 (12%)	48,51,65	2.01	12 (25%)
31	CLA	5	307	-	65,73,73	1.40	8 (12%)	76,113,113	1.42	9 (11%)
31	CLA	b	608	-	65,73,73	1.52	11 (16%)	76,113,113	1.49	8 (10%)
42	KC1	5	313	-	48,53,53	3.04	20 (41%)	55,89,89	5.55	33 (60%)
31	CLA	B	608	-	65,73,73	1.41	9 (13%)	76,113,113	1.52	7 (9%)
31	CLA	B	615	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	11 (14%)
43	A86	5	301	31	44,50,50	1.50	5 (11%)	51,76,76	4.25	27 (52%)
31	CLA	5	311	-	45,53,73	1.76	10 (22%)	52,89,113	1.88	12 (23%)
42	KC1	p	609	-	48,53,53	2.91	20 (41%)	55,89,89	4.84	34 (61%)
31	CLA	0	312	34,26	46,54,73	1.76	6 (13%)	53,90,113	2.02	12 (22%)
31	CLA	7	313	-	50,58,73	1.93	10 (20%)	58,95,113	1.94	14 (24%)
31	CLA	c	503	31	65,73,73	1.53	11 (16%)	76,113,113	2.38	19 (25%)
33	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.46	11 (19%)
31	CLA	14	311	-	46,54,73	1.72	8 (17%)	53,90,113	1.85	11 (20%)
43	A86	16	304	43	44,50,50	1.44	5 (11%)	51,76,76	5.37	24 (47%)
31	CLA	c	512	3	65,73,73	1.47	9 (13%)	76,113,113	1.60	10 (13%)
31	CLA	4	312	27	51,59,73	1.79	10 (19%)	59,96,113	2.13	16 (27%)
42	KC1	16	315	27	48,53,53	3.17	20 (41%)	55,89,89	6.94	34 (61%)
38	LMG	15	314	-	37,37,55	0.98	3 (8%)	45,45,63	1.13	2 (4%)
31	CLA	z	101	-	51,59,73	1.62	9 (17%)	59,96,113	1.57	8 (13%)
38	LMG	5	315	-	37,37,55	1.00	4 (10%)	45,45,63	1.17	3 (6%)
31	CLA	19	308	-	65,73,73	1.43	7 (10%)	76,113,113	1.57	11 (14%)
43	A86	7	301	-	44,50,50	1.42	5 (11%)	51,76,76	3.49	24 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	11	306	-	44,50,50	1.77	8 (18%)	51,76,76	5.16	25 (49%)
31	CLA	1	307	-	43,51,73	1.71	7 (16%)	49,86,113	2.17	15 (30%)
31	CLA	P	607	43	43,51,73	1.74	10 (23%)	49,86,113	1.82	12 (24%)
39	DGD	W	203	-	57,57,67	1.15	8 (14%)	71,71,81	1.48	10 (14%)
31	CLA	11	307	27	43,51,73	1.74	7 (16%)	49,86,113	2.52	18 (36%)
42	KC1	14	313	27	48,53,53	2.88	21 (43%)	55,89,89	5.93	38 (69%)
31	CLA	12	313	-	48,56,73	1.95	10 (20%)	55,92,113	1.56	13 (23%)
33	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.47	9 (16%)
45	KC2	14	308	-	48,53,53	3.10	21 (43%)	54,89,89	5.42	29 (53%)
31	CLA	16	313	-	47,55,73	1.78	8 (17%)	54,91,113	1.51	8 (14%)
31	CLA	B	605	-	65,73,73	1.51	12 (18%)	76,113,113	1.54	7 (9%)
31	CLA	B	612	-	65,73,73	1.39	8 (12%)	76,113,113	1.74	11 (14%)
44	DD6	p	612	-	39,45,45	2.20	6 (15%)	52,67,67	3.59	26 (50%)
31	CLA	C	510	-	65,73,73	1.42	8 (12%)	76,113,113	1.73	11 (14%)
43	A86	1	306	-	44,50,50	1.42	7 (15%)	51,76,76	4.32	25 (49%)
33	BCR	c	516	-	41,41,41	1.24	5 (12%)	56,56,56	1.35	8 (14%)
33	BCR	F	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.42	8 (14%)
31	CLA	a	406	-	60,68,73	1.42	9 (15%)	70,107,113	1.54	7 (10%)
43	A86	10	318	-	44,50,50	1.47	8 (18%)	51,76,76	3.64	24 (47%)
31	CLA	b	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.48	9 (11%)
43	A86	12	301	-	44,50,50	1.36	4 (9%)	51,76,76	4.70	26 (50%)
42	KC1	12	314	-	48,53,53	2.99	19 (39%)	55,89,89	4.98	34 (61%)
31	CLA	13	313	-	65,73,73	1.66	11 (16%)	76,113,113	1.57	15 (19%)
43	A86	14	303	-	44,50,50	1.29	4 (9%)	51,76,76	3.02	20 (39%)
35	PL9	A	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.47	6 (14%)
43	A86	2	305	31	44,50,50	1.46	4 (9%)	51,76,76	3.76	24 (47%)
31	CLA	0	314	-	47,55,73	1.75	9 (19%)	54,91,113	1.71	14 (25%)
43	A86	15	302	-	44,50,50	1.47	5 (11%)	51,76,76	4.46	29 (56%)
43	A86	17	316	-	44,50,50	1.62	7 (15%)	51,76,76	4.91	33 (64%)
38	LMG	f	102	-	46,46,55	0.96	4 (8%)	54,54,63	1.49	9 (16%)
37	BCT	a	411	30	2,3,3	1.38	0	2,3,3	3.94	1 (50%)
38	LMG	D	403	4	40,40,55	1.10	4 (10%)	48,48,63	1.52	7 (14%)
31	CLA	15	309	-	55,63,73	1.52	7 (12%)	64,101,113	1.77	10 (15%)
31	CLA	9	310	-	65,73,73	1.45	5 (7%)	76,113,113	1.54	7 (9%)
43	A86	14	305	-	44,50,50	1.48	8 (18%)	51,76,76	4.18	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	11	313	-	65,73,73	1.60	10 (15%)	76,113,113	1.55	14 (18%)
31	CLA	2	307	-	65,73,73	1.45	10 (15%)	76,113,113	1.64	11 (14%)
38	LMG	M	101	-	40,40,55	0.88	1 (2%)	48,48,63	1.31	5 (10%)
41	HEM	e	101	5,6	41,50,50	1.54	5 (12%)	45,82,82	1.31	7 (15%)
43	A86	9	301	-	44,50,50	1.30	3 (6%)	51,76,76	4.38	25 (49%)
38	LMG	n	701	14	28,28,55	1.11	4 (14%)	36,36,63	1.32	6 (16%)
36	LHG	14	317	-	34,34,48	0.71	1 (2%)	37,40,54	1.27	4 (10%)
38	LMG	4	316	-	49,49,55	0.82	1 (2%)	57,57,63	1.45	13 (22%)
43	A86	4	301	-	44,50,50	1.31	4 (9%)	51,76,76	3.65	22 (43%)
43	A86	11	305	-	44,50,50	1.44	5 (11%)	51,76,76	3.87	34 (66%)
31	CLA	5	314	-	41,49,73	1.85	7 (17%)	47,84,113	1.67	8 (17%)
31	CLA	2	314	-	41,49,73	1.82	6 (14%)	47,84,113	1.78	10 (21%)
38	LMG	J	101	-	50,50,55	0.95	3 (6%)	58,58,63	1.32	4 (6%)
31	CLA	d	404	-	65,73,73	1.57	11 (16%)	76,113,113	1.65	12 (15%)
34	SQD	a	408	39	53,54,54	0.96	6 (11%)	62,65,65	1.56	12 (19%)
31	CLA	14	312	-	51,59,73	1.85	10 (19%)	59,96,113	1.86	14 (23%)
45	KC2	6	312	27	48,53,53	3.18	21 (43%)	54,89,89	5.61	36 (66%)
31	CLA	P	604	-	48,56,73	1.66	8 (16%)	55,92,113	1.76	10 (18%)
43	A86	16	305	-	44,50,50	1.35	6 (13%)	51,76,76	3.49	24 (47%)
43	A86	P	611	-	44,50,50	1.87	10 (22%)	51,76,76	6.02	30 (58%)
36	LHG	18	315	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
38	LMG	j	101	-	50,50,55	0.95	3 (6%)	58,58,63	1.32	4 (6%)
38	LMG	14	316	-	49,49,55	0.79	0	57,57,63	1.41	11 (19%)
31	CLA	p	610	-	41,49,73	1.75	8 (19%)	47,84,113	1.91	9 (19%)
31	CLA	b	611	-	65,73,73	1.47	9 (13%)	76,113,113	1.49	10 (13%)
36	LHG	C	521	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	4 (9%)
31	CLA	1	321	-	61,69,73	1.47	8 (13%)	71,108,113	2.32	20 (28%)
38	LMG	d	408	4	37,37,55	0.90	2 (5%)	45,45,63	1.36	6 (13%)
31	CLA	B	610	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	11 (14%)
43	A86	8	301	-	44,50,50	1.74	7 (15%)	51,76,76	4.70	35 (68%)
31	CLA	11	315	-	41,49,73	1.85	7 (17%)	47,84,113	2.06	13 (27%)
43	A86	17	305	-	44,50,50	1.73	9 (20%)	51,76,76	5.58	24 (47%)
31	CLA	16	308	-	42,50,73	1.81	5 (11%)	48,85,113	2.18	14 (29%)
43	A86	0	301	-	44,50,50	1.37	5 (11%)	51,76,76	4.30	27 (52%)
45	KC2	12	309	-	48,53,53	3.14	19 (39%)	54,89,89	5.10	35 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	10	301	-	44,50,50	1.39	5 (11%)	51,76,76	4.35	28 (54%)
43	A86	6	306	31	44,50,50	1.45	4 (9%)	51,76,76	3.79	22 (43%)
43	A86	1	305	-	44,50,50	1.55	6 (13%)	51,76,76	3.97	34 (66%)
31	CLA	19	312	43	65,73,73	1.45	7 (10%)	76,113,113	1.52	11 (14%)
43	A86	11	302	-	44,50,50	1.48	6 (13%)	51,76,76	5.53	30 (58%)
45	KC2	3	309	-	48,53,53	3.19	22 (45%)	54,89,89	4.78	31 (57%)
31	CLA	13	308	-	43,51,73	1.76	8 (18%)	49,86,113	1.85	9 (18%)
36	LHG	p	615	-	26,26,48	0.87	1 (3%)	29,32,54	1.35	3 (10%)
43	A86	17	303	-	44,50,50	1.41	6 (13%)	51,76,76	3.72	22 (43%)
31	CLA	1	312	-	46,54,73	1.77	10 (21%)	53,90,113	1.67	11 (20%)
45	KC2	9	309	-	48,53,53	3.11	20 (41%)	54,89,89	5.41	34 (62%)
45	KC2	4	308	-	48,53,53	3.10	20 (41%)	54,89,89	5.40	29 (53%)
31	CLA	c	510	-	65,73,73	1.42	8 (12%)	76,113,113	1.72	11 (14%)
45	KC2	0	310	26	48,53,53	2.89	21 (43%)	54,89,89	4.92	32 (59%)
42	KC1	6	315	27	48,53,53	3.18	22 (45%)	55,89,89	7.31	35 (63%)
31	CLA	11	308	-	65,73,73	1.47	8 (12%)	76,113,113	1.71	13 (17%)
45	KC2	10	310	26	48,53,53	2.86	20 (41%)	54,89,89	5.12	33 (61%)
31	CLA	b	605	-	65,73,73	1.63	12 (18%)	76,113,113	2.35	17 (22%)
31	CLA	1	316	43	42,50,73	1.86	8 (19%)	48,85,113	1.68	7 (14%)
31	CLA	P	605	16	41,49,73	1.81	7 (17%)	47,84,113	1.82	13 (27%)
45	KC2	3	311	-	48,53,53	3.17	21 (43%)	54,89,89	5.63	34 (62%)
35	PL9	d	406	-	55,55,55	2.04	15 (27%)	68,69,69	1.42	12 (17%)
31	CLA	8	312	-	55,63,73	1.78	11 (20%)	64,101,113	1.86	18 (28%)
31	CLA	6	313	-	47,55,73	1.76	8 (17%)	54,91,113	1.54	8 (14%)
31	CLA	1	315	27	41,49,73	1.87	6 (14%)	47,84,113	1.70	6 (12%)
31	CLA	6	309	-	65,73,73	1.46	10 (15%)	76,113,113	1.55	10 (13%)
43	A86	6	305	43	44,50,50	1.73	10 (22%)	51,76,76	5.46	30 (58%)
31	CLA	c	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.72	12 (15%)

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
38	LMG	N	101	14	-	6/23/43/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	617	-	1/1/15/20	15/37/115/115	-
31	CLA	8	314	-	1/1/10/20	2/11/89/115	-
31	CLA	15	307	-	1/1/15/20	17/37/115/115	-
36	LHG	15	316	-	-	15/29/29/53	-
33	BCR	b	620	-	-	12/29/63/63	0/2/2/2
43	A86	8	302	-	-	8/34/90/90	0/3/3/3
43	A86	2	301	-	-	10/34/90/90	0/3/3/3
31	CLA	4	314	-	1/1/10/20	5/11/89/115	-
36	LHG	w	202	-	-	20/44/44/53	-
43	A86	13	306	43	-	9/34/90/90	0/3/3/3
43	A86	p	611	-	-	7/34/90/90	1/3/3/3
43	A86	10	303	-	-	7/34/90/90	0/3/3/3
31	CLA	11	310	-	1/1/12/20	5/19/97/115	-
31	CLA	6	316	-	1/1/10/20	4/11/89/115	-
35	PL9	D	406	-	-	9/53/73/73	0/1/1/1
31	CLA	2	306	-	1/1/10/20	4/10/88/115	-
38	LMG	k	101	-	-	23/41/61/70	0/1/1/1
31	CLA	15	306	-	1/1/10/20	4/10/88/115	-
31	CLA	C	512	3	1/1/15/20	6/37/115/115	-
33	BCR	C	516	-	-	9/29/63/63	0/2/2/2
31	CLA	P	606	-	1/1/10/20	6/11/89/115	-
31	CLA	18	309	-	1/1/12/20	7/22/100/115	-
31	CLA	10	317	-	1/1/11/20	5/17/95/115	-
45	KC2	12	311	-	-	8/15/71/71	-
43	A86	13	302	-	-	8/34/90/90	0/3/3/3
31	CLA	6	308	-	1/1/10/20	5/10/88/115	-
43	A86	19	302	-	-	8/34/90/90	0/3/3/3
31	CLA	6	311	-	1/1/10/20	3/8/86/115	-
45	KC2	18	308	-	-	10/15/71/71	-
31	CLA	R	101	-	1/1/11/20	4/16/94/115	-
31	CLA	1	313	-	1/1/15/20	14/37/115/115	-
33	BCR	a	407	-	-	8/29/63/63	0/2/2/2
31	CLA	B	611	-	1/1/15/20	12/37/115/115	-
36	LHG	4	317	-	-	18/38/38/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	504	31	1/1/15/20	23/37/115/115	-
45	KC2	6	310	-	-	10/15/71/71	-
31	CLA	3	307	-	1/1/10/20	5/10/88/115	-
31	CLA	15	311	27	1/1/11/20	5/13/91/115	-
31	CLA	C	502	-	1/1/15/20	13/37/115/115	-
43	A86	12	302	-	-	7/34/90/90	0/3/3/3
43	A86	14	301	-	-	14/34/90/90	0/3/3/3
31	CLA	18	306	42	1/1/12/20	8/19/97/115	-
42	KC1	3	314	27	-	1/15/71/71	-
38	LMG	F	102	-	-	14/41/61/70	0/1/1/1
43	A86	18	302	-	-	8/34/90/90	0/3/3/3
31	CLA	B	604	-	1/1/15/20	14/37/115/115	-
31	CLA	0	311	-	1/1/13/20	6/25/103/115	-
34	SQD	l	101	-	-	25/49/69/69	0/1/1/1
31	CLA	14	314	-	1/1/10/20	5/11/89/115	-
31	CLA	b	614	-	1/1/15/20	10/37/115/115	-
31	CLA	11	312	27	1/1/11/20	7/15/93/115	-
31	CLA	13	312	-	1/1/11/20	6/13/91/115	-
31	CLA	12	307	-	1/1/10/20	1/10/88/115	-
31	CLA	19	307	-	1/1/14/20	10/33/111/115	-
43	A86	5	304	-	-	11/34/90/90	0/3/3/3
43	A86	6	303	-	-	9/34/90/90	0/3/3/3
31	CLA	C	506	-	1/1/15/20	12/37/115/115	-
43	A86	3	306	-	-	8/34/90/90	0/3/3/3
43	A86	19	301	-	-	8/34/90/90	0/3/3/3
31	CLA	5	309	-	1/1/13/20	11/25/103/115	-
34	SQD	L	102	-	-	22/49/69/69	0/1/1/1
31	CLA	15	313	-	1/1/10/20	0/8/86/115	-
43	A86	9	304	-	-	7/34/90/90	0/3/3/3
31	CLA	D	405	-	1/1/15/20	11/37/115/115	-
36	LHG	l	102	-	-	22/53/53/53	-
43	A86	15	305	27	-	6/34/90/90	0/3/3/3
31	CLA	p	602	-	1/1/15/20	14/37/115/115	-
31	CLA	C	504	31	1/1/15/20	23/37/115/115	-
33	BCR	A	407	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	602	-	1/1/15/20	17/37/115/115	-
38	LMG	K	101	-	-	23/41/61/70	0/1/1/1
45	KC2	7	309	-	-	10/15/71/71	-
31	CLA	P	602	-	1/1/15/20	13/37/115/115	-
32	PHO	D	402	-	-	6/37/103/103	0/5/6/6
43	A86	p	613	31	-	8/34/90/90	1/3/3/3
33	BCR	h	101	-	-	10/29/63/63	0/2/2/2
38	LMG	15	315	-	-	18/31/51/70	0/1/1/1
31	CLA	8	307	-	1/1/14/20	8/33/111/115	-
36	LHG	8	316	-	-	20/34/34/53	-
43	A86	4	304	-	-	9/34/90/90	0/3/3/3
42	KC1	17	314	27	-	2/15/71/71	-
38	LMG	1	301	-	-	14/31/51/70	0/1/1/1
31	CLA	18	311	27	-	6/15/93/115	-
45	KC2	7	311	27	-	6/15/71/71	-
31	CLA	C	507	-	1/1/15/20	16/37/115/115	-
36	LHG	a	410	1	-	17/41/41/53	-
43	A86	4	302	-	-	7/34/90/90	0/3/3/3
36	LHG	d	407	-	-	28/53/53/53	-
43	A86	5	318	42	-	10/34/90/90	0/3/3/3
38	LMG	W	201	-	-	25/43/63/70	0/1/1/1
43	A86	12	304	-	-	7/34/90/90	0/3/3/3
43	A86	13	304	-	-	8/34/90/90	0/3/3/3
31	CLA	A	406	-	1/1/14/20	5/31/109/115	-
31	CLA	17	310	-	1/1/11/20	6/13/91/115	-
39	DGD	w	204	-	-	28/45/85/95	0/2/2/2
31	CLA	7	308	-	-	1/8/86/115	-
31	CLA	9	311	43	1/1/11/20	6/15/93/115	-
31	CLA	B	609	-	-	12/37/115/115	-
43	A86	0	303	-	-	7/34/90/90	0/3/3/3
31	CLA	3	316	-	-	15/37/115/115	-
43	A86	12	305	-	-	8/34/90/90	0/3/3/3
45	KC2	5	308	-	-	7/15/71/71	-
39	DGD	C	519	-	-	27/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	503	31	1/1/15/20	11/37/115/115	-
42	KC1	8	313	31,43	-	3/15/71/71	-
31	CLA	3	313	-	1/1/15/20	17/37/115/115	-
31	CLA	4	309	-	1/1/15/20	20/37/115/115	-
33	BCR	H	101	-	-	10/29/63/63	0/2/2/2
31	CLA	0	309	-	-	15/30/108/115	-
31	CLA	0	307	-	1/1/11/20	4/17/95/115	-
31	CLA	Z	101	-	1/1/12/20	6/21/99/115	-
39	DGD	c	518	-	-	22/44/84/95	0/2/2/2
42	KC1	13	314	-	-	4/15/71/71	-
43	A86	4	306	-	-	7/34/90/90	1/3/3/3
43	A86	7	304	-	-	9/34/90/90	0/3/3/3
31	CLA	3	308	-	1/1/10/20	2/11/89/115	-
31	CLA	12	312	-	1/1/11/20	6/13/91/115	-
34	SQD	A	408	39	-	23/49/69/69	0/1/1/1
39	DGD	B	621	-	-	31/43/83/95	0/2/2/2
42	KC1	P	609	-	-	8/15/71/71	-
31	CLA	17	308	-	-	1/8/86/115	-
39	DGD	b	622	34	-	28/44/84/95	0/2/2/2
39	DGD	C	518	-	-	22/44/84/95	0/2/2/2
31	CLA	9	315	-	1/1/10/20	2/8/86/115	-
39	DGD	1	318	-	-	27/43/83/95	0/2/2/2
31	CLA	b	615	-	1/1/15/20	21/37/115/115	-
43	A86	6	301	43	-	9/34/90/90	0/3/3/3
43	A86	17	306	-	-	8/34/90/90	0/3/3/3
43	A86	5	305	-	-	6/34/90/90	0/3/3/3
31	CLA	19	315	-	1/1/10/20	2/8/86/115	-
31	CLA	10	314	-	1/1/11/20	4/16/94/115	-
31	CLA	C	511	-	1/1/15/20	20/37/115/115	-
31	CLA	12	316	-	1/1/11/20	5/15/93/115	-
43	A86	7	306	-	-	7/34/90/90	0/3/3/3
31	CLA	a	403	-	1/1/15/20	10/37/115/115	-
31	CLA	11	316	43	1/1/10/20	0/8/86/115	-
34	SQD	b	601	39	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	15	312	-	-	6/16/94/115	-
31	CLA	12	308	-	1/1/15/20	15/37/115/115	-
31	CLA	P	610	-	1/1/10/20	2/8/86/115	-
31	CLA	16	309	-	1/1/15/20	13/37/115/115	-
43	A86	16	302	43	-	10/34/90/90	0/3/3/3
44	DD6	P	612	-	-	7/26/80/80	0/3/3/3
33	BCR	c	515	-	-	14/29/63/63	0/2/2/2
31	CLA	b	606	-	1/1/15/20	10/37/115/115	-
32	PHO	a	405	-	-	14/37/103/103	0/5/6/6
33	BCR	b	618	-	-	13/29/63/63	0/2/2/2
43	A86	18	305	-	-	12/34/90/90	0/3/3/3
36	LHG	z	102	-	-	16/29/29/53	-
42	KC1	7	314	27	-	2/15/71/71	-
45	KC2	5	310	27	-	7/15/71/71	-
42	KC1	9	314	-	-	5/15/71/71	-
43	A86	3	303	-	-	9/34/90/90	0/3/3/3
31	CLA	10	316	-	1/1/11/20	4/15/93/115	-
43	A86	0	304	-	-	6/34/90/90	0/3/3/3
31	CLA	P	601	16	1/1/15/20	22/37/115/115	-
38	LMG	0	317	-	-	7/26/46/70	0/1/1/1
33	BCR	f	101	-	-	19/29/63/63	0/2/2/2
38	LMG	P	614	-	-	11/26/46/70	0/1/1/1
31	CLA	p	603	-	1/1/12/20	8/19/97/115	-
33	BCR	c	517	-	-	10/29/63/63	0/2/2/2
43	A86	12	303	-	-	5/34/90/90	0/3/3/3
45	KC2	14	310	-	-	6/15/71/71	-
31	CLA	c	502	-	1/1/15/20	13/37/115/115	-
43	A86	4	305	-	-	8/34/90/90	0/3/3/3
38	LMG	c	522	-	-	10/26/46/70	0/1/1/1
42	KC1	4	313	-	-	9/15/71/71	-
38	LMG	w	201	-	-	25/43/63/70	0/1/1/1
38	LMG	Z	102	-	-	10/26/46/70	0/1/1/1
31	CLA	3	310	-	1/1/10/20	3/8/86/115	-
31	CLA	z	103	-	1/1/11/20	5/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	404	-	1/1/11/20	5/18/96/115	-
36	LHG	A	410	1	-	17/41/41/53	-
31	CLA	19	313	-	1/1/15/20	11/37/115/115	-
31	CLA	6	314	-	1/1/10/20	3/10/88/115	-
43	A86	15	301	31	-	6/34/90/90	0/3/3/3
31	CLA	C	509	-	1/1/15/20	11/37/115/115	-
36	LHG	5	317	-	-	15/29/29/53	-
31	CLA	p	604	-	1/1/11/20	5/17/95/115	-
33	BCR	C	515	-	-	14/29/63/63	0/2/2/2
43	A86	13	301	-	-	6/34/90/90	0/3/3/3
31	CLA	B	606	-	1/1/15/20	10/37/115/115	-
43	A86	12	306	-	-	9/34/90/90	0/3/3/3
31	CLA	4	315	-	1/1/10/20	7/11/89/115	-
31	CLA	b	604	-	1/1/15/20	14/37/115/115	-
43	A86	5	303	-	-	8/34/90/90	0/3/3/3
43	A86	3	302	-	-	6/34/90/90	0/3/3/3
39	DGD	H	102	-	-	29/51/91/95	0/2/2/2
45	KC2	13	309	-	-	10/15/71/71	-
43	A86	6	302	-	-	8/34/90/90	0/3/3/3
31	CLA	b	610	-	-	12/37/115/115	-
31	CLA	19	311	43	1/1/11/20	4/15/93/115	-
45	KC2	19	309	-	-	4/15/71/71	-
43	A86	10	302	-	-	7/34/90/90	0/3/3/3
43	A86	1	319	-	-	8/34/90/90	0/3/3/3
31	CLA	8	309	-	1/1/12/20	7/22/100/115	-
31	CLA	c	513	-	1/1/15/20	18/37/115/115	-
31	CLA	p	607	43	1/1/10/20	3/11/89/115	-
36	LHG	b	623	-	-	15/47/47/53	-
31	CLA	13	316	-	-	14/37/115/115	-
38	LMG	B	620	-	-	26/46/66/70	0/1/1/1
31	CLA	13	315	-	-	2/11/90/115	-
31	CLA	4	311	-	1/1/11/20	8/15/93/115	-
43	A86	11	303	-	-	9/34/90/90	0/3/3/3
43	A86	2	304	-	-	6/34/90/90	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	KC2	16	312	-	-	6/15/71/71	-
36	LHG	P	615	-	-	14/31/31/53	-
45	KC2	17	309	-	-	10/15/71/71	-
31	CLA	4	307	-	1/1/15/20	16/37/115/115	-
33	BCR	C	517	-	-	10/29/63/63	0/2/2/2
31	CLA	2	309	-	1/1/10/20	6/11/89/115	-
41	HEM	E	101	5,6	-	5/12/54/54	-
43	A86	2	302	-	-	10/34/90/90	0/3/3/3
31	CLA	B	603	-	1/1/15/20	15/37/115/115	-
38	LMG	C	522	-	-	25/46/66/70	0/1/1/1
39	DGD	11	318	-	-	33/49/89/95	0/2/2/2
45	KC2	1	309	-	-	9/15/71/71	-
43	A86	8	303	-	-	9/34/90/90	0/3/3/3
31	CLA	c	506	-	1/1/15/20	12/37/115/115	-
31	CLA	17	312	-	1/1/11/20	5/16/94/115	-
38	LMG	5	316	-	-	17/31/51/70	0/1/1/1
43	A86	16	306	43	-	8/34/90/90	0/3/3/3
31	CLA	D	404	-	1/1/15/20	12/37/115/115	-
43	A86	18	303	-	-	12/34/90/90	0/3/3/3
36	LHG	8	315	-	-	23/43/43/53	-
31	CLA	p	605	16	1/1/10/20	3/8/86/115	-
42	KC1	16	301	27	-	0/15/71/71	-
31	CLA	c	507	-	1/1/15/20	16/37/115/115	-
36	LHG	18	316	-	-	23/34/34/53	-
31	CLA	13	310	-	1/1/10/20	2/8/86/115	-
36	LHG	Z	103	-	-	16/29/29/53	-
45	KC2	1	311	-	-	4/15/71/71	-
45	KC2	15	308	-	-	7/15/71/71	-
43	A86	7	303	-	-	8/34/90/90	0/3/3/3
41	HEM	v	201	21	-	8/12/54/54	-
31	CLA	a	404	-	1/1/11/20	5/18/96/115	-
43	A86	16	307	31	-	8/34/90/90	0/3/3/3
43	A86	13	303	-	-	6/34/90/90	0/3/3/3
31	CLA	10	311	-	1/1/13/20	6/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	19	303	-	-	7/34/90/90	0/3/3/3
43	A86	11	304	31	-	8/34/90/90	0/3/3/3
39	DGD	c	519	-	-	27/51/91/95	0/2/2/2
31	CLA	D	401	-	1/1/15/20	9/37/115/115	-
31	CLA	c	511	-	1/1/15/20	20/37/115/115	-
43	A86	19	304	-	-	7/34/90/90	0/3/3/3
38	LMG	b	621	-	-	26/46/66/70	0/1/1/1
31	CLA	3	312	-	-	4/13/91/115	-
31	CLA	C	505	-	1/1/15/20	8/37/115/115	-
31	CLA	0	313	-	1/1/10/20	4/10/88/115	-
43	A86	10	304	-	-	6/34/90/90	0/3/3/3
42	KC1	18	313	31,27	-	3/15/71/71	-
31	CLA	10	313	26	1/1/10/20	4/10/88/115	-
31	CLA	1	310	-	1/1/12/20	4/19/97/115	-
31	CLA	2	315	43	-	7/15/93/115	-
43	A86	1	320	-	-	8/34/90/90	0/3/3/3
35	PL9	a	409	-	-	15/27/47/73	0/1/1/1
43	A86	0	305	-	-	9/34/90/90	0/3/3/3
43	A86	0	302	26	-	8/34/90/90	0/3/3/3
31	CLA	5	306	-	1/1/10/20	3/10/88/115	-
43	A86	3	305	-	-	10/34/90/90	0/3/3/3
45	KC2	2	310	-	-	8/15/71/71	-
43	A86	19	306	-	-	8/34/90/90	0/3/3/3
38	LMG	1	317	-	-	26/40/60/70	0/1/1/1
43	A86	7	302	-	-	10/34/90/90	0/3/3/3
43	A86	10	305	-	-	9/34/90/90	0/3/3/3
34	SQD	0	318	31	-	22/36/56/69	0/1/1/1
38	LMG	c	521	-	-	25/46/66/70	0/1/1/1
45	KC2	8	308	-	-	10/15/71/71	-
43	A86	8	304	-	-	8/34/90/90	0/3/3/3
31	CLA	1	308	-	-	15/37/115/115	-
43	A86	P	613	31	-	8/34/90/90	1/3/3/3
43	A86	9	306	-	-	8/34/90/90	0/3/3/3
43	A86	6	307	-	-	13/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	316	-	1/1/11/20	5/15/93/115	-
33	BCR	B	619	-	-	12/29/63/63	0/2/2/2
43	A86	17	302	-	-	6/34/90/90	0/3/3/3
31	CLA	8	306	42	1/1/12/20	5/19/97/115	-
42	KC1	2	313	27	-	4/15/71/71	-
31	CLA	7	310	-	1/1/11/20	6/13/91/115	-
42	KC1	1	314	-	-	7/15/71/71	-
31	CLA	16	314	-	1/1/10/20	3/10/88/115	-
45	KC2	11	309	-	-	10/15/71/71	-
31	CLA	d	405	-	1/1/15/20	11/37/115/115	-
38	LMG	p	614	-	-	11/26/46/70	0/1/1/1
31	CLA	7	307	-	1/1/10/20	4/8/86/115	-
31	CLA	c	509	-	1/1/15/20	11/37/115/115	-
31	CLA	r	101	-	1/1/11/20	4/16/94/115	-
31	CLA	9	307	-	1/1/14/20	10/33/111/115	-
43	A86	6	304	-	-	7/34/90/90	0/3/3/3
31	CLA	0	308	-	1/1/12/20	8/19/97/115	-
31	CLA	10	308	-	1/1/12/20	9/19/97/115	-
43	A86	1	304	31	-	6/34/90/90	0/3/3/3
43	A86	5	302	-	-	8/34/90/90	0/3/3/3
31	CLA	B	613	-	1/1/15/20	10/37/115/115	-
43	A86	15	303	-	-	8/34/90/90	0/3/3/3
31	CLA	W	202	-	1/1/15/20	17/37/115/115	-
31	CLA	8	311	-	-	7/15/93/115	-
43	A86	0	306	-	-	7/34/90/90	0/3/3/3
31	CLA	16	316	-	1/1/10/20	4/11/89/115	-
45	KC2	15	310	27	-	7/15/71/71	-
31	CLA	17	307	-	1/1/10/20	4/8/86/115	-
31	CLA	9	313	-	1/1/15/20	11/37/115/115	-
33	BCR	Y	101	-	-	13/29/63/63	0/2/2/2
31	CLA	b	607	-	1/1/15/20	10/37/115/115	-
43	A86	17	301	-	-	10/34/90/90	0/3/3/3
31	CLA	B	607	-	1/1/15/20	16/37/115/115	-
31	CLA	p	608	16	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	311	-	-	5/13/91/115	-
38	LMG	10	319	-	-	8/26/46/70	0/1/1/1
36	LHG	L	101	-	-	22/53/53/53	-
38	LMG	11	301	-	-	14/31/51/70	0/1/1/1
31	CLA	18	312	27	1/1/13/20	8/25/103/115	-
33	BCR	y	101	-	-	13/29/63/63	0/2/2/2
43	A86	14	302	43	-	7/34/90/90	0/3/3/3
31	CLA	p	601	16	1/1/15/20	22/37/115/115	-
43	A86	11	319	-	-	6/34/90/90	0/3/3/3
31	CLA	5	312	-	-	4/16/94/115	-
31	CLA	2	312	-	-	10/17/95/115	-
42	KC1	0	315	-	-	4/15/71/71	-
31	CLA	B	601	-	1/1/15/20	20/37/115/115	-
31	CLA	P	608	16	1/1/12/20	5/21/99/115	-
36	LHG	D	407	-	-	28/53/53/53	-
45	KC2	17	311	27	-	6/15/71/71	-
31	CLA	b	616	-	1/1/15/20	7/37/115/115	-
39	DGD	h	102	-	-	29/51/91/95	0/2/2/2
34	SQD	B	623	-	-	25/49/69/69	0/1/1/1
38	LMG	d	403	-	-	17/35/55/70	0/1/1/1
31	CLA	16	311	-	1/1/10/20	3/8/86/115	-
31	CLA	B	614	-	1/1/15/20	20/37/115/115	-
34	SQD	i	101	-	-	21/35/55/69	0/1/1/1
31	CLA	10	309	-	-	16/30/108/115	-
31	CLA	b	612	-	1/1/15/20	12/37/115/115	-
31	CLA	c	508	-	1/1/15/20	14/37/115/115	-
32	PHO	A	405	-	-	14/37/103/103	0/5/6/6
43	A86	2	303	-	-	7/34/90/90	0/3/3/3
45	KC2	16	310	-	-	10/15/71/71	-
32	PHO	d	402	-	-	6/37/103/103	0/5/6/6
31	CLA	7	315	-	1/1/10/20	4/8/86/115	-
31	CLA	p	606	-	1/1/10/20	6/11/89/115	-
36	LHG	B	622	-	-	15/47/47/53	-
43	A86	10	306	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	HEM	V	201	21	-	8/12/54/54	-
31	CLA	13	307	-	1/1/10/20	1/10/88/115	-
31	CLA	18	314	27	1/1/10/20	7/11/89/115	-
43	A86	7	305	-	-	8/34/90/90	0/3/3/3
43	A86	14	304	-	-	7/34/90/90	0/3/3/3
31	CLA	b	609	-	1/1/15/20	16/37/115/115	-
43	A86	9	305	-	-	9/34/90/90	0/3/3/3
38	LMG	11	317	-	-	24/40/60/70	0/1/1/1
43	A86	9	302	-	-	6/34/90/90	0/3/3/3
43	A86	11	320	-	-	8/34/90/90	0/3/3/3
43	A86	13	305	-	-	9/34/90/90	0/3/3/3
45	KC2	18	310	27	-	7/15/71/71	-
31	CLA	9	308	-	1/1/15/20	18/37/115/115	-
31	CLA	14	309	-	1/1/15/20	20/37/115/115	-
31	CLA	A	403	-	1/1/15/20	10/37/115/115	-
43	A86	16	303	-	-	8/34/90/90	0/3/3/3
31	CLA	7	312	-	1/1/11/20	8/16/94/115	-
31	CLA	d	401	-	1/1/15/20	9/37/115/115	-
31	CLA	9	312	43	1/1/15/20	6/37/115/115	-
31	CLA	17	315	-	1/1/10/20	4/8/86/115	-
45	KC2	4	310	-	-	6/15/71/71	-
43	A86	8	305	-	-	8/34/90/90	0/3/3/3
39	DGD	c	520	34	-	32/51/91/95	0/2/2/2
31	CLA	B	616	-	1/1/15/20	14/37/115/115	-
31	CLA	18	307	-	1/1/14/20	9/33/111/115	-
31	CLA	b	613	-	1/1/15/20	16/37/115/115	-
31	CLA	14	315	-	1/1/10/20	7/11/89/115	-
42	KC1	11	314	-	-	8/15/71/71	-
31	CLA	C	513	-	1/1/15/20	18/37/115/115	-
43	A86	18	301	-	-	5/34/90/90	0/3/3/3
43	A86	1	303	-	-	8/34/90/90	0/3/3/3
43	A86	3	301	-	-	10/34/90/90	0/3/3/3
43	A86	15	304	-	-	10/34/90/90	1/3/3/3
31	CLA	14	306	-	1/1/14/20	15/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	514	-	1/1/11/20	5/18/96/115	-
45	KC2	11	311	-	-	4/15/71/71	-
31	CLA	w	203	-	1/1/15/20	17/37/115/115	-
31	CLA	C	508	-	1/1/15/20	14/37/115/115	-
31	CLA	12	315	-	-	1/8/86/115	-
38	LMG	D	408	4	-	16/32/52/70	0/1/1/1
45	KC2	8	310	-	-	6/15/71/71	-
31	CLA	3	315	-	1/1/10/20	5/11/90/115	-
31	CLA	10	312	34,26	1/1/11/20	6/15/93/115	-
42	KC1	19	314	-	-	5/15/71/71	-
33	BCR	B	617	-	-	13/29/63/63	0/2/2/2
43	A86	19	305	-	-	9/34/90/90	0/3/3/3
42	KC1	10	315	-	-	4/15/71/71	-
43	A86	18	304	-	-	6/34/90/90	0/3/3/3
43	A86	3	304	-	-	6/34/90/90	0/3/3/3
43	A86	17	304	-	-	8/34/90/90	0/3/3/3
31	CLA	14	307	-	1/1/15/20	16/37/115/115	-
31	CLA	P	603	-	1/1/12/20	8/19/97/115	-
39	DGD	C	520	34	-	32/51/91/95	0/2/2/2
45	KC2	2	308	-	-	10/15/71/71	-
43	A86	9	303	-	-	8/34/90/90	0/3/3/3
31	CLA	12	310	-	1/1/10/20	6/11/89/115	-
31	CLA	19	310	-	1/1/15/20	15/37/115/115	-
34	SQD	10	320	31	-	24/36/56/69	0/1/1/1
38	LMG	m	101	-	-	19/35/55/70	0/1/1/1
43	A86	4	303	-	-	12/34/90/90	0/3/3/3
31	CLA	17	313	27	1/1/12/20	6/19/97/115	-
43	A86	1	302	-	-	8/34/90/90	0/3/3/3
31	CLA	10	307	-	1/1/11/20	7/17/95/115	-
31	CLA	C	514	-	1/1/11/20	5/18/96/115	-
45	KC2	13	311	-	-	7/15/71/71	-
31	CLA	b	603	-	1/1/15/20	17/37/115/115	-
34	SQD	A	411	-	-	22/35/55/69	0/1/1/1
31	CLA	5	307	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	608	-	1/1/15/20	17/37/115/115	-
42	KC1	5	313	-	-	3/15/71/71	-
31	CLA	B	608	-	1/1/15/20	16/37/115/115	-
31	CLA	B	615	-	1/1/15/20	7/37/115/115	-
43	A86	5	301	31	-	6/34/90/90	0/3/3/3
31	CLA	5	311	-	1/1/11/20	5/13/91/115	-
42	KC1	p	609	-	-	8/15/71/71	-
31	CLA	0	312	34,26	1/1/11/20	7/15/93/115	-
31	CLA	7	313	-	1/1/12/20	7/19/97/115	-
31	CLA	c	503	31	1/1/15/20	11/37/115/115	-
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
31	CLA	14	311	-	1/1/11/20	10/15/93/115	-
43	A86	16	304	43	-	8/34/90/90	0/3/3/3
31	CLA	c	512	3	1/1/15/20	6/37/115/115	-
31	CLA	4	312	27	1/1/12/20	9/21/99/115	-
42	KC1	16	315	27	-	1/15/71/71	-
38	LMG	15	314	-	-	17/32/52/70	0/1/1/1
31	CLA	z	101	-	1/1/12/20	6/21/99/115	-
38	LMG	5	315	-	-	16/32/52/70	0/1/1/1
31	CLA	19	308	-	1/1/15/20	15/37/115/115	-
43	A86	7	301	-	-	6/34/90/90	0/3/3/3
43	A86	11	306	-	-	8/34/90/90	0/3/3/3
31	CLA	1	307	-	1/1/10/20	2/11/89/115	-
31	CLA	P	607	43	1/1/10/20	3/11/89/115	-
39	DGD	W	203	-	-	28/45/85/95	0/2/2/2
31	CLA	11	307	27	1/1/10/20	3/11/89/115	-
42	KC1	14	313	27	-	9/15/71/71	-
31	CLA	12	313	-	-	10/17/95/115	-
33	BCR	B	618	-	-	9/29/63/63	0/2/2/2
45	KC2	14	308	-	-	7/15/71/71	-
31	CLA	16	313	-	1/1/11/20	6/16/94/115	-
31	CLA	B	605	-	1/1/15/20	10/37/115/115	-
31	CLA	B	612	-	1/1/15/20	16/37/115/115	-
44	DD6	p	612	-	-	10/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	510	-	1/1/15/20	7/37/115/115	-
43	A86	1	306	-	-	8/34/90/90	0/3/3/3
33	BCR	c	516	-	-	9/29/63/63	0/2/2/2
33	BCR	F	101	-	-	19/29/63/63	0/2/2/2
31	CLA	a	406	-	1/1/14/20	5/31/109/115	-
43	A86	10	318	-	-	8/34/90/90	0/3/3/3
31	CLA	b	602	-	1/1/15/20	20/37/115/115	-
43	A86	12	301	-	-	8/34/90/90	0/3/3/3
42	KC1	12	314	-	-	3/15/71/71	-
31	CLA	13	313	-	-	16/37/115/115	-
43	A86	14	303	-	-	9/34/90/90	0/3/3/3
35	PL9	A	409	-	-	16/27/47/73	0/1/1/1
43	A86	2	305	31	-	7/34/90/90	0/3/3/3
31	CLA	0	314	-	-	5/16/94/115	-
43	A86	15	302	-	-	9/34/90/90	1/3/3/3
43	A86	17	316	-	-	9/34/90/90	0/3/3/3
38	LMG	f	102	-	-	14/41/61/70	0/1/1/1
38	LMG	D	403	4	-	22/35/55/70	0/1/1/1
31	CLA	15	309	-	1/1/13/20	11/25/103/115	-
31	CLA	9	310	-	1/1/15/20	15/37/115/115	-
43	A86	14	305	-	-	6/34/90/90	1/3/3/3
31	CLA	11	313	-	1/1/15/20	12/37/115/115	-
31	CLA	2	307	-	1/1/15/20	15/37/115/115	-
38	LMG	M	101	-	-	18/35/55/70	0/1/1/1
41	HEM	e	101	5,6	-	5/12/54/54	-
43	A86	9	301	-	-	8/34/90/90	0/3/3/3
38	LMG	n	701	14	-	6/23/43/70	0/1/1/1
36	LHG	14	317	-	-	22/38/38/53	-
38	LMG	4	316	-	-	24/44/64/70	0/1/1/1
43	A86	4	301	-	-	8/34/90/90	0/3/3/3
43	A86	11	305	-	-	9/34/90/90	0/3/3/3
31	CLA	5	314	-	1/1/10/20	1/8/86/115	-
31	CLA	2	314	-	-	4/8/86/115	-
38	LMG	J	101	-	-	29/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	d	404	-	1/1/15/20	12/37/115/115	-
34	SQD	a	408	39	-	23/49/69/69	0/1/1/1
31	CLA	14	312	-	1/1/12/20	8/21/99/115	-
45	KC2	6	312	27	-	6/15/71/71	-
31	CLA	P	604	-	1/1/11/20	5/17/95/115	-
43	A86	16	305	-	-	7/34/90/90	0/3/3/3
43	A86	P	611	-	-	7/34/90/90	1/3/3/3
36	LHG	18	315	-	-	21/43/43/53	-
38	LMG	j	101	-	-	29/45/65/70	0/1/1/1
38	LMG	14	316	-	-	24/44/64/70	0/1/1/1
31	CLA	p	610	-	1/1/10/20	2/8/86/115	-
31	CLA	b	611	-	-	9/37/115/115	-
36	LHG	C	521	-	-	20/44/44/53	-
31	CLA	1	321	-	1/1/14/20	13/33/111/115	-
38	LMG	d	408	4	-	16/32/52/70	0/1/1/1
31	CLA	B	610	-	-	9/37/115/115	-
43	A86	8	301	-	-	11/34/90/90	0/3/3/3
31	CLA	11	315	-	1/1/10/20	5/8/86/115	-
43	A86	17	305	-	-	8/34/90/90	0/3/3/3
31	CLA	16	308	-	1/1/10/20	5/10/88/115	-
43	A86	0	301	-	-	7/34/90/90	0/3/3/3
45	KC2	12	309	-	-	6/15/71/71	-
43	A86	10	301	-	-	7/34/90/90	0/3/3/3
43	A86	6	306	31	-	8/34/90/90	0/3/3/3
43	A86	1	305	-	-	10/34/90/90	0/3/3/3
31	CLA	19	312	43	1/1/15/20	8/37/115/115	-
43	A86	11	302	-	-	6/34/90/90	0/3/3/3
45	KC2	3	309	-	-	10/15/71/71	-
31	CLA	13	308	-	1/1/10/20	3/11/89/115	-
36	LHG	p	615	-	-	14/31/31/53	-
43	A86	17	303	-	-	10/34/90/90	0/3/3/3
31	CLA	1	312	-	1/1/11/20	6/15/93/115	-
45	KC2	9	309	-	-	5/15/71/71	-
45	KC2	4	308	-	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	510	-	1/1/15/20	7/37/115/115	-
45	KC2	0	310	26	-	9/15/71/71	-
42	KC1	6	315	27	-	1/15/71/71	-
31	CLA	11	308	-	1/1/15/20	22/37/115/115	-
45	KC2	10	310	26	-	7/15/71/71	-
31	CLA	b	605	-	1/1/15/20	14/37/115/115	-
31	CLA	1	316	43	1/1/10/20	3/10/88/115	-
31	CLA	P	605	16	1/1/10/20	3/8/86/115	-
45	KC2	3	311	-	-	6/15/71/71	-
35	PL9	d	406	-	-	9/53/73/73	0/1/1/1
31	CLA	8	312	-	1/1/13/20	10/25/103/115	-
31	CLA	6	313	-	1/1/11/20	6/16/94/115	-
31	CLA	1	315	27	-	3/8/86/115	-
31	CLA	6	309	-	1/1/15/20	13/37/115/115	-
43	A86	6	305	43	-	8/34/90/90	0/3/3/3
31	CLA	c	505	-	1/1/15/20	8/37/115/115	-

All (4266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	12	313	CLA	C4B-NB	8.87	1.43	1.35
31	17	313	CLA	C4B-NB	8.86	1.43	1.35
42	6	315	KC1	C4D-ND	8.81	1.43	1.35
44	p	612	DD6	C29-C27	-8.80	1.25	1.42
44	P	612	DD6	C29-C27	-8.78	1.25	1.42
31	2	315	CLA	C4B-NB	8.69	1.43	1.35
31	2	312	CLA	C4B-NB	8.67	1.42	1.35
31	7	313	CLA	C4B-NB	8.57	1.42	1.35
31	13	313	CLA	C4B-NB	8.42	1.42	1.35
31	11	316	CLA	C4B-NB	8.28	1.42	1.35
31	3	313	CLA	C4B-NB	8.18	1.42	1.35
31	12	316	CLA	C4B-NB	8.04	1.42	1.35
42	7	314	KC1	C4D-ND	8.00	1.42	1.35
44	P	612	DD6	C30-C31	-8.00	1.25	1.42
44	p	612	DD6	C30-C31	-7.98	1.25	1.42
45	15	308	KC2	C4C-NC	7.97	1.49	1.37
45	5	308	KC2	C4C-NC	7.96	1.49	1.37
31	3	312	CLA	C4B-NB	7.92	1.42	1.35
31	13	315	CLA	C4B-NB	7.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	13	311	KC2	C4C-NC	7.88	1.49	1.37
31	15	311	CLA	C4B-NB	7.88	1.42	1.35
45	1	309	KC2	C4C-NC	7.85	1.49	1.37
42	3	314	KC1	C4D-ND	7.84	1.42	1.35
31	14	315	CLA	C4B-NB	7.82	1.42	1.35
31	10	313	CLA	C4B-NB	7.82	1.42	1.35
31	4	315	CLA	C4B-NB	7.80	1.42	1.35
45	7	311	KC2	C4C-NC	7.78	1.49	1.37
45	17	311	KC2	C4C-NC	7.78	1.49	1.37
43	p	611	A86	O1-C20	-7.76	1.35	1.46
42	8	313	KC1	C4D-ND	7.74	1.42	1.35
31	P	606	CLA	CAA-C2A	7.73	1.68	1.54
45	2	310	KC2	C4C-NC	7.71	1.49	1.37
31	p	606	CLA	CAA-C2A	7.71	1.68	1.54
45	16	312	KC2	C4C-NC	7.70	1.49	1.37
45	2	308	KC2	C4C-NC	7.69	1.49	1.37
31	7	312	CLA	C4B-NB	7.68	1.42	1.35
45	17	309	KC2	C4C-NC	7.68	1.49	1.37
45	6	312	KC2	C4C-NC	7.68	1.49	1.37
42	9	314	KC1	C4C-NC	7.67	1.49	1.37
45	12	311	KC2	C4C-NC	7.66	1.49	1.37
43	P	611	A86	O1-C20	-7.66	1.35	1.46
42	16	315	KC1	C4D-ND	7.65	1.42	1.35
31	14	312	CLA	C4B-NB	7.63	1.42	1.35
45	19	309	KC2	C4C-NC	7.62	1.49	1.37
45	7	309	KC2	C4C-NC	7.62	1.49	1.37
31	17	312	CLA	C4B-NB	7.62	1.42	1.35
45	3	311	KC2	C4C-NC	7.62	1.49	1.37
42	16	301	KC1	C4C-NC	7.62	1.49	1.37
42	18	313	KC1	C4D-ND	7.61	1.42	1.35
42	19	314	KC1	C4C-NC	7.61	1.49	1.37
31	11	312	CLA	C4B-NB	7.60	1.42	1.35
42	14	313	KC1	C4C-NC	7.59	1.49	1.37
45	9	309	KC2	C4C-NC	7.59	1.49	1.37
45	6	310	KC2	C4C-NC	7.56	1.49	1.37
31	1	315	CLA	C4B-NB	7.54	1.41	1.35
31	18	312	CLA	C4B-NB	7.53	1.41	1.35
45	3	309	KC2	C4C-NC	7.53	1.49	1.37
31	16	308	CLA	C4B-NB	7.51	1.41	1.35
31	6	314	CLA	C4B-NB	7.51	1.41	1.35
31	19	310	CLA	C4B-NB	7.50	1.41	1.35
42	13	314	KC1	C4C-NC	7.50	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	13	309	KC2	C4C-NC	7.49	1.49	1.37
31	9	311	CLA	C4B-NB	7.48	1.41	1.35
42	1	314	KC1	C4C-NC	7.48	1.49	1.37
45	14	308	KC2	C4C-NC	7.48	1.49	1.37
45	16	310	KC2	C4C-NC	7.48	1.49	1.37
45	15	310	KC2	C4C-NC	7.47	1.49	1.37
31	14	306	CLA	C4B-NB	7.47	1.41	1.35
42	5	313	KC1	C4C-NC	7.47	1.49	1.37
31	12	315	CLA	C4B-NB	7.47	1.41	1.35
45	5	310	KC2	C4C-NC	7.47	1.49	1.37
31	13	307	CLA	C4B-NB	7.46	1.41	1.35
42	4	313	KC1	C4C-NC	7.46	1.49	1.37
42	11	314	KC1	C4C-NC	7.46	1.48	1.37
45	4	308	KC2	C4C-NC	7.45	1.48	1.37
45	18	310	KC2	C4C-NC	7.45	1.48	1.37
31	5	314	CLA	C4B-NB	7.43	1.41	1.35
45	8	310	KC2	C4C-NC	7.43	1.48	1.37
31	2	311	CLA	C4B-NB	7.43	1.41	1.35
31	19	315	CLA	C4B-NB	7.42	1.41	1.35
42	16	315	KC1	C4C-NC	7.40	1.48	1.37
31	1	313	CLA	C4B-NB	7.40	1.41	1.35
31	9	315	CLA	C4B-NB	7.40	1.41	1.35
31	6	316	CLA	C4B-NB	7.39	1.41	1.35
31	16	313	CLA	C4B-NB	7.39	1.41	1.35
42	12	314	KC1	C4C-NC	7.38	1.48	1.37
31	15	312	CLA	C4B-NB	7.38	1.41	1.35
45	12	309	KC2	C4C-NC	7.36	1.48	1.37
31	6	313	CLA	C4B-NB	7.35	1.41	1.35
31	11	313	CLA	C4B-NB	7.35	1.41	1.35
45	8	308	KC2	C4C-NC	7.34	1.48	1.37
45	11	309	KC2	C4C-NC	7.34	1.48	1.37
31	19	307	CLA	C4B-NB	7.33	1.41	1.35
31	19	311	CLA	C4B-NB	7.33	1.41	1.35
31	9	310	CLA	C4B-NB	7.31	1.41	1.35
31	0	313	CLA	C4B-NB	7.30	1.41	1.35
31	13	312	CLA	C4B-NB	7.29	1.41	1.35
42	2	313	KC1	C4C-NC	7.27	1.48	1.37
31	14	314	CLA	C4B-NB	7.27	1.41	1.35
45	10	310	KC2	C4C-NC	7.26	1.48	1.37
45	0	310	KC2	C4C-NC	7.26	1.48	1.37
31	9	312	CLA	C4B-NB	7.26	1.41	1.35
45	18	308	KC2	C4C-NC	7.25	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	10	315	KC1	C4C-NC	7.25	1.48	1.37
31	3	315	CLA	C4B-NB	7.25	1.41	1.35
31	15	313	CLA	C4B-NB	7.24	1.41	1.35
31	11	315	CLA	C4B-NB	7.24	1.41	1.35
31	16	316	CLA	C4B-NB	7.24	1.41	1.35
31	8	311	CLA	C4B-NB	7.23	1.41	1.35
45	14	310	KC2	C4C-NC	7.22	1.48	1.37
31	10	308	CLA	C4B-NB	7.21	1.41	1.35
31	19	312	CLA	C4B-NB	7.21	1.41	1.35
31	0	307	CLA	C4B-NB	7.21	1.41	1.35
31	10	317	CLA	C4B-NB	7.21	1.41	1.35
31	4	312	CLA	C4B-NB	7.21	1.41	1.35
42	9	314	KC1	C4D-ND	7.20	1.41	1.35
31	17	307	CLA	C4B-NB	7.20	1.41	1.35
31	z	103	CLA	C4B-NB	7.20	1.41	1.35
45	11	311	KC2	C4C-NC	7.20	1.48	1.37
31	1	316	CLA	C4B-NB	7.19	1.41	1.35
45	4	310	KC2	C4C-NC	7.17	1.48	1.37
31	12	307	CLA	C4B-NB	7.16	1.41	1.35
31	10	314	CLA	C4B-NB	7.15	1.41	1.35
31	7	307	CLA	C4B-NB	7.15	1.41	1.35
35	D	406	PL9	C3-C4	-7.14	1.37	1.49
31	14	311	CLA	C4B-NB	7.13	1.41	1.35
31	7	315	CLA	C4B-NB	7.13	1.41	1.35
42	6	315	KC1	C4C-NC	7.13	1.48	1.37
31	5	312	CLA	C4B-NB	7.13	1.41	1.35
31	2	314	CLA	C4B-NB	7.12	1.41	1.35
31	16	314	CLA	C4B-NB	7.12	1.41	1.35
35	d	406	PL9	C3-C4	-7.12	1.37	1.49
45	1	311	KC2	C4C-NC	7.10	1.48	1.37
31	0	308	CLA	C4B-NB	7.10	1.41	1.35
31	p	605	CLA	C4B-NB	7.09	1.41	1.35
31	1	312	CLA	C4B-NB	7.09	1.41	1.35
31	0	312	CLA	C4B-NB	7.09	1.41	1.35
31	10	312	CLA	C4B-NB	7.09	1.41	1.35
31	15	306	CLA	C4B-NB	7.09	1.41	1.35
31	11	308	CLA	C4B-NB	7.06	1.41	1.35
31	P	605	CLA	C4B-NB	7.06	1.41	1.35
31	12	312	CLA	C4B-NB	7.06	1.41	1.35
31	3	307	CLA	C4B-NB	7.06	1.41	1.35
31	3	310	CLA	C4B-NB	7.05	1.41	1.35
31	4	314	CLA	C4B-NB	7.05	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	608	CLA	C4B-NB	7.05	1.41	1.35
42	0	315	KC1	C4C-NC	7.05	1.48	1.37
31	13	316	CLA	C4B-NB	7.05	1.41	1.35
31	3	316	CLA	C4B-NB	7.04	1.41	1.35
31	D	404	CLA	C4B-NB	7.03	1.41	1.35
31	d	404	CLA	C4B-NB	7.03	1.41	1.35
31	B	607	CLA	C4B-NB	7.02	1.41	1.35
45	16	312	KC2	C4D-ND	7.02	1.41	1.35
42	1	314	KC1	C4D-ND	7.02	1.41	1.35
31	11	307	CLA	C4B-NB	7.01	1.41	1.35
42	17	314	KC1	C4C-NC	7.01	1.48	1.37
42	7	314	KC1	C4C-NC	7.01	1.48	1.37
31	1	308	CLA	C4B-NB	7.01	1.41	1.35
31	4	311	CLA	C4B-NB	7.01	1.41	1.35
42	19	314	KC1	C4D-ND	7.01	1.41	1.35
31	2	309	CLA	C4B-NB	6.98	1.41	1.35
45	11	311	KC2	C4D-ND	6.98	1.41	1.35
31	5	311	CLA	C4B-NB	6.96	1.41	1.35
45	1	309	KC2	C4D-ND	6.95	1.41	1.35
45	6	312	KC2	C4D-ND	6.95	1.41	1.35
31	9	307	CLA	C4B-NB	6.94	1.41	1.35
42	18	313	KC1	C4C-NC	6.93	1.48	1.37
31	10	307	CLA	C4B-NB	6.93	1.41	1.35
31	17	310	CLA	C4B-NB	6.93	1.41	1.35
31	B	601	CLA	C4B-NB	6.92	1.41	1.35
31	12	310	CLA	C4B-NB	6.92	1.41	1.35
42	3	314	KC1	C4C-NC	6.92	1.48	1.37
31	17	315	CLA	C4B-NB	6.91	1.41	1.35
31	0	314	CLA	C4B-NB	6.91	1.41	1.35
31	r	101	CLA	C4B-NB	6.91	1.41	1.35
31	7	310	CLA	C4B-NB	6.89	1.41	1.35
42	2	313	KC1	C4D-ND	6.87	1.41	1.35
45	1	311	KC2	C4D-ND	6.85	1.41	1.35
31	R	101	CLA	C4B-NB	6.83	1.41	1.35
42	P	609	KC1	C4C-NC	6.83	1.48	1.37
45	12	309	KC2	C4D-ND	6.81	1.41	1.35
42	p	609	KC1	C4C-NC	6.80	1.48	1.37
31	1	307	CLA	C4B-NB	6.79	1.41	1.35
31	7	308	CLA	C4B-NB	6.79	1.41	1.35
31	8	314	CLA	C4B-NB	6.77	1.41	1.35
31	13	310	CLA	C4B-NB	6.77	1.41	1.35
31	b	602	CLA	C4B-NB	6.77	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	611	CLA	C4B-NB	6.74	1.41	1.35
45	3	311	KC2	C4D-ND	6.74	1.41	1.35
31	B	610	CLA	C4B-NB	6.73	1.41	1.35
31	Z	101	CLA	C4B-NB	6.73	1.41	1.35
31	19	308	CLA	C4B-NB	6.72	1.41	1.35
31	p	608	CLA	C4B-NB	6.71	1.41	1.35
31	8	312	CLA	C4B-NB	6.71	1.41	1.35
31	17	308	CLA	C4B-NB	6.71	1.41	1.35
31	B	616	CLA	C4B-NB	6.71	1.41	1.35
31	8	306	CLA	C4B-NB	6.69	1.41	1.35
31	9	308	CLA	C4B-NB	6.69	1.41	1.35
31	13	308	CLA	C4B-NB	6.69	1.41	1.35
31	5	306	CLA	C4B-NB	6.68	1.41	1.35
31	18	314	CLA	C4B-NB	6.68	1.41	1.35
31	p	601	CLA	C4B-NB	6.68	1.41	1.35
31	w	203	CLA	C4B-NB	6.67	1.41	1.35
31	P	608	CLA	C4B-NB	6.67	1.41	1.35
31	16	311	CLA	C4B-NB	6.67	1.41	1.35
31	z	101	CLA	C4B-NB	6.67	1.41	1.35
31	2	306	CLA	C4B-NB	6.66	1.41	1.35
31	P	601	CLA	C4B-NB	6.65	1.41	1.35
31	b	617	CLA	C4B-NB	6.65	1.41	1.35
45	7	309	KC2	C4D-ND	6.64	1.41	1.35
31	12	308	CLA	C4B-NB	6.64	1.41	1.35
31	C	504	CLA	C4B-NB	6.62	1.41	1.35
42	13	314	KC1	C4D-ND	6.61	1.41	1.35
31	B	609	CLA	C4B-NB	6.60	1.41	1.35
45	17	309	KC2	C4D-ND	6.60	1.41	1.35
31	4	307	CLA	C4B-NB	6.59	1.41	1.35
31	6	309	CLA	C4B-NB	6.59	1.41	1.35
31	10	309	CLA	C4B-NB	6.59	1.41	1.35
31	p	610	CLA	C4B-NB	6.59	1.41	1.35
31	P	610	CLA	C4B-NB	6.58	1.41	1.35
31	W	202	CLA	C4B-NB	6.58	1.41	1.35
31	2	307	CLA	C4B-NB	6.58	1.41	1.35
31	14	307	CLA	C4B-NB	6.58	1.41	1.35
31	6	311	CLA	C4B-NB	6.58	1.41	1.35
45	7	311	KC2	C4D-ND	6.57	1.41	1.35
31	c	504	CLA	C4B-NB	6.57	1.41	1.35
31	p	602	CLA	C4B-NB	6.57	1.41	1.35
31	8	309	CLA	C4B-NB	6.56	1.41	1.35
31	C	507	CLA	C4B-NB	6.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	0	309	CLA	C4B-NB	6.55	1.41	1.35
31	c	507	CLA	C4B-NB	6.55	1.41	1.35
31	B	611	CLA	C4B-NB	6.53	1.41	1.35
31	6	308	CLA	C4B-NB	6.52	1.41	1.35
31	18	306	CLA	C4B-NB	6.51	1.41	1.35
31	b	610	CLA	C4B-NB	6.50	1.41	1.35
31	C	505	CLA	C4B-NB	6.50	1.41	1.35
31	b	612	CLA	C4B-NB	6.50	1.41	1.35
31	c	505	CLA	C4B-NB	6.50	1.41	1.35
31	16	309	CLA	C4B-NB	6.49	1.41	1.35
31	10	311	CLA	C4B-NB	6.49	1.41	1.35
31	18	311	CLA	C4B-NB	6.48	1.41	1.35
31	P	602	CLA	C4B-NB	6.47	1.41	1.35
45	15	308	KC2	C4D-ND	6.44	1.41	1.35
31	3	308	CLA	C4B-NB	6.44	1.41	1.35
31	0	311	CLA	C4B-NB	6.43	1.40	1.35
45	2	308	KC2	C4D-ND	6.43	1.40	1.35
31	b	616	CLA	C4B-NB	6.42	1.40	1.35
45	2	310	KC2	C4D-ND	6.42	1.40	1.35
31	15	309	CLA	C4B-NB	6.41	1.40	1.35
31	b	609	CLA	C4B-NB	6.40	1.40	1.35
45	17	311	KC2	C4D-ND	6.39	1.40	1.35
31	11	310	CLA	C4B-NB	6.38	1.40	1.35
31	C	506	CLA	C4B-NB	6.37	1.40	1.35
31	c	506	CLA	C4B-NB	6.37	1.40	1.35
31	B	615	CLA	C4B-NB	6.36	1.40	1.35
31	B	608	CLA	C4B-NB	6.36	1.40	1.35
31	D	405	CLA	C4B-NB	6.35	1.40	1.35
42	p	609	KC1	C4D-ND	6.35	1.40	1.35
31	C	509	CLA	C4B-NB	6.35	1.40	1.35
31	d	405	CLA	C4B-NB	6.34	1.40	1.35
31	p	603	CLA	C4B-NB	6.33	1.40	1.35
45	3	309	KC2	C4D-ND	6.32	1.40	1.35
31	p	604	CLA	C4B-NB	6.32	1.40	1.35
31	p	607	CLA	C4B-NB	6.31	1.40	1.35
43	8	301	A86	O4-C38	6.31	1.49	1.35
31	18	309	CLA	C4B-NB	6.31	1.40	1.35
42	P	609	KC1	C4D-ND	6.31	1.40	1.35
31	C	511	CLA	C4B-NB	6.31	1.40	1.35
31	c	511	CLA	C4B-NB	6.31	1.40	1.35
31	0	316	CLA	C4B-NB	6.31	1.40	1.35
31	C	514	CLA	C4B-NB	6.30	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	514	CLA	C4B-NB	6.30	1.40	1.35
31	P	604	CLA	C4B-NB	6.29	1.40	1.35
31	P	607	CLA	C4B-NB	6.29	1.40	1.35
45	18	310	KC2	C4D-ND	6.29	1.40	1.35
45	12	311	KC2	C4D-ND	6.28	1.40	1.35
45	4	308	KC2	C4D-ND	6.28	1.40	1.35
45	5	308	KC2	C4D-ND	6.28	1.40	1.35
45	14	308	KC2	C4D-ND	6.28	1.40	1.35
45	8	308	KC2	C4D-ND	6.27	1.40	1.35
31	10	316	CLA	C4B-NB	6.26	1.40	1.35
42	3	314	KC1	C2A-C3A	6.25	1.49	1.37
42	16	315	KC1	C2A-C3A	6.25	1.49	1.37
45	5	310	KC2	C4D-ND	6.25	1.40	1.35
45	9	309	KC2	C4D-ND	6.24	1.40	1.35
31	c	508	CLA	C4B-NB	6.24	1.40	1.35
31	c	509	CLA	C4B-NB	6.24	1.40	1.35
45	17	311	KC2	C1A-NA	6.24	1.50	1.38
31	15	307	CLA	C4B-NB	6.24	1.40	1.35
45	16	310	KC2	C4D-ND	6.23	1.40	1.35
45	8	310	KC2	C4D-ND	6.23	1.40	1.35
31	P	603	CLA	C4B-NB	6.22	1.40	1.35
42	4	313	KC1	C4D-ND	6.22	1.40	1.35
42	7	314	KC1	C2A-C3A	6.21	1.49	1.37
31	5	309	CLA	C4B-NB	6.21	1.40	1.35
31	4	309	CLA	C4B-NB	6.19	1.40	1.35
31	C	508	CLA	C4B-NB	6.19	1.40	1.35
45	18	308	KC2	C4D-ND	6.19	1.40	1.35
31	B	613	CLA	C4B-NB	6.17	1.40	1.35
45	6	310	KC2	C4D-ND	6.16	1.40	1.35
31	1	310	CLA	C4B-NB	6.15	1.40	1.35
42	2	313	KC1	C2A-C3A	6.15	1.49	1.37
31	14	309	CLA	C4B-NB	6.14	1.40	1.35
45	13	309	KC2	C4D-ND	6.14	1.40	1.35
31	B	605	CLA	C4B-NB	6.13	1.40	1.35
42	16	315	KC1	C1A-NA	6.12	1.50	1.38
42	17	314	KC1	C4D-ND	6.12	1.40	1.35
31	C	512	CLA	C4B-NB	6.11	1.40	1.35
31	b	606	CLA	C4B-NB	6.11	1.40	1.35
31	c	512	CLA	C4B-NB	6.11	1.40	1.35
31	1	321	CLA	C4B-NB	6.11	1.40	1.35
45	2	308	KC2	CHD-C4C	6.11	1.50	1.35
45	13	311	KC2	C3C-C2C	6.10	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	10	315	KC1	C1A-NA	6.09	1.49	1.38
31	b	614	CLA	C4B-NB	6.09	1.40	1.35
31	B	614	CLA	C4B-NB	6.08	1.40	1.35
45	15	310	KC2	C4D-ND	6.08	1.40	1.35
43	11	306	A86	O1-C20	-6.08	1.37	1.46
42	8	313	KC1	C4C-NC	6.07	1.46	1.37
31	A	404	CLA	C4B-NB	6.06	1.40	1.35
31	a	404	CLA	C4B-NB	6.06	1.40	1.35
31	b	615	CLA	C4B-NB	6.06	1.40	1.35
31	C	510	CLA	C4B-NB	6.05	1.40	1.35
31	C	502	CLA	C4B-NB	6.04	1.40	1.35
31	c	502	CLA	C4B-NB	6.04	1.40	1.35
45	3	309	KC2	CHD-C4C	6.03	1.50	1.35
45	19	309	KC2	C4D-ND	6.02	1.40	1.35
45	18	310	KC2	C1A-NA	6.02	1.49	1.38
45	16	310	KC2	CHD-C4C	6.02	1.50	1.35
45	17	309	KC2	CHD-C4C	6.02	1.50	1.35
42	5	313	KC1	C1A-NA	6.02	1.49	1.38
45	7	309	KC2	CHD-C4C	6.01	1.50	1.35
31	18	307	CLA	C4B-NB	6.01	1.40	1.35
42	17	314	KC1	C2A-C3A	6.00	1.49	1.37
45	13	311	KC2	CHD-C4C	6.00	1.50	1.35
45	6	310	KC2	CHD-C4C	6.00	1.50	1.35
31	b	604	CLA	C4B-NB	5.99	1.40	1.35
31	c	510	CLA	C4B-NB	5.98	1.40	1.35
45	13	311	KC2	C4D-ND	5.98	1.40	1.35
42	6	315	KC1	C2A-C3A	5.97	1.49	1.37
42	0	315	KC1	C4D-ND	5.96	1.40	1.35
31	B	604	CLA	C4B-NB	5.96	1.40	1.35
45	5	308	KC2	CHD-C4C	5.95	1.50	1.35
45	12	311	KC2	C1A-NA	5.95	1.49	1.38
31	B	603	CLA	C4B-NB	5.95	1.40	1.35
45	2	310	KC2	CHD-C4C	5.95	1.50	1.35
45	15	308	KC2	CHD-C4C	5.94	1.50	1.35
31	a	403	CLA	C4B-NB	5.94	1.40	1.35
42	17	314	KC1	C1A-NA	5.93	1.49	1.38
45	13	311	KC2	C2A-C3A	5.93	1.49	1.37
45	18	308	KC2	CHD-C4C	5.92	1.50	1.35
45	6	312	KC2	CHD-C4C	5.92	1.50	1.35
45	2	308	KC2	C3C-C2C	5.91	1.49	1.37
31	8	307	CLA	C4B-NB	5.91	1.40	1.35
45	1	309	KC2	CHD-C4C	5.91	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	3	309	KC2	C3C-C2C	5.90	1.49	1.37
45	13	309	KC2	C2A-C3A	5.90	1.49	1.37
45	16	312	KC2	CHD-C4C	5.90	1.50	1.35
31	b	605	CLA	C4B-NB	5.90	1.40	1.35
45	4	308	KC2	CHD-C4C	5.90	1.50	1.35
45	5	310	KC2	CHD-C4C	5.89	1.50	1.35
31	A	403	CLA	C4B-NB	5.88	1.40	1.35
31	9	313	CLA	C4B-NB	5.88	1.40	1.35
42	5	313	KC1	C4D-ND	5.88	1.40	1.35
45	4	310	KC2	CHD-C4C	5.87	1.50	1.35
45	2	310	KC2	C1A-NA	5.87	1.49	1.38
45	15	310	KC2	CHD-C4C	5.86	1.50	1.35
45	14	308	KC2	CHD-C4C	5.86	1.50	1.35
45	12	309	KC2	CHD-C4C	5.86	1.50	1.35
45	8	308	KC2	CHD-C4C	5.86	1.50	1.35
42	2	313	KC1	C1A-NA	5.86	1.49	1.38
45	9	309	KC2	CHD-C4C	5.85	1.50	1.35
42	16	301	KC1	C1A-NA	5.85	1.49	1.38
31	d	401	CLA	C4B-NB	5.85	1.40	1.35
45	4	310	KC2	C4D-ND	5.85	1.40	1.35
45	19	309	KC2	CHD-C4C	5.84	1.49	1.35
45	19	309	KC2	C3C-C2C	5.83	1.49	1.37
43	3	304	A86	O4-C38	5.83	1.48	1.35
45	14	310	KC2	CHD-C4C	5.82	1.49	1.35
31	D	401	CLA	C4B-NB	5.82	1.40	1.35
42	8	313	KC1	C2A-C3A	5.82	1.49	1.37
42	18	313	KC1	C2A-C3A	5.82	1.49	1.37
31	5	307	CLA	C4B-NB	5.81	1.40	1.35
45	3	309	KC2	C2A-C3A	5.81	1.49	1.37
45	7	309	KC2	C3C-C2C	5.80	1.49	1.37
45	17	309	KC2	C2A-C3A	5.80	1.49	1.37
45	8	310	KC2	C1A-NA	5.80	1.49	1.38
45	12	311	KC2	CHD-C4C	5.80	1.49	1.35
45	11	309	KC2	C4D-ND	5.79	1.40	1.35
31	b	607	CLA	C4B-NB	5.79	1.40	1.35
45	3	311	KC2	C2A-C3A	5.79	1.49	1.37
42	19	314	KC1	C2A-C3A	5.79	1.49	1.37
31	B	602	CLA	C4B-NB	5.79	1.40	1.35
45	6	310	KC2	C3C-C2C	5.78	1.49	1.37
43	15	305	A86	O4-C38	5.78	1.48	1.35
45	7	311	KC2	C1A-NA	5.78	1.49	1.38
45	7	311	KC2	CHD-C4C	5.77	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	314	KC1	C2A-C3A	5.77	1.49	1.37
31	B	606	CLA	C4B-NB	5.76	1.40	1.35
45	14	310	KC2	C4D-ND	5.76	1.40	1.35
45	13	309	KC2	CHD-C4C	5.76	1.49	1.35
45	12	311	KC2	C3C-C2C	5.76	1.48	1.37
45	17	309	KC2	C3C-C2C	5.76	1.48	1.37
42	0	315	KC1	CHD-C4C	5.76	1.49	1.35
45	7	309	KC2	C2A-C3A	5.75	1.48	1.37
45	17	311	KC2	CHD-C4C	5.75	1.49	1.35
42	16	301	KC1	CHD-C4C	5.75	1.49	1.35
31	c	513	CLA	C4B-NB	5.75	1.40	1.35
31	b	603	CLA	C4B-NB	5.74	1.40	1.35
42	12	314	KC1	C4D-ND	5.73	1.40	1.35
45	16	310	KC2	C3C-C2C	5.73	1.48	1.37
45	6	312	KC2	C1A-NA	5.73	1.49	1.38
45	3	311	KC2	C1A-NA	5.73	1.49	1.38
42	9	314	KC1	C2A-C3A	5.72	1.48	1.37
45	16	312	KC2	C2A-C3A	5.72	1.48	1.37
45	11	311	KC2	CHD-C4C	5.72	1.49	1.35
45	11	309	KC2	CHD-C4C	5.72	1.49	1.35
45	16	312	KC2	C1A-NA	5.72	1.49	1.38
45	3	311	KC2	CHD-C4C	5.72	1.49	1.35
42	19	314	KC1	CHD-C4C	5.72	1.49	1.35
45	14	308	KC2	C3C-C2C	5.71	1.48	1.37
42	9	314	KC1	CHD-C4C	5.71	1.49	1.35
45	9	309	KC2	C3C-C2C	5.71	1.48	1.37
42	1	314	KC1	CHD-C4C	5.70	1.49	1.35
45	16	312	KC2	C3C-C2C	5.70	1.48	1.37
43	11	302	A86	O4-C38	5.70	1.48	1.35
42	16	315	KC1	CHD-C4C	5.69	1.49	1.35
45	4	308	KC2	C3C-C2C	5.69	1.48	1.37
45	6	312	KC2	C2A-C3A	5.69	1.48	1.37
31	B	612	CLA	C4B-NB	5.69	1.40	1.35
42	3	314	KC1	C1A-NA	5.69	1.49	1.38
45	4	310	KC2	C3C-C2C	5.68	1.48	1.37
42	5	313	KC1	CHD-C4C	5.68	1.49	1.35
31	C	513	CLA	C4B-NB	5.68	1.40	1.35
42	11	314	KC1	C4D-ND	5.68	1.40	1.35
42	4	313	KC1	CHD-C4C	5.68	1.49	1.35
45	8	310	KC2	CHD-C4C	5.68	1.49	1.35
45	6	312	KC2	C3C-C2C	5.68	1.48	1.37
42	11	314	KC1	CHD-C4C	5.67	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	406	CLA	C4B-NB	5.67	1.40	1.35
35	d	406	PL9	C7-C3	-5.67	1.45	1.51
45	14	310	KC2	C3C-C2C	5.67	1.48	1.37
45	19	309	KC2	C1A-NA	5.66	1.49	1.38
43	2	302	A86	O4-C38	5.66	1.48	1.35
45	2	308	KC2	C2A-C3A	5.66	1.48	1.37
42	12	314	KC1	C1A-NA	5.66	1.49	1.38
31	19	313	CLA	C4B-NB	5.66	1.40	1.35
42	13	314	KC1	C1A-NA	5.65	1.49	1.38
45	9	309	KC2	C1A-NA	5.65	1.49	1.38
31	b	613	CLA	C4B-NB	5.65	1.40	1.35
45	3	311	KC2	C3C-C2C	5.65	1.48	1.37
42	14	313	KC1	C4D-ND	5.65	1.40	1.35
43	11	320	A86	O4-C38	5.64	1.48	1.35
45	13	309	KC2	C3C-C2C	5.64	1.48	1.37
42	14	313	KC1	CHD-C4C	5.64	1.49	1.35
45	12	311	KC2	C2A-C3A	5.63	1.48	1.37
45	2	310	KC2	C3C-C2C	5.62	1.48	1.37
45	17	311	KC2	C3C-C2C	5.62	1.48	1.37
45	4	310	KC2	C1A-NA	5.62	1.49	1.38
42	p	609	KC1	CHD-C4C	5.61	1.49	1.35
45	18	310	KC2	CHD-C4C	5.61	1.49	1.35
43	10	306	A86	O4-C38	5.61	1.47	1.35
45	11	309	KC2	C1A-NA	5.60	1.49	1.38
45	19	309	KC2	C2A-C3A	5.60	1.48	1.37
45	4	310	KC2	C2A-C3A	5.60	1.48	1.37
45	14	310	KC2	C2A-C3A	5.59	1.48	1.37
42	11	314	KC1	C2A-C3A	5.59	1.48	1.37
45	1	311	KC2	CHD-C4C	5.59	1.49	1.35
43	15	301	A86	O4-C38	5.59	1.47	1.35
42	19	314	KC1	C1A-NA	5.59	1.48	1.38
35	D	406	PL9	C7-C3	-5.59	1.45	1.51
45	0	310	KC2	C1A-NA	5.58	1.48	1.38
45	1	311	KC2	C1A-NA	5.58	1.48	1.38
42	P	609	KC1	CHD-C4C	5.58	1.49	1.35
45	6	310	KC2	C2A-C3A	5.58	1.48	1.37
31	A	406	CLA	C4B-NB	5.58	1.40	1.35
42	16	301	KC1	C3C-C2C	5.58	1.48	1.36
42	10	315	KC1	C2A-C3A	5.57	1.48	1.37
45	7	311	KC2	C3C-C2C	5.57	1.48	1.37
45	16	310	KC2	C2A-C3A	5.57	1.48	1.37
42	7	314	KC1	C1A-NA	5.57	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	9	309	KC2	C2A-C3A	5.56	1.48	1.37
42	2	313	KC1	CHD-C4C	5.56	1.49	1.35
45	11	311	KC2	C1A-NA	5.56	1.48	1.38
45	12	309	KC2	C2A-C3A	5.55	1.48	1.37
42	9	314	KC1	C1A-NA	5.55	1.48	1.38
43	9	301	A86	O4-C38	5.55	1.47	1.35
42	P	609	KC1	C2A-C3A	5.54	1.48	1.37
43	1	304	A86	O4-C38	5.54	1.47	1.35
45	12	309	KC2	C3C-C2C	5.54	1.48	1.37
43	7	305	A86	O4-C38	5.53	1.47	1.35
42	16	301	KC1	C4D-ND	5.53	1.40	1.35
45	7	311	KC2	C2A-C3A	5.53	1.48	1.37
45	10	310	KC2	CHD-C4C	5.52	1.49	1.35
45	1	309	KC2	C3C-C2C	5.52	1.48	1.37
42	12	314	KC1	CHD-C4C	5.51	1.49	1.35
45	12	309	KC2	C1A-NA	5.51	1.48	1.38
45	0	310	KC2	C3C-C2C	5.51	1.48	1.37
43	0	306	A86	O4-C38	5.51	1.47	1.35
45	8	308	KC2	C2A-C3A	5.50	1.48	1.37
42	7	314	KC1	CHD-C4C	5.50	1.49	1.35
43	17	306	A86	O4-C38	5.50	1.47	1.35
45	10	310	KC2	C3C-C2C	5.50	1.48	1.37
43	6	302	A86	O4-C38	5.50	1.47	1.35
43	17	302	A86	C30-C29	-5.49	1.22	1.32
42	p	609	KC1	C2A-C3A	5.49	1.48	1.37
45	18	308	KC2	C2A-C3A	5.49	1.48	1.37
45	14	308	KC2	C2A-C3A	5.48	1.48	1.37
45	13	309	KC2	C1A-NA	5.48	1.48	1.38
45	14	310	KC2	C1A-NA	5.48	1.48	1.38
45	2	310	KC2	C2A-C3A	5.48	1.48	1.37
42	9	314	KC1	C3C-C2C	5.47	1.48	1.36
45	10	310	KC2	C1A-NA	5.47	1.48	1.38
45	0	310	KC2	C2A-C3A	5.47	1.48	1.37
43	12	301	A86	O4-C38	5.47	1.47	1.35
45	5	310	KC2	C3C-C2C	5.47	1.48	1.37
45	0	310	KC2	CHD-C4C	5.46	1.49	1.35
42	18	313	KC1	CHD-C4C	5.46	1.49	1.35
43	2	305	A86	O4-C38	5.46	1.47	1.35
45	8	310	KC2	C2A-C3A	5.46	1.48	1.37
43	13	306	A86	O4-C38	5.45	1.47	1.35
45	5	308	KC2	C3C-C2C	5.44	1.48	1.37
45	15	308	KC2	C2A-C3A	5.44	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	314	KC1	C3C-C2C	5.44	1.48	1.36
43	7	301	A86	O4-C38	5.44	1.47	1.35
42	1	314	KC1	C3C-C2C	5.44	1.48	1.36
42	7	314	KC1	C3C-C2C	5.44	1.48	1.36
45	18	308	KC2	C3C-C2C	5.43	1.48	1.37
45	15	308	KC2	C3C-C2C	5.43	1.48	1.37
42	10	315	KC1	CHD-C4C	5.43	1.48	1.35
42	6	315	KC1	CHD-C4C	5.43	1.48	1.35
42	16	301	KC1	C2A-C3A	5.43	1.48	1.37
45	4	308	KC2	C2A-C3A	5.43	1.48	1.37
42	6	315	KC1	C1A-NA	5.42	1.48	1.38
43	9	305	A86	O1-C20	-5.42	1.38	1.46
42	5	313	KC1	C3C-C2C	5.42	1.48	1.36
43	14	305	A86	O4-C38	5.42	1.47	1.35
43	17	302	A86	O4-C38	5.41	1.47	1.35
43	19	305	A86	O1-C20	-5.41	1.38	1.46
45	13	311	KC2	C3B-C2B	5.41	1.48	1.37
43	8	305	A86	O4-C38	5.40	1.47	1.35
42	2	313	KC1	C3C-C2C	5.40	1.48	1.36
42	12	314	KC1	C3C-C2C	5.40	1.48	1.36
42	P	609	KC1	C3C-C2C	5.39	1.48	1.36
45	8	310	KC2	C3C-C2C	5.39	1.48	1.37
43	10	301	A86	O4-C38	5.39	1.47	1.35
43	12	303	A86	O4-C38	5.39	1.47	1.35
43	2	301	A86	O4-C38	5.39	1.47	1.35
42	p	609	KC1	C3C-C2C	5.39	1.48	1.36
43	13	301	A86	O4-C38	5.39	1.47	1.35
45	15	310	KC2	C3C-C2C	5.39	1.48	1.37
45	13	311	KC2	C1A-NA	5.38	1.48	1.38
42	13	314	KC1	CHD-C4C	5.38	1.48	1.35
43	17	316	A86	O4-C38	5.38	1.47	1.35
45	18	310	KC2	C2A-C3A	5.37	1.48	1.37
42	17	314	KC1	CHD-C4C	5.37	1.48	1.35
42	4	313	KC1	C2A-C3A	5.37	1.48	1.37
42	9	314	KC1	C3B-C2B	5.36	1.48	1.37
43	0	301	A86	O4-C38	5.36	1.47	1.35
45	10	310	KC2	C2A-C3A	5.36	1.48	1.37
43	19	302	A86	O4-C38	5.35	1.47	1.35
42	16	315	KC1	C3B-C2B	5.35	1.48	1.37
42	19	314	KC1	C3B-C2B	5.35	1.48	1.37
43	2	304	A86	O4-C38	5.35	1.47	1.35
45	18	310	KC2	C3C-C2C	5.35	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	5	301	A86	O4-C38	5.35	1.47	1.35
45	15	310	KC2	C1A-NA	5.35	1.48	1.38
43	4	302	A86	O4-C38	5.35	1.47	1.35
43	10	318	A86	O4-C38	5.35	1.47	1.35
43	19	301	A86	O4-C38	5.34	1.47	1.35
42	6	315	KC1	C3B-C2B	5.34	1.48	1.37
42	12	314	KC1	C2A-C3A	5.33	1.48	1.37
45	15	308	KC2	C1A-NA	5.33	1.48	1.38
42	11	314	KC1	C3C-C2C	5.32	1.48	1.36
43	17	304	A86	O4-C38	5.32	1.47	1.35
42	6	315	KC1	C3C-C2C	5.32	1.48	1.36
43	19	304	A86	O4-C38	5.32	1.47	1.35
42	5	313	KC1	C2A-C3A	5.32	1.48	1.37
42	13	314	KC1	C3C-C2C	5.32	1.48	1.36
31	B	611	CLA	CMC-C2C	-5.32	1.39	1.50
42	5	313	KC1	C3D-C2D	5.31	1.49	1.39
45	17	311	KC2	C2A-C3A	5.31	1.48	1.37
45	5	308	KC2	C2A-C3A	5.31	1.48	1.37
43	6	305	A86	O1-C20	-5.30	1.38	1.46
42	3	314	KC1	C3B-C2B	5.30	1.48	1.37
42	16	301	KC1	C3D-C2D	5.30	1.48	1.39
43	16	306	A86	O4-C38	5.30	1.47	1.35
43	3	302	A86	O4-C38	5.29	1.47	1.35
42	0	315	KC1	C3C-C2C	5.29	1.48	1.36
31	b	612	CLA	CMC-C2C	-5.28	1.39	1.50
45	11	309	KC2	C3C-C2C	5.28	1.48	1.37
42	11	314	KC1	C1A-NA	5.28	1.48	1.38
42	18	313	KC1	C1A-NA	5.28	1.48	1.38
43	13	303	A86	O4-C38	5.28	1.47	1.35
42	3	314	KC1	C3C-C2C	5.28	1.48	1.36
45	15	308	KC2	O2D-CGD	5.28	1.46	1.33
43	1	320	A86	O4-C38	5.28	1.47	1.35
42	17	314	KC1	C3C-C2C	5.27	1.47	1.36
45	8	308	KC2	C3C-C2C	5.27	1.47	1.37
45	1	311	KC2	C2A-C3A	5.27	1.47	1.37
45	1	311	KC2	C3C-C2C	5.25	1.47	1.37
42	4	313	KC1	C3C-C2C	5.25	1.47	1.36
43	11	319	A86	O4-C38	5.25	1.47	1.35
42	5	313	KC1	OBD-CAD	5.25	1.29	1.22
42	16	315	KC1	C3C-C2C	5.25	1.47	1.36
43	6	305	A86	O4-C38	5.25	1.47	1.35
45	5	308	KC2	O2D-CGD	5.25	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	0	315	KC1	C2A-C3A	5.25	1.47	1.37
42	14	313	KC1	C2A-C3A	5.24	1.47	1.37
42	17	314	KC1	O2D-CGD	5.24	1.46	1.33
42	14	313	KC1	C3C-C2C	5.24	1.47	1.36
45	3	309	KC2	O2D-CGD	5.24	1.46	1.33
45	5	310	KC2	C2A-C3A	5.22	1.47	1.37
45	11	311	KC2	C3C-C2C	5.22	1.47	1.37
43	p	613	A86	O4-C38	5.22	1.47	1.35
45	19	309	KC2	C3B-C2B	5.22	1.47	1.37
43	17	305	A86	O4-C38	5.21	1.47	1.35
45	16	310	KC2	C3D-C2D	5.21	1.48	1.39
43	P	613	A86	O4-C38	5.19	1.46	1.35
43	16	306	A86	O1-C20	-5.19	1.38	1.46
42	18	313	KC1	C3C-C2C	5.19	1.47	1.36
42	13	314	KC1	OBD-CAD	5.19	1.29	1.22
45	2	308	KC2	C3B-C2B	5.19	1.47	1.37
45	5	310	KC2	C1A-NA	5.19	1.48	1.38
42	13	314	KC1	C3B-C2B	5.19	1.47	1.37
43	14	303	A86	O4-C38	5.19	1.46	1.35
45	17	309	KC2	C3B-C2B	5.19	1.47	1.37
45	6	312	KC2	O2D-CGD	5.19	1.45	1.33
45	16	312	KC2	O2D-CGD	5.19	1.45	1.33
45	3	311	KC2	O2D-CGD	5.18	1.45	1.33
42	6	315	KC1	OBD-CAD	5.18	1.29	1.22
42	10	315	KC1	C3C-C2C	5.18	1.47	1.36
45	7	309	KC2	C3B-C2B	5.18	1.47	1.37
45	9	309	KC2	C3B-C2B	5.17	1.47	1.37
45	2	308	KC2	C3D-C2D	5.17	1.48	1.39
43	7	303	A86	O4-C38	5.17	1.46	1.35
42	18	313	KC1	C3B-C2B	5.17	1.47	1.37
45	13	311	KC2	C3D-C2D	5.17	1.48	1.39
43	11	304	A86	O4-C38	5.17	1.46	1.35
45	16	310	KC2	O2D-CGD	5.16	1.45	1.33
45	3	309	KC2	C3D-C2D	5.16	1.48	1.39
45	5	308	KC2	C1A-NA	5.16	1.48	1.38
42	13	314	KC1	C2A-C3A	5.16	1.47	1.37
43	5	305	A86	O4-C38	5.16	1.46	1.35
45	13	309	KC2	O2D-CGD	5.15	1.45	1.33
45	2	308	KC2	C1A-NA	5.15	1.48	1.38
45	17	311	KC2	O2D-CGD	5.15	1.45	1.33
45	13	311	KC2	O2D-CGD	5.15	1.45	1.33
45	11	311	KC2	C2A-C3A	5.15	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	16	307	A86	O4-C38	5.15	1.46	1.35
45	2	308	KC2	O2D-CGD	5.15	1.45	1.33
45	6	310	KC2	C3D-C2D	5.15	1.48	1.39
45	6	310	KC2	O2D-CGD	5.15	1.45	1.33
45	6	310	KC2	C3B-C2B	5.15	1.47	1.37
45	1	309	KC2	C2A-C3A	5.14	1.47	1.37
42	0	315	KC1	C1A-NA	5.14	1.48	1.38
31	P	606	CLA	C2A-C1A	-5.13	1.40	1.52
43	0	302	A86	O4-C38	5.13	1.46	1.35
45	2	310	KC2	O2D-CGD	5.13	1.45	1.33
45	12	309	KC2	C3B-C2B	5.13	1.47	1.37
45	14	308	KC2	C1A-NA	5.13	1.48	1.38
45	7	309	KC2	C3D-C2D	5.13	1.48	1.39
45	3	311	KC2	C3B-C2B	5.12	1.47	1.37
45	16	310	KC2	C1A-NA	5.12	1.48	1.38
45	4	310	KC2	C3B-C2B	5.12	1.47	1.37
45	14	310	KC2	C3B-C2B	5.12	1.47	1.37
31	p	606	CLA	C2A-C1A	-5.11	1.40	1.52
43	4	304	A86	O4-C38	5.11	1.46	1.35
42	7	314	KC1	O2D-CGD	5.11	1.45	1.33
45	17	309	KC2	C1A-NA	5.10	1.48	1.38
45	12	309	KC2	O2D-CGD	5.10	1.45	1.33
43	19	303	A86	O4-C38	5.10	1.46	1.35
45	6	310	KC2	C1A-NA	5.10	1.48	1.38
42	2	313	KC1	C3B-C2B	5.10	1.47	1.37
45	3	309	KC2	C3B-C2B	5.10	1.47	1.37
43	13	305	A86	O4-C38	5.10	1.46	1.35
45	16	310	KC2	C3B-C2B	5.10	1.47	1.37
35	D	406	PL9	C6-C1	-5.09	1.39	1.48
45	11	309	KC2	C2A-C3A	5.09	1.47	1.37
42	9	314	KC1	O2D-CGD	5.09	1.45	1.33
42	p	609	KC1	C1A-NA	5.09	1.48	1.38
45	9	309	KC2	O2D-CGD	5.09	1.45	1.33
42	8	313	KC1	C3C-C2C	5.09	1.47	1.36
45	15	310	KC2	C2A-C3A	5.09	1.47	1.37
42	3	314	KC1	CHD-C4C	5.09	1.48	1.35
43	14	304	A86	O4-C38	5.09	1.46	1.35
42	19	314	KC1	O2D-CGD	5.09	1.45	1.33
45	17	309	KC2	C3D-C2D	5.08	1.48	1.39
43	15	304	A86	O4-C38	5.08	1.46	1.35
45	7	309	KC2	C1A-NA	5.08	1.47	1.38
42	3	314	KC1	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	17	309	KC2	O2D-CGD	5.08	1.45	1.33
45	4	308	KC2	C3B-C2B	5.08	1.47	1.37
42	8	313	KC1	C1A-NA	5.07	1.47	1.38
35	d	406	PL9	C6-C1	-5.07	1.39	1.48
42	14	313	KC1	C3B-C2B	5.07	1.47	1.37
42	14	313	KC1	O2D-CGD	5.07	1.45	1.33
45	7	309	KC2	O2D-CGD	5.07	1.45	1.33
43	9	302	A86	O4-C38	5.06	1.46	1.35
45	4	308	KC2	C1A-NA	5.06	1.47	1.38
42	16	315	KC1	CHB-C1B	5.06	1.48	1.38
43	9	304	A86	O4-C38	5.06	1.46	1.35
43	15	303	A86	O4-C38	5.06	1.46	1.35
42	16	301	KC1	C3B-C2B	5.05	1.47	1.37
45	19	309	KC2	O2D-CGD	5.05	1.45	1.33
45	3	309	KC2	C1A-NA	5.05	1.47	1.38
45	14	308	KC2	C3B-C2B	5.04	1.47	1.37
43	1	302	A86	O4-C38	5.04	1.46	1.35
42	P	609	KC1	C1A-NA	5.04	1.47	1.38
42	4	313	KC1	C3B-C2B	5.04	1.47	1.37
42	7	314	KC1	CHB-C1B	5.04	1.48	1.38
45	7	311	KC2	O2D-CGD	5.04	1.45	1.33
42	4	313	KC1	O2D-CGD	5.03	1.45	1.33
45	16	312	KC2	C3B-C2B	5.03	1.47	1.37
43	5	304	A86	O4-C38	5.03	1.46	1.35
42	2	313	KC1	O2D-CGD	5.03	1.45	1.33
43	8	304	A86	O4-C38	5.03	1.46	1.35
42	17	314	KC1	C3B-C2B	5.03	1.47	1.37
45	11	311	KC2	C3B-C2B	5.03	1.47	1.37
45	13	309	KC2	C3B-C2B	5.03	1.47	1.37
42	12	314	KC1	O2D-CGD	5.02	1.45	1.33
45	18	310	KC2	O2D-CGD	5.02	1.45	1.33
43	8	301	A86	C32-C31	5.02	1.62	1.54
43	16	303	A86	C30-C29	-5.02	1.23	1.32
43	9	305	A86	O4-C38	5.01	1.46	1.35
43	17	301	A86	O4-C38	5.01	1.46	1.35
43	18	301	A86	O4-C38	5.01	1.46	1.35
45	2	308	KC2	CHC-C4B	5.00	1.48	1.38
42	p	609	KC1	O2D-CGD	5.00	1.45	1.33
45	11	309	KC2	O2D-CGD	5.00	1.45	1.33
42	P	609	KC1	O2D-CGD	5.00	1.45	1.33
45	8	310	KC2	O2D-CGD	5.00	1.45	1.33
42	11	314	KC1	C3B-C2B	4.99	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	313	KC1	C1A-NA	4.99	1.47	1.38
43	14	301	A86	O4-C38	4.98	1.46	1.35
45	1	311	KC2	C3B-C2B	4.98	1.47	1.37
45	1	309	KC2	C3B-C2B	4.98	1.47	1.37
45	15	308	KC2	C3B-C2B	4.98	1.47	1.37
43	10	302	A86	O4-C38	4.98	1.46	1.35
42	5	313	KC1	C3B-C2B	4.98	1.47	1.37
45	4	308	KC2	O2D-CGD	4.98	1.45	1.33
43	6	306	A86	O4-C38	4.98	1.46	1.35
43	11	305	A86	O4-C38	4.97	1.46	1.35
42	16	315	KC1	OBD-CAD	4.97	1.29	1.22
43	5	302	A86	O4-C38	4.97	1.46	1.35
45	14	308	KC2	O2D-CGD	4.97	1.45	1.33
43	2	303	A86	O4-C38	4.96	1.46	1.35
42	7	314	KC1	C3B-C2B	4.96	1.47	1.37
43	7	302	A86	O4-C38	4.96	1.46	1.35
45	18	308	KC2	O2D-CGD	4.96	1.45	1.33
45	11	309	KC2	C3B-C2B	4.95	1.47	1.37
42	19	314	KC1	CHC-C4B	4.95	1.48	1.38
45	6	312	KC2	C3B-C2B	4.95	1.47	1.37
43	19	306	A86	O4-C38	4.95	1.46	1.35
42	1	314	KC1	C1A-NA	4.95	1.47	1.38
45	1	309	KC2	O2D-CGD	4.94	1.45	1.33
42	8	313	KC1	C3B-C2B	4.94	1.47	1.37
45	13	309	KC2	C3D-C2D	4.94	1.48	1.39
42	1	314	KC1	O2D-CGD	4.94	1.45	1.33
42	6	315	KC1	CHB-C1B	4.93	1.48	1.38
42	0	315	KC1	C3B-C2B	4.93	1.47	1.37
45	17	309	KC2	CHC-C4B	4.93	1.48	1.38
43	4	305	A86	O4-C38	4.93	1.46	1.35
45	8	308	KC2	O2D-CGD	4.93	1.45	1.33
43	4	301	A86	O4-C38	4.93	1.46	1.35
45	7	311	KC2	C3B-C2B	4.92	1.47	1.37
43	3	305	A86	O1-C20	-4.92	1.39	1.46
43	9	306	A86	O4-C38	4.92	1.46	1.35
42	13	314	KC1	O2D-CGD	4.91	1.45	1.33
42	3	314	KC1	CHB-C1B	4.91	1.47	1.38
45	1	311	KC2	O2D-CGD	4.90	1.45	1.33
31	p	606	CLA	C4B-NB	4.90	1.39	1.35
43	16	303	A86	O4-C38	4.90	1.46	1.35
42	9	314	KC1	CHC-C4B	4.90	1.47	1.38
45	12	311	KC2	C3B-C2B	4.90	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	15	310	KC2	C3B-C2B	4.90	1.47	1.37
42	12	314	KC1	C3B-C2B	4.90	1.47	1.37
43	19	305	A86	O4-C38	4.90	1.46	1.35
42	10	315	KC1	C3B-C2B	4.89	1.47	1.37
45	2	310	KC2	C3B-C2B	4.89	1.47	1.37
42	11	314	KC1	CHB-C1B	4.89	1.47	1.38
45	5	308	KC2	C3D-C2D	4.89	1.48	1.39
45	17	311	KC2	C3B-C2B	4.89	1.47	1.37
43	1	305	A86	O4-C38	4.89	1.46	1.35
45	17	311	KC2	C3D-C2D	4.88	1.48	1.39
45	7	309	KC2	CHC-C4B	4.88	1.47	1.38
45	1	309	KC2	C3D-C2D	4.88	1.48	1.39
43	11	306	A86	O4-C38	4.87	1.46	1.35
43	9	303	A86	O4-C38	4.86	1.46	1.35
42	8	313	KC1	O2D-CGD	4.86	1.45	1.33
42	17	314	KC1	C3D-C2D	4.86	1.48	1.39
45	12	309	KC2	CHC-C4B	4.86	1.47	1.38
45	6	310	KC2	CHC-C4B	4.86	1.47	1.38
42	11	314	KC1	O2D-CGD	4.85	1.45	1.33
45	12	309	KC2	C3D-C2D	4.85	1.48	1.39
42	19	314	KC1	C3D-C2D	4.85	1.48	1.39
42	9	314	KC1	C3D-C2D	4.85	1.48	1.39
45	19	309	KC2	C3D-C2D	4.85	1.48	1.39
45	11	311	KC2	O2D-CGD	4.85	1.45	1.33
43	8	303	A86	O4-C38	4.85	1.46	1.35
42	1	314	KC1	C3B-C2B	4.85	1.47	1.37
31	P	606	CLA	C4B-NB	4.84	1.39	1.35
43	7	306	A86	O4-C38	4.84	1.46	1.35
43	18	305	A86	O4-C38	4.84	1.46	1.35
45	9	309	KC2	C3D-C2D	4.84	1.48	1.39
43	1	303	A86	O1-C20	-4.84	1.39	1.46
42	7	314	KC1	OBD-CAD	4.84	1.29	1.22
45	2	310	KC2	C3D-C2D	4.84	1.48	1.39
45	15	308	KC2	C3D-C2D	4.83	1.48	1.39
45	18	308	KC2	C1A-NA	4.83	1.47	1.38
43	6	307	A86	O4-C38	4.82	1.46	1.35
43	1	306	A86	O4-C38	4.82	1.46	1.35
43	6	303	A86	O4-C38	4.82	1.46	1.35
42	P	609	KC1	C3B-C2B	4.82	1.47	1.37
45	12	311	KC2	O2D-CGD	4.82	1.45	1.33
43	3	301	A86	O4-C38	4.82	1.46	1.35
45	7	309	KC2	CHB-C1B	4.82	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	5	313	KC1	O2D-CGD	4.82	1.45	1.33
45	16	310	KC2	CHC-C4B	4.82	1.47	1.38
43	5	301	A86	C33-C34	4.82	1.60	1.51
45	17	309	KC2	CHB-C1B	4.81	1.47	1.38
42	1	314	KC1	C3D-C2D	4.81	1.48	1.39
45	5	308	KC2	C3B-C2B	4.81	1.47	1.37
42	p	609	KC1	C3B-C2B	4.81	1.47	1.37
45	5	310	KC2	C3D-C2D	4.81	1.48	1.39
43	12	305	A86	O4-C38	4.81	1.46	1.35
43	12	304	A86	O4-C38	4.81	1.46	1.35
42	9	314	KC1	CHB-C1B	4.81	1.47	1.38
42	16	315	KC1	O2D-CGD	4.81	1.44	1.33
45	15	310	KC2	C3D-C2D	4.81	1.48	1.39
45	3	309	KC2	CHC-C4B	4.81	1.47	1.38
43	16	302	A86	O4-C38	4.81	1.46	1.35
45	12	311	KC2	C3D-C2D	4.80	1.48	1.39
45	17	311	KC2	OBD-CAD	4.80	1.29	1.22
45	18	308	KC2	C3B-C2B	4.80	1.47	1.37
43	14	302	A86	O1-C20	-4.80	1.39	1.46
43	5	318	A86	O4-C38	4.80	1.46	1.35
43	0	303	A86	O4-C38	4.80	1.46	1.35
43	11	303	A86	O1-C20	-4.79	1.39	1.46
45	14	308	KC2	C3D-C2D	4.79	1.48	1.39
45	7	311	KC2	OBD-CAD	4.79	1.29	1.22
43	14	302	A86	O4-C38	4.79	1.46	1.35
45	4	310	KC2	O2D-CGD	4.79	1.44	1.33
31	16	314	CLA	CMD-C2D	-4.78	1.40	1.50
42	1	314	KC1	CHB-C1B	4.78	1.47	1.38
45	5	310	KC2	C3B-C2B	4.78	1.47	1.37
42	9	314	KC1	OBD-CAD	4.78	1.29	1.22
42	13	314	KC1	CHC-C4B	4.78	1.47	1.38
45	16	312	KC2	C3D-C2D	4.78	1.48	1.39
42	11	314	KC1	CHC-C4B	4.78	1.47	1.38
45	8	308	KC2	C3B-C2B	4.78	1.47	1.37
42	14	313	KC1	C3D-C2D	4.78	1.48	1.39
43	13	304	A86	O1-C20	-4.77	1.39	1.46
45	14	310	KC2	O2D-CGD	4.77	1.44	1.33
45	8	308	KC2	C1A-NA	4.77	1.47	1.38
42	0	315	KC1	C3D-C2D	4.77	1.48	1.39
45	6	312	KC2	C3D-C2D	4.77	1.48	1.39
45	13	311	KC2	CHB-C1B	4.77	1.47	1.38
42	17	314	KC1	CHB-C1B	4.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	10	303	A86	O4-C38	4.76	1.46	1.35
42	19	314	KC1	CHB-C1B	4.76	1.47	1.38
45	16	312	KC2	CHB-C1B	4.76	1.47	1.38
43	13	302	A86	O4-C38	4.76	1.45	1.35
45	7	311	KC2	C3D-C2D	4.76	1.48	1.39
45	18	310	KC2	C3B-C2B	4.76	1.46	1.37
45	13	311	KC2	CHC-C4B	4.76	1.47	1.38
45	14	308	KC2	CHC-C4B	4.76	1.47	1.38
45	4	308	KC2	CHC-C4B	4.75	1.47	1.38
43	12	302	A86	O4-C38	4.75	1.45	1.35
45	8	310	KC2	C3B-C2B	4.75	1.46	1.37
45	3	309	KC2	OBD-CAD	4.75	1.28	1.22
42	19	314	KC1	OBD-CAD	4.75	1.28	1.22
43	P	613	A86	O1-C20	-4.75	1.39	1.46
45	6	312	KC2	CHB-C1B	4.75	1.47	1.38
42	10	315	KC1	O2D-CGD	4.74	1.44	1.33
43	10	304	A86	O4-C38	4.74	1.45	1.35
45	3	311	KC2	C3D-C2D	4.74	1.47	1.39
43	p	613	A86	O1-C20	-4.74	1.39	1.46
43	18	302	A86	O4-C38	4.74	1.45	1.35
45	3	311	KC2	OBD-CAD	4.73	1.28	1.22
42	6	315	KC1	O2D-CGD	4.73	1.44	1.33
45	8	310	KC2	C3D-C2D	4.73	1.47	1.39
45	14	308	KC2	CHB-C1B	4.72	1.47	1.38
45	5	310	KC2	O2D-CGD	4.72	1.44	1.33
45	14	310	KC2	CHB-C1B	4.72	1.47	1.38
45	2	308	KC2	CHB-C1B	4.72	1.47	1.38
42	3	314	KC1	CHC-C4B	4.72	1.47	1.38
45	1	309	KC2	C1A-NA	4.72	1.47	1.38
45	19	309	KC2	CHC-C4B	4.72	1.47	1.38
45	14	310	KC2	CHC-C4B	4.71	1.47	1.38
43	15	302	A86	O4-C38	4.71	1.45	1.35
45	4	310	KC2	CHC-C4B	4.71	1.47	1.38
42	7	314	KC1	CHC-C4B	4.71	1.47	1.38
45	12	309	KC2	OBD-CAD	4.71	1.28	1.22
45	4	310	KC2	CHB-C1B	4.70	1.47	1.38
45	13	309	KC2	OBD-CAD	4.69	1.28	1.22
45	13	311	KC2	OBD-CAD	4.69	1.28	1.22
45	15	310	KC2	O2D-CGD	4.69	1.44	1.33
45	16	310	KC2	CHB-C1B	4.69	1.47	1.38
45	4	308	KC2	CHB-C1B	4.68	1.47	1.38
42	16	301	KC1	O2D-CGD	4.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	18	303	A86	O4-C38	4.68	1.45	1.35
45	4	308	KC2	C3D-C2D	4.68	1.47	1.39
43	0	304	A86	O4-C38	4.68	1.45	1.35
43	3	306	A86	O4-C38	4.67	1.45	1.35
45	9	309	KC2	CHC-C4B	4.67	1.47	1.38
45	13	309	KC2	CHC-C4B	4.67	1.47	1.38
42	1	314	KC1	OBD-CAD	4.67	1.28	1.22
45	18	310	KC2	C3D-C2D	4.67	1.47	1.39
43	4	303	A86	O4-C38	4.67	1.45	1.35
42	0	315	KC1	O2D-CGD	4.66	1.44	1.33
43	6	301	A86	O4-C38	4.66	1.45	1.35
45	5	308	KC2	CHB-C1B	4.66	1.47	1.38
42	12	314	KC1	CHB-C1B	4.66	1.47	1.38
45	9	309	KC2	CHB-C1B	4.66	1.47	1.38
42	6	315	KC1	CHC-C4B	4.66	1.47	1.38
42	16	301	KC1	CHC-C4B	4.66	1.47	1.38
45	13	309	KC2	CHB-C1B	4.66	1.47	1.38
42	4	313	KC1	C1A-NA	4.66	1.47	1.38
45	18	308	KC2	CHC-C4B	4.66	1.47	1.38
42	13	314	KC1	C3D-C2D	4.65	1.47	1.39
45	19	309	KC2	CHB-C1B	4.65	1.47	1.38
43	10	305	A86	O4-C38	4.64	1.45	1.35
43	16	305	A86	O4-C38	4.64	1.45	1.35
38	0	317	LMG	C4-C5	4.63	1.62	1.53
45	4	310	KC2	C3D-C2D	4.63	1.47	1.39
31	4	312	CLA	C4D-ND	-4.63	1.31	1.37
42	1	314	KC1	CHC-C4B	4.63	1.47	1.38
45	6	310	KC2	CHB-C1B	4.63	1.47	1.38
45	1	309	KC2	CHC-C4B	4.63	1.47	1.38
45	1	311	KC2	CHC-C4B	4.63	1.47	1.38
45	14	310	KC2	OBD-CAD	4.63	1.28	1.22
43	6	304	A86	O4-C38	4.63	1.45	1.35
42	4	313	KC1	C3D-C2D	4.62	1.47	1.39
45	11	309	KC2	C3D-C2D	4.62	1.47	1.39
43	1	319	A86	O1-C20	-4.62	1.39	1.46
45	8	308	KC2	CHC-C4B	4.62	1.47	1.38
42	3	314	KC1	OBD-CAD	4.61	1.28	1.22
45	3	311	KC2	CHB-C1B	4.61	1.47	1.38
42	13	314	KC1	CHB-C1B	4.61	1.47	1.38
45	11	309	KC2	CHC-C4B	4.60	1.47	1.38
45	14	310	KC2	C3D-C2D	4.60	1.47	1.39
42	14	313	KC1	CHC-C4B	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	17	316	A86	O1-C20	-4.60	1.39	1.46
42	4	313	KC1	CHC-C4B	4.59	1.47	1.38
42	2	313	KC1	OBD-CAD	4.59	1.28	1.22
42	16	301	KC1	OBD-CAD	4.59	1.28	1.22
43	8	302	A86	O4-C38	4.59	1.45	1.35
45	17	311	KC2	CHC-C4B	4.58	1.47	1.38
45	16	312	KC2	CHC-C4B	4.58	1.47	1.38
43	0	305	A86	O4-C38	4.58	1.45	1.35
42	16	301	KC1	CHB-C1B	4.57	1.47	1.38
45	1	311	KC2	C3D-C2D	4.57	1.47	1.39
43	5	303	A86	O4-C38	4.57	1.45	1.35
42	16	315	KC1	CHC-C4B	4.57	1.47	1.38
45	6	312	KC2	CHC-C4B	4.57	1.47	1.38
42	12	314	KC1	CHC-C4B	4.56	1.47	1.38
42	12	314	KC1	OBD-CAD	4.56	1.28	1.22
45	18	308	KC2	C3D-C2D	4.56	1.47	1.39
45	15	308	KC2	CHB-C1B	4.56	1.47	1.38
45	7	311	KC2	CHC-C4B	4.55	1.47	1.38
45	4	310	KC2	OBD-CAD	4.55	1.28	1.22
45	3	311	KC2	CHC-C4B	4.55	1.47	1.38
45	11	311	KC2	CHC-C4B	4.55	1.47	1.38
31	c	509	CLA	CMC-C2C	-4.54	1.41	1.50
42	18	313	KC1	CHC-C4B	4.54	1.47	1.38
45	12	311	KC2	OBD-CAD	4.54	1.28	1.22
38	10	319	LMG	C4-C5	4.54	1.62	1.53
45	2	308	KC2	OBD-CAD	4.53	1.28	1.22
42	5	313	KC1	CHC-C4B	4.53	1.47	1.38
45	0	310	KC2	C3B-C2B	4.53	1.46	1.37
31	15	311	CLA	CMB-C2B	-4.53	1.42	1.51
43	12	302	A86	O1-C20	-4.52	1.39	1.46
43	13	302	A86	O1-C20	-4.52	1.39	1.46
45	10	310	KC2	C3D-C2D	4.52	1.47	1.39
45	11	309	KC2	OBD-CAD	4.52	1.28	1.22
43	8	304	A86	C32-C31	-4.52	1.47	1.54
43	0	305	A86	O1-C20	-4.51	1.39	1.46
45	15	308	KC2	CHC-C4B	4.51	1.47	1.38
43	7	304	A86	O1-C20	-4.51	1.39	1.46
45	16	312	KC2	OBD-CAD	4.51	1.28	1.22
43	3	305	A86	O4-C38	4.51	1.45	1.35
45	10	310	KC2	O2D-CGD	4.51	1.44	1.33
45	2	310	KC2	CHC-C4B	4.50	1.47	1.38
45	11	311	KC2	C3D-C2D	4.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	v	201	HEM	C3C-C2C	-4.50	1.34	1.40
42	17	314	KC1	CHC-C4B	4.50	1.47	1.38
45	5	308	KC2	OBD-CAD	4.49	1.28	1.22
42	8	313	KC1	CHC-C4B	4.49	1.47	1.38
42	12	314	KC1	C3D-C2D	4.49	1.47	1.39
43	8	302	A86	O1-C20	-4.49	1.39	1.46
42	8	313	KC1	CHD-C4C	4.49	1.46	1.35
31	C	509	CLA	CMC-C2C	-4.49	1.41	1.50
42	2	313	KC1	CHC-C4B	4.48	1.47	1.38
42	2	313	KC1	CHB-C1B	4.48	1.47	1.38
45	6	312	KC2	OBD-CAD	4.47	1.28	1.22
42	18	313	KC1	O2D-CGD	4.47	1.44	1.33
43	1	319	A86	O4-C38	4.47	1.45	1.35
43	3	303	A86	O4-C38	4.47	1.45	1.35
42	2	313	KC1	C3D-C2D	4.46	1.47	1.39
45	3	309	KC2	CHB-C1B	4.46	1.47	1.38
45	10	310	KC2	C3B-C2B	4.46	1.46	1.37
41	V	201	HEM	C3C-C2C	-4.46	1.34	1.40
45	5	308	KC2	CHC-C4B	4.45	1.47	1.38
45	7	311	KC2	CHB-C1B	4.45	1.47	1.38
43	4	302	A86	C30-C29	-4.45	1.24	1.32
45	2	308	KC2	CBC-CAC	4.45	1.52	1.30
45	8	310	KC2	CHB-C1B	4.44	1.47	1.38
43	10	305	A86	O1-C20	-4.44	1.39	1.46
45	8	310	KC2	OBD-CAD	4.44	1.28	1.22
45	0	310	KC2	CHC-C4B	4.43	1.47	1.38
43	3	303	A86	O1-C20	-4.43	1.39	1.46
42	8	313	KC1	OBD-CAD	4.43	1.28	1.22
45	6	310	KC2	CBC-CAC	4.42	1.52	1.30
45	11	311	KC2	CHB-C1B	4.42	1.47	1.38
43	12	306	A86	O4-C38	4.42	1.45	1.35
45	16	310	KC2	CBC-CAC	4.42	1.52	1.30
45	1	311	KC2	OBD-CAD	4.42	1.28	1.22
45	2	310	KC2	OBD-CAD	4.41	1.28	1.22
45	15	308	KC2	OBD-CAD	4.41	1.28	1.22
45	7	309	KC2	CBC-CAC	4.41	1.52	1.30
45	17	309	KC2	CBC-CAC	4.41	1.52	1.30
42	18	313	KC1	OBD-CAD	4.40	1.28	1.22
45	13	311	KC2	CBC-CAC	4.40	1.52	1.30
45	0	310	KC2	C3D-C2D	4.40	1.47	1.39
45	3	309	KC2	CBC-CAC	4.39	1.52	1.30
45	2	310	KC2	CHB-C1B	4.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	15	308	KC2	CBC-CAC	4.39	1.52	1.30
45	16	310	KC2	OBD-CAD	4.39	1.28	1.22
42	5	313	KC1	CHB-C1B	4.39	1.46	1.38
45	11	311	KC2	OBD-CAD	4.39	1.28	1.22
43	18	304	A86	O4-C38	4.39	1.45	1.35
45	5	308	KC2	CBC-CAC	4.38	1.52	1.30
45	8	310	KC2	CHC-C4B	4.38	1.46	1.38
43	17	305	A86	O1-C20	-4.38	1.39	1.46
42	14	313	KC1	CHB-C1B	4.38	1.46	1.38
45	12	311	KC2	CHC-C4B	4.37	1.46	1.38
45	1	309	KC2	OBD-CAD	4.37	1.28	1.22
43	0	306	A86	C30-C29	-4.37	1.24	1.32
31	C	503	CLA	C4B-CHC	-4.37	1.28	1.41
42	P	609	KC1	CHB-C1B	4.36	1.46	1.38
45	18	310	KC2	CHC-C4B	4.36	1.46	1.38
45	0	310	KC2	O2D-CGD	4.35	1.43	1.33
31	C	509	CLA	C4D-ND	-4.35	1.31	1.37
45	10	310	KC2	CHC-C4B	4.35	1.46	1.38
45	7	311	KC2	CBC-CAC	4.35	1.51	1.30
31	c	503	CLA	C4B-CHC	-4.35	1.28	1.41
45	3	311	KC2	CBC-CAC	4.34	1.51	1.30
42	p	609	KC1	C3D-C2D	4.34	1.47	1.39
43	4	306	A86	O4-C38	4.34	1.45	1.35
45	8	308	KC2	CHB-C1B	4.33	1.46	1.38
45	0	310	KC2	C4D-ND	4.33	1.39	1.35
43	11	303	A86	O4-C38	4.33	1.45	1.35
45	12	309	KC2	CBC-CAC	4.33	1.51	1.30
31	c	509	CLA	C4D-ND	-4.33	1.31	1.37
45	4	308	KC2	CBC-CAC	4.33	1.51	1.30
45	17	311	KC2	CBC-CAC	4.33	1.51	1.30
45	14	308	KC2	CBC-CAC	4.33	1.51	1.30
42	p	609	KC1	CHB-C1B	4.32	1.46	1.38
45	18	310	KC2	OBD-CAD	4.32	1.28	1.22
42	4	313	KC1	CHB-C1B	4.32	1.46	1.38
45	2	310	KC2	CBC-CAC	4.32	1.51	1.30
45	12	311	KC2	CBC-CAC	4.32	1.51	1.30
45	12	311	KC2	CHB-C1B	4.32	1.46	1.38
45	8	308	KC2	C3D-C2D	4.31	1.47	1.39
43	17	303	A86	O4-C38	4.31	1.44	1.35
45	17	311	KC2	CHB-C1B	4.31	1.46	1.38
45	18	308	KC2	CBC-CAC	4.31	1.51	1.30
45	16	312	KC2	CBC-CAC	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	8	308	KC2	CBC-CAC	4.31	1.51	1.30
43	17	305	A86	C32-C31	-4.30	1.47	1.54
43	18	303	A86	C30-C29	-4.30	1.24	1.32
45	1	309	KC2	CHB-C1B	4.29	1.46	1.38
45	18	310	KC2	CBC-CAC	4.29	1.51	1.30
45	4	308	KC2	OBD-CAD	4.29	1.28	1.22
42	0	315	KC1	CHC-C4B	4.29	1.46	1.38
45	12	309	KC2	CHB-C1B	4.29	1.46	1.38
45	10	310	KC2	CHB-C1B	4.29	1.46	1.38
45	8	310	KC2	CBC-CAC	4.29	1.51	1.30
42	P	609	KC1	C3D-C2D	4.28	1.47	1.39
45	5	310	KC2	CBC-CAC	4.28	1.51	1.30
45	18	308	KC2	CHB-C1B	4.28	1.46	1.38
45	14	308	KC2	OBD-CAD	4.28	1.28	1.22
45	6	312	KC2	CBC-CAC	4.28	1.51	1.30
42	10	315	KC1	C3D-C2D	4.28	1.47	1.39
31	18	312	CLA	C4D-ND	-4.27	1.31	1.37
31	B	611	CLA	C4D-ND	-4.27	1.31	1.37
45	18	310	KC2	CHB-C1B	4.27	1.46	1.38
42	18	313	KC1	CHB-C1B	4.27	1.46	1.38
45	15	310	KC2	CHB-C1B	4.27	1.46	1.38
45	5	310	KC2	CHB-C1B	4.27	1.46	1.38
45	14	310	KC2	CBC-CAC	4.27	1.51	1.30
45	18	308	KC2	OBD-CAD	4.27	1.28	1.22
45	0	310	KC2	CHB-C1B	4.26	1.46	1.38
45	6	310	KC2	OBD-CAD	4.26	1.28	1.22
45	10	310	KC2	OBD-CAD	4.26	1.28	1.22
45	1	309	KC2	CBC-CAC	4.26	1.51	1.30
45	11	309	KC2	CBC-CAC	4.25	1.51	1.30
45	1	311	KC2	CHB-C1B	4.25	1.46	1.38
45	0	310	KC2	OBD-CAD	4.25	1.28	1.22
31	b	612	CLA	C4D-ND	-4.24	1.31	1.37
31	2	306	CLA	C1D-ND	4.24	1.43	1.37
45	13	309	KC2	CBC-CAC	4.24	1.51	1.30
42	0	315	KC1	CHB-C1B	4.24	1.46	1.38
45	4	310	KC2	CBC-CAC	4.24	1.51	1.30
31	B	604	CLA	C4D-ND	-4.24	1.31	1.37
31	B	604	CLA	CMB-C2B	-4.24	1.42	1.51
42	10	315	KC1	CHC-C4B	4.23	1.46	1.38
43	5	303	A86	O1-C20	-4.23	1.40	1.46
45	15	310	KC2	CBC-CAC	4.23	1.51	1.30
31	15	306	CLA	C1D-ND	4.22	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	15	310	KC2	CHC-C4B	4.22	1.46	1.38
31	b	605	CLA	C4D-ND	-4.22	1.31	1.37
42	8	313	KC1	C3D-C2D	4.21	1.47	1.39
43	P	611	A86	O4-C38	4.21	1.44	1.35
45	5	310	KC2	OBD-CAD	4.21	1.28	1.22
45	15	310	KC2	OBD-CAD	4.21	1.28	1.22
45	5	310	KC2	CHC-C4B	4.21	1.46	1.38
31	b	605	CLA	CMB-C2B	-4.20	1.42	1.51
45	19	309	KC2	CBC-CAC	4.19	1.51	1.30
45	11	311	KC2	CBC-CAC	4.19	1.51	1.30
45	9	309	KC2	CBC-CAC	4.19	1.51	1.30
42	11	314	KC1	C3D-C2D	4.18	1.46	1.39
43	13	304	A86	O4-C38	4.18	1.44	1.35
45	17	309	KC2	OBD-CAD	4.18	1.28	1.22
45	7	309	KC2	OBD-CAD	4.18	1.28	1.22
31	12	316	CLA	C1D-ND	4.17	1.42	1.37
43	15	303	A86	O1-C20	-4.17	1.40	1.46
43	18	305	A86	C30-C29	-4.17	1.25	1.32
43	p	611	A86	O4-C38	4.16	1.44	1.35
45	1	311	KC2	CBC-CAC	4.16	1.50	1.30
42	p	609	KC1	CHC-C4B	4.16	1.46	1.38
45	8	308	KC2	OBD-CAD	4.15	1.28	1.22
31	B	605	CLA	C4D-ND	-4.15	1.32	1.37
42	17	314	KC1	OBD-CAD	4.15	1.28	1.22
31	19	311	CLA	C1D-ND	4.15	1.42	1.37
31	C	503	CLA	C3B-C2B	-4.13	1.34	1.40
31	c	503	CLA	C3B-C2B	-4.13	1.34	1.40
31	b	606	CLA	C4D-ND	-4.13	1.32	1.37
31	D	404	CLA	C4D-ND	-4.12	1.32	1.37
31	6	314	CLA	CMB-C2B	-4.12	1.43	1.51
43	5	305	A86	C30-C29	-4.12	1.25	1.32
31	P	602	CLA	C4D-ND	-4.11	1.32	1.37
42	P	609	KC1	CHC-C4B	4.11	1.46	1.38
43	7	302	A86	O1-C20	-4.11	1.40	1.46
31	3	315	CLA	C1D-ND	4.11	1.42	1.37
31	5	306	CLA	C1D-ND	4.10	1.42	1.37
31	C	503	CLA	C4D-ND	-4.09	1.32	1.37
45	10	310	KC2	CBC-CAC	4.09	1.50	1.30
45	0	310	KC2	CBC-CAC	4.09	1.50	1.30
31	0	312	CLA	C1D-ND	4.09	1.42	1.37
31	13	312	CLA	C1D-ND	4.08	1.42	1.37
31	C	503	CLA	C4B-NB	4.07	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	602	CLA	C4D-ND	-4.07	1.32	1.37
43	8	305	A86	O1-C20	-4.07	1.40	1.46
43	3	303	A86	C30-C29	-4.07	1.25	1.32
31	c	503	CLA	C4D-ND	-4.07	1.32	1.37
31	d	404	CLA	C4D-ND	-4.06	1.32	1.37
31	16	316	CLA	C1D-ND	4.06	1.42	1.37
43	7	302	A86	C30-C29	-4.06	1.25	1.32
31	3	313	CLA	C4D-ND	-4.06	1.32	1.37
31	1	321	CLA	C4D-ND	-4.06	1.32	1.37
31	17	307	CLA	C1D-ND	4.06	1.42	1.37
43	2	302	A86	C30-C29	-4.05	1.25	1.32
43	5	302	A86	O1-C20	-4.05	1.40	1.46
43	13	302	A86	C30-C29	-4.05	1.25	1.32
31	13	315	CLA	C1D-ND	4.04	1.42	1.37
42	3	314	KC1	C3D-C2D	4.04	1.46	1.39
43	18	302	A86	C30-C29	-4.04	1.25	1.32
45	11	309	KC2	CHB-C1B	4.03	1.46	1.38
31	2	312	CLA	CMB-C2B	-4.03	1.43	1.51
45	10	310	KC2	C4D-ND	4.02	1.38	1.35
31	15	313	CLA	C1D-ND	4.01	1.42	1.37
45	9	309	KC2	OBD-CAD	4.01	1.27	1.22
31	9	315	CLA	C1D-ND	4.01	1.42	1.37
43	18	301	A86	O1-C20	-4.00	1.40	1.46
31	2	314	CLA	C1D-ND	4.00	1.42	1.37
43	0	303	A86	O1-C20	-4.00	1.40	1.46
31	10	312	CLA	C1D-ND	4.00	1.42	1.37
31	p	604	CLA	C4D-ND	-3.99	1.32	1.37
42	10	315	KC1	CHB-C1B	3.99	1.46	1.38
31	6	316	CLA	C1D-ND	3.99	1.42	1.37
43	10	306	A86	C30-C29	-3.99	1.25	1.32
31	c	503	CLA	C4B-NB	3.98	1.38	1.35
43	14	301	A86	C30-C29	-3.98	1.25	1.32
31	P	604	CLA	C4D-ND	-3.98	1.32	1.37
41	e	101	HEM	C3C-CAC	3.98	1.56	1.47
43	16	304	A86	O1-C20	-3.97	1.40	1.46
43	7	304	A86	O4-C38	3.96	1.44	1.35
31	12	307	CLA	C1D-ND	3.95	1.42	1.37
41	E	101	HEM	C3C-CAC	3.95	1.55	1.47
31	13	316	CLA	C1D-ND	3.94	1.42	1.37
43	3	304	A86	C32-C31	-3.94	1.47	1.54
31	0	314	CLA	C1D-ND	3.94	1.42	1.37
31	7	307	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	404	CLA	C4D-ND	-3.93	1.32	1.37
31	a	404	CLA	C4D-ND	-3.93	1.32	1.37
31	11	316	CLA	C1D-ND	3.93	1.42	1.37
31	19	315	CLA	C1D-ND	3.93	1.42	1.37
42	0	315	KC1	OBD-CAD	3.93	1.27	1.22
45	19	309	KC2	OBD-CAD	3.93	1.27	1.22
31	16	308	CLA	C1D-ND	3.92	1.42	1.37
31	5	307	CLA	C4D-ND	-3.92	1.32	1.37
31	19	310	CLA	C1D-ND	3.92	1.42	1.37
42	16	315	KC1	CHB-C4A	3.92	1.48	1.39
31	16	314	CLA	CMB-C2B	-3.91	1.43	1.51
31	9	307	CLA	C1D-ND	3.91	1.42	1.37
31	7	313	CLA	C4D-ND	-3.90	1.32	1.37
43	6	306	A86	C30-C29	-3.90	1.25	1.32
42	3	314	KC1	CHB-C4A	3.90	1.48	1.39
31	6	314	CLA	CMD-C2D	-3.90	1.42	1.50
42	P	609	KC1	OBD-CAD	3.90	1.27	1.22
31	C	513	CLA	C4D-ND	-3.89	1.32	1.37
31	6	308	CLA	C1D-ND	3.89	1.42	1.37
41	e	101	HEM	C3C-C2C	-3.89	1.35	1.40
38	15	315	LMG	C4-C5	3.89	1.61	1.53
43	6	303	A86	C30-C29	-3.89	1.25	1.32
31	c	508	CLA	C4D-ND	-3.88	1.32	1.37
31	11	313	CLA	C4D-ND	-3.88	1.32	1.37
42	p	609	KC1	OBD-CAD	3.88	1.27	1.22
31	15	312	CLA	CMB-C2B	-3.88	1.43	1.51
31	B	613	CLA	C4D-ND	-3.88	1.32	1.37
31	9	310	CLA	C1D-ND	3.88	1.42	1.37
31	5	314	CLA	C1D-ND	3.87	1.42	1.37
31	13	307	CLA	C1D-ND	3.87	1.42	1.37
43	8	301	A86	C30-C29	-3.87	1.25	1.32
31	3	307	CLA	C1D-ND	3.86	1.42	1.37
43	1	303	A86	O4-C38	3.86	1.43	1.35
43	7	304	A86	C40-C32	-3.86	1.46	1.53
43	1	303	A86	C30-C29	-3.85	1.25	1.32
43	8	303	A86	C30-C29	-3.85	1.25	1.32
31	b	614	CLA	C4D-ND	-3.85	1.32	1.37
43	10	303	A86	O1-C20	-3.85	1.40	1.46
43	14	302	A86	C30-C29	-3.85	1.25	1.32
31	B	602	CLA	C4D-ND	-3.85	1.32	1.37
43	6	301	A86	O1-C20	-3.85	1.40	1.46
42	7	314	KC1	CHB-C4A	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	10	302	A86	O1-C20	-3.85	1.40	1.46
43	16	306	A86	C19-C20	3.84	1.57	1.52
43	10	318	A86	O1-C20	-3.84	1.40	1.46
31	12	313	CLA	CHC-C1C	3.84	1.44	1.35
43	3	305	A86	C19-C20	3.84	1.57	1.52
43	2	305	A86	O1-C20	-3.84	1.40	1.46
31	C	507	CLA	C4D-ND	-3.83	1.32	1.37
31	c	507	CLA	C4D-ND	-3.83	1.32	1.37
31	17	315	CLA	C1D-ND	3.83	1.42	1.37
31	3	312	CLA	C1D-ND	3.83	1.42	1.37
31	c	513	CLA	C4D-ND	-3.83	1.32	1.37
31	19	308	CLA	C1D-ND	3.83	1.42	1.37
43	6	305	A86	C19-C20	3.83	1.57	1.52
31	19	307	CLA	C1D-ND	3.83	1.42	1.37
31	9	308	CLA	C1D-ND	3.82	1.42	1.37
31	C	508	CLA	C4D-ND	-3.82	1.32	1.37
41	E	101	HEM	C3C-C2C	-3.82	1.35	1.40
43	13	304	A86	C30-C29	-3.82	1.25	1.32
43	5	302	A86	C30-C29	-3.82	1.25	1.32
31	1	315	CLA	C1D-ND	3.81	1.42	1.37
31	16	314	CLA	MG-ND	-3.81	1.98	2.05
31	b	603	CLA	C4D-ND	-3.81	1.32	1.37
45	4	310	KC2	CHB-C4A	3.80	1.47	1.39
43	13	301	A86	C30-C29	-3.80	1.25	1.32
43	12	306	A86	O1-C20	-3.80	1.40	1.46
42	6	315	KC1	CHB-C4A	3.80	1.47	1.39
31	7	315	CLA	C1D-ND	3.80	1.42	1.37
42	7	314	KC1	C3D-C2D	3.80	1.46	1.39
31	1	316	CLA	C1D-ND	3.80	1.42	1.37
43	15	301	A86	C33-C34	3.80	1.58	1.51
42	11	314	KC1	CHB-C4A	3.79	1.47	1.39
45	6	312	KC2	CHB-C4A	3.79	1.47	1.39
43	6	303	A86	O1-C20	-3.79	1.40	1.46
45	14	310	KC2	CHB-C4A	3.78	1.47	1.39
31	2	312	CLA	CHC-C1C	3.78	1.44	1.35
31	14	312	CLA	C4D-ND	-3.78	1.32	1.37
43	16	304	A86	O4-C38	3.77	1.43	1.35
31	1	308	CLA	C1D-ND	3.77	1.42	1.37
31	b	616	CLA	C4D-ND	-3.77	1.32	1.37
31	B	611	CLA	CMB-C2B	-3.77	1.43	1.51
31	17	313	CLA	CMD-C2D	-3.77	1.42	1.50
31	c	504	CLA	C4D-ND	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	18	304	A86	C30-C29	-3.77	1.25	1.32
45	16	312	KC2	CHB-C4A	3.76	1.47	1.39
43	3	305	A86	C40-C32	-3.76	1.46	1.53
31	D	401	CLA	C4D-ND	-3.76	1.32	1.37
31	3	308	CLA	C4D-ND	-3.76	1.32	1.37
43	11	305	A86	C30-C29	-3.75	1.25	1.32
31	C	510	CLA	C4D-ND	-3.75	1.32	1.37
43	6	307	A86	C30-C29	-3.75	1.25	1.32
31	0	311	CLA	C4D-ND	-3.75	1.32	1.37
31	15	307	CLA	C4D-ND	-3.75	1.32	1.37
43	7	305	A86	O1-C20	-3.74	1.40	1.46
43	17	306	A86	O1-C20	-3.74	1.40	1.46
31	14	306	CLA	C4D-ND	-3.74	1.32	1.37
43	19	306	A86	O1-C20	-3.74	1.40	1.46
31	11	308	CLA	C4D-ND	-3.74	1.32	1.37
43	12	305	A86	C30-C29	-3.74	1.25	1.32
31	b	612	CLA	CMB-C2B	-3.74	1.43	1.51
31	2	309	CLA	C1D-ND	3.74	1.42	1.37
42	11	314	KC1	OBD-CAD	3.74	1.27	1.22
45	17	309	KC2	CHB-C4A	3.74	1.47	1.39
43	8	304	A86	C30-C29	-3.74	1.25	1.32
31	c	510	CLA	C4D-ND	-3.74	1.32	1.37
45	3	311	KC2	CHB-C4A	3.73	1.47	1.39
43	1	305	A86	C30-C29	-3.73	1.25	1.32
42	8	313	KC1	CHB-C1B	3.73	1.45	1.38
31	16	311	CLA	C1D-ND	3.73	1.42	1.37
31	7	312	CLA	C1D-ND	3.72	1.42	1.37
31	1	313	CLA	C4D-ND	-3.72	1.32	1.37
43	18	301	A86	O1-C15	-3.72	1.39	1.45
43	9	306	A86	C28-C27	3.72	1.58	1.50
42	17	314	KC1	CHB-C4A	3.72	1.47	1.39
31	B	615	CLA	C4D-ND	-3.72	1.32	1.37
31	p	607	CLA	C4D-ND	-3.71	1.32	1.37
31	10	311	CLA	C4D-ND	-3.71	1.32	1.37
43	8	303	A86	O1-C20	-3.71	1.40	1.46
31	13	310	CLA	C1D-ND	3.71	1.42	1.37
31	d	401	CLA	C4D-ND	-3.71	1.32	1.37
31	9	311	CLA	C1D-ND	3.71	1.42	1.37
43	3	301	A86	C30-C29	-3.71	1.25	1.32
31	C	507	CLA	CMB-C2B	-3.70	1.43	1.51
31	0	313	CLA	C1D-ND	3.70	1.42	1.37
31	18	307	CLA	C4D-ND	-3.70	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	311	CLA	C4D-ND	-3.70	1.32	1.37
43	16	304	A86	O1-C15	-3.70	1.39	1.45
31	12	310	CLA	C1D-ND	3.70	1.42	1.37
31	17	313	CLA	CHC-C1C	3.70	1.44	1.35
31	14	307	CLA	C4D-ND	-3.70	1.32	1.37
31	17	310	CLA	C1D-ND	3.69	1.42	1.37
31	10	308	CLA	C1D-ND	3.69	1.42	1.37
43	4	303	A86	C30-C29	-3.69	1.25	1.32
42	1	314	KC1	CHB-C4A	3.68	1.47	1.39
31	4	307	CLA	C4D-ND	-3.68	1.32	1.37
43	19	306	A86	C30-C29	-3.68	1.25	1.32
31	13	313	CLA	CHC-C1C	3.68	1.44	1.35
45	13	311	KC2	CHC-C1C	3.68	1.47	1.39
31	C	504	CLA	C4D-ND	-3.68	1.32	1.37
45	3	309	KC2	C4D-CHA	3.68	1.49	1.45
45	7	309	KC2	CHB-C4A	3.68	1.47	1.39
31	0	308	CLA	C1D-ND	3.67	1.42	1.37
31	18	311	CLA	C4D-ND	-3.67	1.32	1.37
31	6	311	CLA	C1D-ND	3.67	1.42	1.37
45	13	309	KC2	CHB-C4A	3.67	1.47	1.39
31	8	312	CLA	CMB-C2B	-3.66	1.44	1.51
31	c	507	CLA	CMB-C2B	-3.66	1.44	1.51
35	a	409	PL9	C3-C4	-3.66	1.43	1.49
45	6	312	KC2	C4D-CHA	3.66	1.49	1.45
43	7	303	A86	O1-C20	-3.66	1.41	1.46
42	12	314	KC1	CHB-C4A	3.66	1.47	1.39
31	8	307	CLA	C4D-ND	-3.66	1.32	1.37
42	9	314	KC1	CHB-C4A	3.66	1.47	1.39
31	18	312	CLA	CMB-C2B	-3.66	1.44	1.51
35	A	409	PL9	C3-C4	-3.65	1.43	1.49
45	2	308	KC2	CHC-C1C	3.65	1.47	1.39
31	2	312	CLA	CMD-C2D	-3.65	1.43	1.50
45	9	309	KC2	CHB-C4A	3.65	1.47	1.39
31	P	607	CLA	C4D-ND	-3.65	1.32	1.37
43	9	302	A86	O1-C20	-3.65	1.41	1.46
43	16	307	A86	O1-C20	-3.65	1.41	1.46
31	W	202	CLA	C4D-ND	-3.65	1.32	1.37
43	17	303	A86	O1-C20	-3.65	1.41	1.46
42	19	314	KC1	CHB-C4A	3.65	1.47	1.39
31	11	315	CLA	C1D-ND	3.65	1.42	1.37
31	8	312	CLA	CMD-C2D	-3.64	1.43	1.50
31	10	314	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	w	203	CLA	C4D-ND	-3.64	1.32	1.37
45	19	309	KC2	CHB-C4A	3.64	1.47	1.39
43	17	304	A86	O1-C20	-3.64	1.41	1.46
31	b	604	CLA	C4D-ND	-3.63	1.32	1.37
43	6	305	A86	C30-C29	-3.63	1.25	1.32
45	17	309	KC2	C4D-CHA	3.63	1.49	1.45
43	15	302	A86	O1-C20	-3.62	1.41	1.46
43	2	304	A86	C35-C34	3.62	1.58	1.51
33	Y	101	BCR	C30-C25	-3.62	1.48	1.53
31	B	601	CLA	C4D-ND	-3.62	1.32	1.37
31	b	602	CLA	C4D-ND	-3.62	1.32	1.37
43	19	302	A86	O1-C20	-3.62	1.41	1.46
43	16	307	A86	C30-C29	-3.62	1.25	1.32
31	B	612	CLA	C4D-ND	-3.62	1.32	1.37
43	6	306	A86	O1-C20	-3.62	1.41	1.46
45	13	311	KC2	CHB-C4A	3.62	1.47	1.39
45	7	309	KC2	C4D-CHA	3.62	1.49	1.45
43	5	318	A86	O1-C20	-3.62	1.41	1.46
45	4	310	KC2	C4D-CHA	3.61	1.49	1.45
39	b	622	DGD	O3G-C1D	3.61	1.46	1.40
45	16	312	KC2	C4D-CHA	3.61	1.49	1.45
31	P	601	CLA	C4D-ND	-3.60	1.32	1.37
31	c	512	CLA	C4D-ND	-3.60	1.32	1.37
31	B	603	CLA	C4D-ND	-3.60	1.32	1.37
31	3	310	CLA	C1D-ND	3.60	1.42	1.37
45	2	308	KC2	CHB-C4A	3.60	1.47	1.39
42	2	313	KC1	CHB-C4A	3.60	1.47	1.39
43	3	302	A86	C30-C29	-3.60	1.26	1.32
31	15	312	CLA	C3B-C2B	-3.59	1.35	1.40
43	9	306	A86	O1-C20	-3.59	1.41	1.46
43	9	305	A86	C19-C20	3.59	1.57	1.52
31	2	307	CLA	C4D-ND	-3.59	1.32	1.37
31	12	312	CLA	C1D-ND	3.59	1.42	1.37
31	A	403	CLA	C4D-ND	-3.59	1.32	1.37
43	8	302	A86	C30-C29	-3.58	1.26	1.32
43	11	306	A86	C19-C20	3.58	1.57	1.52
43	3	306	A86	O1-C20	-3.58	1.41	1.46
31	7	310	CLA	C1D-ND	3.58	1.42	1.37
31	14	312	CLA	CMB-C2B	-3.58	1.44	1.51
31	0	316	CLA	C1D-ND	3.58	1.42	1.37
31	C	512	CLA	C4D-ND	-3.58	1.32	1.37
43	13	305	A86	O1-C20	-3.58	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	621	DGD	C4D-C5D	3.58	1.60	1.53
31	3	316	CLA	C4D-ND	-3.57	1.32	1.37
42	16	301	KC1	CHB-C4A	3.57	1.47	1.39
31	4	312	CLA	MG-ND	-3.57	1.98	2.05
31	b	615	CLA	C4D-ND	-3.57	1.32	1.37
31	P	608	CLA	C4D-ND	-3.57	1.32	1.37
42	10	315	KC1	OBD-CAD	3.57	1.27	1.22
31	P	603	CLA	C4D-ND	-3.57	1.32	1.37
43	16	302	A86	C30-C29	-3.57	1.26	1.32
31	b	613	CLA	C4D-ND	-3.57	1.32	1.37
31	13	313	CLA	CMD-C2D	-3.56	1.43	1.50
31	C	511	CLA	C4D-ND	-3.56	1.32	1.37
31	D	405	CLA	C4D-ND	-3.56	1.32	1.37
31	d	405	CLA	C4D-ND	-3.56	1.32	1.37
45	2	308	KC2	C4D-CHA	3.56	1.49	1.45
45	3	311	KC2	C4D-CHA	3.56	1.49	1.45
31	8	312	CLA	C4D-ND	-3.56	1.32	1.37
31	p	603	CLA	C4D-ND	-3.56	1.32	1.37
43	13	304	A86	C19-C20	3.56	1.57	1.52
43	2	303	A86	O1-C20	-3.56	1.41	1.46
31	p	608	CLA	C4D-ND	-3.56	1.32	1.37
31	a	403	CLA	C4D-ND	-3.56	1.32	1.37
31	1	312	CLA	C4D-ND	-3.56	1.32	1.37
31	13	308	CLA	C4D-ND	-3.56	1.32	1.37
43	11	303	A86	C30-C29	-3.56	1.26	1.32
43	7	304	A86	C19-C20	3.55	1.57	1.52
31	0	314	CLA	C4D-ND	-3.55	1.32	1.37
31	15	311	CLA	C3B-C2B	-3.55	1.35	1.40
38	K	101	LMG	O7-C8	-3.55	1.37	1.46
38	k	101	LMG	O7-C8	-3.55	1.37	1.46
31	B	607	CLA	C4D-ND	-3.55	1.32	1.37
31	2	315	CLA	C4D-ND	-3.55	1.32	1.37
42	19	314	KC1	CHC-C1C	3.55	1.47	1.39
31	p	601	CLA	C4D-ND	-3.55	1.32	1.37
45	14	310	KC2	C4D-CHA	3.55	1.49	1.45
31	10	316	CLA	C1D-ND	3.55	1.42	1.37
31	11	312	CLA	C4D-ND	-3.55	1.32	1.37
31	P	605	CLA	C1D-ND	3.55	1.42	1.37
31	b	608	CLA	C4D-ND	-3.54	1.32	1.37
33	y	101	BCR	C30-C25	-3.54	1.48	1.53
42	13	314	KC1	CHB-C4A	3.54	1.47	1.39
45	2	310	KC2	CHB-C4A	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	314	CLA	C1D-ND	3.54	1.42	1.37
43	11	306	A86	C30-C29	-3.54	1.26	1.32
31	p	605	CLA	C1D-ND	3.54	1.42	1.37
31	p	610	CLA	C4D-ND	-3.54	1.32	1.37
43	4	306	A86	O1-C20	-3.53	1.41	1.46
31	11	310	CLA	C1D-ND	3.53	1.42	1.37
31	2	315	CLA	CHC-C1C	3.53	1.44	1.35
31	c	511	CLA	C4D-ND	-3.53	1.32	1.37
31	14	314	CLA	C1D-ND	3.53	1.42	1.37
45	5	308	KC2	CHB-C4A	3.53	1.47	1.39
31	b	605	CLA	C3B-C2B	-3.53	1.35	1.40
39	C	520	DGD	O5D-C6D	-3.52	1.37	1.43
31	C	502	CLA	C4D-ND	-3.52	1.32	1.37
31	z	101	CLA	C4D-ND	-3.52	1.32	1.37
43	15	302	A86	C30-C29	-3.52	1.26	1.32
45	12	311	KC2	CHB-C4A	3.52	1.47	1.39
43	19	305	A86	C19-C20	3.52	1.57	1.52
43	18	303	A86	C14-C13	3.52	1.55	1.51
45	15	308	KC2	C4D-CHA	3.52	1.49	1.45
45	7	309	KC2	CHC-C1C	3.52	1.47	1.39
39	c	520	DGD	O5D-C6D	-3.51	1.37	1.43
43	2	304	A86	C37-C36	3.51	1.58	1.52
31	p	608	CLA	C1D-ND	3.51	1.42	1.37
43	2	305	A86	C30-C29	-3.51	1.26	1.32
31	P	610	CLA	C4D-ND	-3.51	1.32	1.37
43	17	303	A86	C30-C29	-3.51	1.26	1.32
31	a	404	CLA	C1D-ND	3.51	1.42	1.37
45	17	309	KC2	CHC-C1C	3.50	1.47	1.39
41	v	201	HEM	C3C-CAC	3.50	1.55	1.47
31	18	306	CLA	C1D-ND	3.50	1.42	1.37
31	B	614	CLA	C4D-ND	-3.50	1.32	1.37
43	1	305	A86	C13-C11	-3.50	1.42	1.49
43	14	303	A86	O1-C20	-3.50	1.41	1.46
45	16	310	KC2	C4D-CHA	3.50	1.49	1.45
31	10	307	CLA	CMB-C2B	-3.50	1.44	1.51
43	3	301	A86	C13-C11	-3.49	1.42	1.49
45	6	310	KC2	CHB-C4A	3.49	1.47	1.39
43	0	302	A86	O1-C20	-3.49	1.41	1.46
31	2	311	CLA	C1D-ND	3.49	1.42	1.37
43	7	306	A86	O1-C20	-3.49	1.41	1.46
31	3	308	CLA	CHC-C1C	3.49	1.43	1.35
31	B	606	CLA	C4D-ND	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	V	201	HEM	C3C-CAC	3.49	1.55	1.47
45	12	309	KC2	CHC-C1C	3.49	1.47	1.39
45	1	309	KC2	CHC-C1C	3.49	1.47	1.39
45	17	311	KC2	C4D-CHA	3.49	1.49	1.45
45	6	310	KC2	CHC-C1C	3.48	1.47	1.39
31	w	203	CLA	C1D-ND	3.48	1.42	1.37
43	9	303	A86	O1-C20	-3.48	1.41	1.46
31	14	309	CLA	C1D-ND	3.48	1.42	1.37
42	7	314	KC1	CHC-C1C	3.48	1.47	1.39
38	1	301	LMG	C4-C5	3.48	1.60	1.53
31	6	314	CLA	C4D-ND	-3.48	1.32	1.37
43	0	301	A86	C30-C29	-3.48	1.26	1.32
39	B	621	DGD	O3G-C1D	3.48	1.46	1.40
31	Z	101	CLA	C4D-ND	-3.48	1.32	1.37
42	13	314	KC1	CHC-C1C	3.48	1.47	1.39
42	9	314	KC1	CHC-C1C	3.48	1.47	1.39
31	B	604	CLA	C3B-C2B	-3.48	1.35	1.40
45	11	309	KC2	CHC-C1C	3.48	1.47	1.39
45	16	310	KC2	CHB-C4A	3.48	1.47	1.39
45	6	310	KC2	C4D-CHA	3.48	1.49	1.45
31	17	312	CLA	C1D-ND	3.48	1.42	1.37
31	18	312	CLA	C3B-C2B	-3.48	1.35	1.40
43	6	307	A86	C2-C1	-3.47	1.31	1.35
31	16	314	CLA	C4D-ND	-3.47	1.32	1.37
43	12	305	A86	O1-C20	-3.47	1.41	1.46
31	7	313	CLA	CHC-C1C	3.47	1.43	1.35
43	3	304	A86	C30-C29	-3.47	1.26	1.32
31	A	404	CLA	C1D-ND	3.47	1.42	1.37
38	11	301	LMG	C4-C5	3.46	1.60	1.53
43	17	301	A86	C40-C32	-3.46	1.46	1.53
31	4	309	CLA	C1D-ND	3.46	1.42	1.37
31	c	502	CLA	C4D-ND	-3.46	1.32	1.37
45	4	308	KC2	CHC-C1C	3.46	1.47	1.39
42	5	313	KC1	CHB-C4A	3.46	1.47	1.39
31	c	514	CLA	C4D-ND	-3.46	1.32	1.37
31	16	309	CLA	C4D-ND	-3.46	1.32	1.37
43	1	304	A86	C30-C29	-3.45	1.26	1.32
43	4	306	A86	C30-C29	-3.45	1.26	1.32
45	12	309	KC2	C4D-CHA	3.45	1.49	1.45
42	18	313	KC1	CHB-C4A	3.45	1.47	1.39
31	1	310	CLA	C1D-ND	3.45	1.42	1.37
31	11	313	CLA	CHC-C1C	3.45	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	4	305	A86	O1-C20	-3.45	1.41	1.46
43	19	303	A86	O1-C20	-3.44	1.41	1.46
31	P	608	CLA	C1D-ND	3.44	1.42	1.37
39	b	622	DGD	C4E-C5E	3.44	1.60	1.53
45	7	311	KC2	CHB-C4A	3.44	1.47	1.39
31	0	309	CLA	C4D-ND	-3.44	1.33	1.37
31	B	610	CLA	C4D-ND	-3.44	1.33	1.37
31	1	315	CLA	C4D-ND	-3.44	1.33	1.37
33	y	101	BCR	C1-C6	-3.43	1.49	1.53
31	15	309	CLA	C1D-ND	3.43	1.42	1.37
31	C	505	CLA	C4D-ND	-3.43	1.33	1.37
31	17	308	CLA	C4D-ND	-3.43	1.33	1.37
31	C	514	CLA	C4D-ND	-3.43	1.33	1.37
31	b	617	CLA	C4D-ND	-3.43	1.33	1.37
45	15	308	KC2	CHB-C4A	3.43	1.47	1.39
42	18	313	KC1	C1B-NB	-3.43	1.33	1.37
31	14	309	CLA	C4D-ND	-3.43	1.33	1.37
45	14	308	KC2	CHB-C4A	3.42	1.47	1.39
31	7	308	CLA	C4D-ND	-3.42	1.33	1.37
31	18	309	CLA	C4D-ND	-3.42	1.33	1.37
43	6	304	A86	C30-C29	-3.42	1.26	1.32
43	4	304	A86	O1-C20	-3.42	1.41	1.46
31	18	311	CLA	C1D-ND	3.42	1.42	1.37
31	5	312	CLA	CMB-C2B	-3.42	1.44	1.51
33	Y	101	BCR	C1-C6	-3.42	1.49	1.53
31	1	308	CLA	CHC-C1C	3.41	1.43	1.35
31	W	202	CLA	C1D-ND	3.41	1.42	1.37
31	6	309	CLA	C4D-ND	-3.41	1.33	1.37
31	B	604	CLA	C4B-CHC	-3.41	1.31	1.41
45	4	308	KC2	CHB-C4A	3.41	1.47	1.39
43	14	304	A86	O1-C20	-3.41	1.41	1.46
31	4	309	CLA	C4D-ND	-3.41	1.33	1.37
31	8	312	CLA	C3B-C2B	-3.41	1.35	1.40
31	1	313	CLA	CHC-C1C	3.41	1.43	1.35
31	b	607	CLA	C4D-ND	-3.41	1.33	1.37
31	8	314	CLA	C1D-ND	3.40	1.42	1.37
43	0	301	A86	O1-C15	-3.40	1.39	1.45
31	b	605	CLA	C4B-CHC	-3.40	1.31	1.41
43	18	304	A86	C32-C31	-3.40	1.48	1.54
45	13	309	KC2	C4D-CHA	3.40	1.49	1.45
31	0	307	CLA	C4D-ND	-3.40	1.33	1.37
31	B	609	CLA	C4D-ND	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	605	CLA	C4D-ND	-3.40	1.33	1.37
31	b	610	CLA	C4D-ND	-3.40	1.33	1.37
31	8	309	CLA	C4D-ND	-3.40	1.33	1.37
43	0	303	A86	C13-C11	-3.40	1.43	1.49
31	c	505	CLA	C4D-ND	-3.39	1.33	1.37
39	B	621	DGD	C4E-C5E	3.39	1.60	1.53
31	b	611	CLA	C4D-ND	-3.39	1.33	1.37
31	17	308	CLA	CHC-C1C	3.39	1.43	1.35
31	3	313	CLA	CHC-C1C	3.39	1.43	1.35
31	p	606	CLA	CMC-C2C	-3.39	1.43	1.50
43	12	301	A86	C30-C29	-3.39	1.26	1.32
45	12	309	KC2	CHB-C4A	3.39	1.47	1.39
31	18	306	CLA	C4D-ND	-3.39	1.33	1.37
45	14	308	KC2	C4D-CHA	3.39	1.49	1.45
31	1	308	CLA	C4D-ND	-3.39	1.33	1.37
31	P	606	CLA	CMC-C2C	-3.39	1.43	1.50
45	16	310	KC2	CHC-C1C	3.39	1.47	1.39
31	12	315	CLA	C1D-ND	3.39	1.41	1.37
31	5	312	CLA	C4D-ND	-3.39	1.33	1.37
31	B	607	CLA	CMB-C2B	-3.39	1.44	1.51
31	6	313	CLA	C1D-ND	3.39	1.41	1.37
31	12	313	CLA	C4D-ND	-3.39	1.33	1.37
42	9	314	KC1	C4D-CHA	3.38	1.49	1.45
45	8	310	KC2	CHB-C4A	3.38	1.47	1.39
31	8	306	CLA	C1D-ND	3.38	1.41	1.37
43	13	304	A86	C13-C11	-3.38	1.43	1.49
31	12	308	CLA	C4D-ND	-3.38	1.33	1.37
43	6	302	A86	C30-C29	-3.38	1.26	1.32
45	3	309	KC2	CHC-C1C	3.38	1.46	1.39
45	5	308	KC2	C4D-CHA	3.38	1.49	1.45
45	4	308	KC2	C4D-CHA	3.38	1.49	1.45
38	5	316	LMG	C4-C5	3.38	1.60	1.53
38	5	316	LMG	O1-C7	-3.37	1.37	1.43
31	7	308	CLA	CHC-C1C	3.37	1.43	1.35
43	6	307	A86	C26-C27	-3.37	1.31	1.35
31	14	314	CLA	CHC-C1C	3.37	1.43	1.35
42	10	315	KC1	CHB-C4A	3.37	1.46	1.39
45	3	309	KC2	CHB-C4A	3.37	1.46	1.39
31	p	605	CLA	C4D-ND	-3.37	1.33	1.37
31	0	309	CLA	CHC-C1C	3.37	1.43	1.35
31	6	314	CLA	MG-ND	-3.37	1.99	2.05
31	5	309	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	314	CLA	C4D-ND	-3.37	1.33	1.37
33	b	620	BCR	C1-C6	-3.37	1.49	1.53
45	17	311	KC2	CHB-C4A	3.36	1.46	1.39
31	10	313	CLA	C1D-ND	3.36	1.41	1.37
43	p	611	A86	C19-C20	3.36	1.56	1.52
31	2	312	CLA	C4D-ND	-3.36	1.33	1.37
31	0	313	CLA	CMB-C2B	-3.36	1.44	1.51
42	16	315	KC1	C3D-C2D	3.36	1.45	1.39
45	7	311	KC2	C4D-CHA	3.36	1.49	1.45
31	3	316	CLA	C1D-ND	3.36	1.41	1.37
31	3	313	CLA	CMB-C2B	-3.36	1.44	1.51
31	10	309	CLA	C4D-ND	-3.35	1.33	1.37
33	B	619	BCR	C1-C6	-3.35	1.49	1.53
43	17	306	A86	C30-C29	-3.35	1.26	1.32
31	c	511	CLA	C1D-ND	3.35	1.41	1.37
45	2	310	KC2	C4D-CHA	3.35	1.49	1.45
31	b	608	CLA	CMB-C2B	-3.35	1.44	1.51
43	15	304	A86	C30-C29	-3.35	1.26	1.32
31	B	616	CLA	C4D-ND	-3.35	1.33	1.37
43	P	611	A86	C19-C20	3.35	1.56	1.52
31	11	308	CLA	CHC-C1C	3.35	1.43	1.35
42	p	609	KC1	C4D-CHA	3.35	1.49	1.45
43	0	303	A86	C30-C29	-3.34	1.26	1.32
42	P	609	KC1	C1B-NB	-3.34	1.33	1.37
31	10	309	CLA	CHC-C1C	3.34	1.43	1.35
42	P	609	KC1	C4D-CHA	3.34	1.49	1.45
42	1	314	KC1	CHC-C1C	3.34	1.46	1.39
43	17	305	A86	C33-C34	3.34	1.57	1.51
45	14	308	KC2	CHC-C1C	3.34	1.46	1.39
31	b	609	CLA	C4D-ND	-3.34	1.33	1.37
31	10	317	CLA	C4D-ND	-3.34	1.33	1.37
31	z	103	CLA	C1D-ND	3.33	1.41	1.37
45	4	310	KC2	CHC-C1C	3.33	1.46	1.39
43	10	301	A86	C30-C29	-3.33	1.26	1.32
31	4	314	CLA	C4D-ND	-3.33	1.33	1.37
45	18	310	KC2	CHB-C4A	3.33	1.46	1.39
43	12	303	A86	O1-C20	-3.33	1.41	1.46
42	11	314	KC1	CHC-C1C	3.33	1.46	1.39
45	15	308	KC2	C1B-NB	-3.33	1.33	1.37
31	13	313	CLA	C4D-ND	-3.33	1.33	1.37
42	p	609	KC1	C1B-NB	-3.33	1.33	1.37
45	1	309	KC2	CHB-C4A	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	5	310	KC2	CHB-C4A	3.32	1.46	1.39
31	z	103	CLA	C4D-ND	-3.32	1.33	1.37
31	5	306	CLA	C4D-ND	-3.32	1.33	1.37
31	C	511	CLA	C1D-ND	3.32	1.41	1.37
45	11	311	KC2	CHB-C4A	3.32	1.46	1.39
31	4	312	CLA	CHC-C1C	3.32	1.43	1.35
43	0	306	A86	O1-C20	-3.32	1.41	1.46
43	10	306	A86	O1-C20	-3.32	1.41	1.46
31	p	604	CLA	C1D-ND	3.32	1.41	1.37
31	C	504	CLA	C1D-ND	3.32	1.41	1.37
45	15	310	KC2	CHB-C4A	3.32	1.46	1.39
31	B	608	CLA	C4D-ND	-3.32	1.33	1.37
33	A	407	BCR	C30-C25	-3.32	1.49	1.53
33	a	407	BCR	C30-C25	-3.32	1.49	1.53
43	13	301	A86	O1-C20	-3.32	1.41	1.46
43	1	305	A86	C40-C32	-3.31	1.47	1.53
31	18	312	CLA	CHC-C1C	3.31	1.43	1.35
42	P	609	KC1	CHB-C4A	3.31	1.46	1.39
43	6	304	A86	O1-C20	-3.31	1.41	1.46
43	12	302	A86	C30-C29	-3.31	1.26	1.32
31	C	506	CLA	C4D-ND	-3.31	1.33	1.37
31	c	506	CLA	C4D-ND	-3.31	1.33	1.37
45	14	310	KC2	CHC-C1C	3.31	1.46	1.39
42	p	609	KC1	CHB-C4A	3.31	1.46	1.39
45	0	310	KC2	CHB-C4A	3.31	1.46	1.39
31	B	607	CLA	C3B-C2B	-3.31	1.35	1.40
33	B	617	BCR	C1-C6	-3.30	1.49	1.53
33	F	101	BCR	C30-C25	-3.30	1.49	1.53
42	17	314	KC1	CHC-C1C	3.30	1.46	1.39
31	2	315	CLA	C1D-ND	3.30	1.41	1.37
31	16	313	CLA	C1D-ND	3.30	1.41	1.37
42	12	314	KC1	CHC-C1C	3.30	1.46	1.39
43	16	305	A86	O1-C20	-3.30	1.41	1.46
31	c	509	CLA	CMB-C2B	-3.30	1.44	1.51
31	5	311	CLA	C4D-ND	-3.30	1.33	1.37
31	A	406	CLA	C4D-ND	-3.30	1.33	1.37
31	2	312	CLA	C3B-C2B	-3.30	1.35	1.40
45	15	308	KC2	CHC-C1C	3.30	1.46	1.39
31	D	404	CLA	CHC-C1C	3.30	1.43	1.35
31	17	312	CLA	C4D-ND	-3.30	1.33	1.37
31	17	313	CLA	CMB-C2B	-3.30	1.44	1.51
31	8	312	CLA	C1D-ND	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	11	309	KC2	CHB-C4A	3.30	1.46	1.39
39	b	622	DGD	C4D-C5D	3.30	1.60	1.53
45	1	311	KC2	C4D-CHA	3.30	1.49	1.45
31	0	312	CLA	C4D-ND	-3.30	1.33	1.37
42	14	313	KC1	CHB-C4A	3.29	1.46	1.39
43	2	301	A86	C30-C29	-3.29	1.26	1.32
31	a	406	CLA	C4D-ND	-3.29	1.33	1.37
31	7	313	CLA	CMD-C2D	-3.29	1.43	1.50
31	0	307	CLA	CMB-C2B	-3.29	1.44	1.51
31	B	605	CLA	C3B-C2B	-3.29	1.35	1.40
31	P	604	CLA	C1D-ND	3.29	1.41	1.37
42	16	301	KC1	CHC-C1C	3.29	1.46	1.39
31	13	308	CLA	C1D-ND	3.29	1.41	1.37
33	f	101	BCR	C30-C25	-3.29	1.49	1.53
42	17	314	KC1	C4D-CHA	3.29	1.49	1.45
31	9	311	CLA	CHC-C1C	3.29	1.43	1.35
31	C	509	CLA	CMB-C2B	-3.28	1.44	1.51
31	1	307	CLA	C1D-ND	3.28	1.41	1.37
43	11	304	A86	C30-C29	-3.28	1.26	1.32
31	Z	101	CLA	C1D-ND	3.28	1.41	1.37
45	13	309	KC2	CHC-C1C	3.28	1.46	1.39
43	13	304	A86	C40-C32	-3.28	1.47	1.53
33	C	515	BCR	C30-C25	-3.28	1.49	1.53
33	c	515	BCR	C30-C25	-3.28	1.49	1.53
43	17	301	A86	O1-C20	-3.28	1.41	1.46
31	b	608	CLA	C1D-ND	3.28	1.41	1.37
45	5	308	KC2	CHC-C1C	3.28	1.46	1.39
31	d	404	CLA	CHC-C1C	3.28	1.43	1.35
31	10	317	CLA	C1D-ND	3.27	1.41	1.37
31	4	314	CLA	CHC-C1C	3.27	1.43	1.35
31	14	306	CLA	CHC-C1C	3.27	1.43	1.35
31	z	103	CLA	CMB-C2B	-3.27	1.44	1.51
33	C	517	BCR	C1-C6	-3.27	1.49	1.53
31	c	504	CLA	C1D-ND	3.27	1.41	1.37
45	1	311	KC2	CHB-C4A	3.26	1.46	1.39
31	1	316	CLA	C4D-ND	-3.26	1.33	1.37
42	8	313	KC1	C1B-NB	-3.26	1.33	1.37
43	17	305	A86	C19-C20	3.26	1.56	1.52
42	3	314	KC1	CHC-C1C	3.26	1.46	1.39
31	15	312	CLA	CHC-C1C	3.26	1.43	1.35
45	18	310	KC2	C4D-CHA	3.26	1.49	1.45
31	p	606	CLA	C3B-C2B	-3.26	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	18	314	CLA	C4D-ND	-3.26	1.33	1.37
43	10	303	A86	C30-C29	-3.26	1.26	1.32
42	4	313	KC1	C4D-CHA	3.26	1.49	1.45
31	B	607	CLA	C1D-ND	3.26	1.41	1.37
35	A	409	PL9	C7-C3	-3.25	1.48	1.51
42	10	315	KC1	C1B-NB	-3.25	1.33	1.37
31	B	606	CLA	C1D-ND	3.25	1.41	1.37
31	18	314	CLA	C1D-ND	3.25	1.41	1.37
31	b	606	CLA	C3B-C2B	-3.25	1.35	1.40
31	8	306	CLA	C4D-ND	-3.25	1.33	1.37
31	5	309	CLA	C4D-ND	-3.25	1.33	1.37
42	2	313	KC1	CHC-C1C	3.25	1.46	1.39
31	13	310	CLA	C4D-ND	-3.25	1.33	1.37
43	7	302	A86	C19-C20	3.25	1.56	1.52
31	P	606	CLA	C3B-C2B	-3.25	1.35	1.40
31	z	101	CLA	C1D-ND	3.25	1.41	1.37
31	7	312	CLA	C4D-ND	-3.25	1.33	1.37
42	10	315	KC1	C4D-ND	3.24	1.38	1.35
31	9	312	CLA	C1D-ND	3.24	1.41	1.37
45	12	311	KC2	CHC-C1C	3.24	1.46	1.39
31	3	316	CLA	CAC-C3C	-3.24	1.42	1.51
43	5	301	A86	O1-C20	-3.24	1.41	1.46
33	b	618	BCR	C1-C6	-3.24	1.49	1.53
42	2	313	KC1	C4D-CHA	3.24	1.49	1.45
43	6	307	A86	O1-C20	-3.24	1.41	1.46
31	18	312	CLA	C1D-ND	3.24	1.41	1.37
43	0	302	A86	C32-C31	-3.24	1.49	1.54
31	10	316	CLA	C4D-ND	-3.24	1.33	1.37
35	a	409	PL9	C7-C3	-3.24	1.48	1.51
45	11	309	KC2	C1B-NB	-3.24	1.33	1.37
31	b	608	CLA	C3B-C2B	-3.24	1.35	1.40
42	0	315	KC1	CHB-C4A	3.24	1.46	1.39
43	10	301	A86	O1-C15	-3.24	1.40	1.45
31	8	306	CLA	CMB-C2B	-3.23	1.44	1.51
31	0	316	CLA	C4D-ND	-3.23	1.33	1.37
42	6	315	KC1	C1D-CHD	3.23	1.50	1.41
31	10	307	CLA	C4D-ND	-3.23	1.33	1.37
43	1	306	A86	C30-C29	-3.23	1.26	1.32
43	0	306	A86	C26-C27	-3.23	1.31	1.35
31	2	307	CLA	CHC-C1C	3.23	1.43	1.35
33	c	517	BCR	C1-C6	-3.23	1.49	1.53
31	P	606	CLA	C1D-ND	3.23	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	314	KC1	C4D-CHA	3.23	1.49	1.45
31	8	312	CLA	CHC-C1C	3.23	1.43	1.35
31	19	311	CLA	CHC-C1C	3.23	1.43	1.35
42	12	314	KC1	C1A-CHA	3.23	1.49	1.40
31	b	607	CLA	C1D-ND	3.23	1.41	1.37
31	c	503	CLA	CMB-C2B	-3.22	1.44	1.51
31	7	313	CLA	CMB-C2B	-3.22	1.44	1.51
31	1	310	CLA	C4D-ND	-3.22	1.33	1.37
31	10	312	CLA	C4D-ND	-3.22	1.33	1.37
45	10	310	KC2	CHB-C4A	3.22	1.46	1.39
31	1	316	CLA	CMB-C2B	-3.22	1.44	1.51
31	b	611	CLA	C1D-ND	3.22	1.41	1.37
43	2	304	A86	C30-C29	-3.22	1.26	1.32
31	B	602	CLA	C1D-ND	3.22	1.41	1.37
31	9	312	CLA	CMD-C2D	-3.22	1.44	1.50
43	9	302	A86	C30-C29	-3.22	1.26	1.32
45	3	311	KC2	CHC-C1C	3.22	1.46	1.39
31	19	308	CLA	CHC-C1C	3.21	1.43	1.35
31	14	314	CLA	C4D-ND	-3.21	1.33	1.37
45	9	309	KC2	C4D-CHA	3.21	1.49	1.45
43	9	306	A86	O3-C36	-3.21	1.37	1.43
31	5	312	CLA	CHC-C1C	3.21	1.43	1.35
43	16	304	A86	C30-C29	-3.20	1.26	1.32
31	9	308	CLA	C4D-ND	-3.20	1.33	1.37
31	12	308	CLA	CHC-C1C	3.20	1.43	1.35
31	16	311	CLA	C4D-ND	-3.20	1.33	1.37
31	19	313	CLA	CHC-C1C	3.20	1.43	1.35
31	B	603	CLA	CMB-C2B	-3.20	1.45	1.51
42	16	315	KC1	CHC-C1C	3.20	1.46	1.39
31	18	307	CLA	CMB-C2B	-3.20	1.45	1.51
45	11	311	KC2	C4D-CHA	3.20	1.49	1.45
45	8	310	KC2	C4D-CHA	3.20	1.49	1.45
45	13	311	KC2	C4D-CHA	3.20	1.49	1.45
43	11	304	A86	O1-C20	-3.20	1.41	1.46
31	9	313	CLA	CHC-C1C	3.20	1.43	1.35
45	7	311	KC2	CHC-C1C	3.20	1.46	1.39
43	15	303	A86	C30-C29	-3.20	1.26	1.32
31	9	315	CLA	CHC-C1C	3.19	1.43	1.35
43	10	303	A86	C13-C11	-3.19	1.43	1.49
31	15	306	CLA	C4D-ND	-3.19	1.33	1.37
43	16	306	A86	C30-C29	-3.19	1.26	1.32
31	b	604	CLA	CMB-C2B	-3.19	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	503	CLA	CMB-C2B	-3.19	1.45	1.51
31	p	607	CLA	CHC-C1C	3.19	1.43	1.35
31	r	101	CLA	C1D-ND	3.19	1.41	1.37
31	19	312	CLA	C1D-ND	3.19	1.41	1.37
31	b	616	CLA	CMC-C2C	-3.18	1.44	1.50
45	18	308	KC2	C4D-CHA	3.18	1.49	1.45
31	19	315	CLA	CHC-C1C	3.18	1.43	1.35
31	b	603	CLA	C1D-ND	3.18	1.41	1.37
31	p	606	CLA	C1D-ND	3.18	1.41	1.37
43	2	301	A86	O1-C20	-3.18	1.41	1.46
31	16	313	CLA	CMD-C2D	-3.18	1.44	1.50
45	1	311	KC2	CHC-C1C	3.18	1.46	1.39
45	1	309	KC2	C4D-CHA	3.18	1.49	1.45
43	15	301	A86	O1-C20	-3.18	1.41	1.46
31	B	613	CLA	C1D-ND	3.17	1.41	1.37
31	6	313	CLA	C4D-ND	-3.17	1.33	1.37
31	19	312	CLA	CMD-C2D	-3.17	1.44	1.50
31	4	311	CLA	C1D-ND	3.17	1.41	1.37
42	4	313	KC1	CHB-C4A	3.17	1.46	1.39
43	16	302	A86	O1-C20	-3.17	1.41	1.46
31	C	512	CLA	CMD-C2D	-3.17	1.44	1.50
31	9	308	CLA	CHC-C1C	3.17	1.43	1.35
31	14	311	CLA	C1D-ND	3.17	1.41	1.37
31	6	311	CLA	C4D-ND	-3.17	1.33	1.37
31	5	311	CLA	CMB-C2B	-3.17	1.45	1.51
31	11	316	CLA	CHC-C1C	3.16	1.43	1.35
43	19	301	A86	C30-C29	-3.16	1.26	1.32
43	4	302	A86	O1-C20	-3.16	1.41	1.46
31	1	312	CLA	C1D-ND	3.16	1.41	1.37
31	17	310	CLA	C4D-ND	-3.16	1.33	1.37
31	15	312	CLA	C4D-ND	-3.16	1.33	1.37
31	8	309	CLA	C1D-ND	3.16	1.41	1.37
31	4	312	CLA	CMB-C2B	-3.16	1.45	1.51
42	5	313	KC1	CHC-C1C	3.16	1.46	1.39
31	16	314	CLA	CHC-C1C	3.16	1.43	1.35
31	P	607	CLA	CHC-C1C	3.16	1.43	1.35
44	p	612	DD6	C13-C11	3.16	1.52	1.45
38	10	319	LMG	C4-C3	3.16	1.60	1.52
43	7	305	A86	C30-C29	-3.15	1.26	1.32
43	1	320	A86	O1-C20	-3.15	1.41	1.46
31	b	609	CLA	CMB-C2B	-3.15	1.45	1.51
31	3	307	CLA	C4D-ND	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	310	CLA	C4D-ND	-3.15	1.33	1.37
31	b	616	CLA	C3B-C2B	-3.14	1.36	1.40
31	13	315	CLA	CHC-C1C	3.14	1.43	1.35
31	B	610	CLA	C1D-ND	3.14	1.41	1.37
45	19	309	KC2	C4D-CHA	3.14	1.49	1.45
31	8	311	CLA	C1D-ND	3.14	1.41	1.37
42	6	315	KC1	CHC-C1C	3.14	1.46	1.39
31	R	101	CLA	C1D-ND	3.14	1.41	1.37
45	6	312	KC2	CHC-C1C	3.14	1.46	1.39
43	6	303	A86	C19-C20	3.14	1.56	1.52
31	7	315	CLA	C4D-ND	-3.13	1.33	1.37
45	19	309	KC2	CHC-C1C	3.13	1.46	1.39
31	6	309	CLA	CHC-C1C	3.13	1.43	1.35
45	17	311	KC2	CHC-C1C	3.13	1.46	1.39
43	17	302	A86	C32-C31	-3.13	1.49	1.54
43	17	304	A86	C30-C29	-3.13	1.26	1.32
31	15	309	CLA	C4D-ND	-3.13	1.33	1.37
31	11	310	CLA	C4D-ND	-3.13	1.33	1.37
43	6	307	A86	C13-C11	-3.13	1.43	1.49
31	1	307	CLA	C4D-ND	-3.13	1.33	1.37
45	8	308	KC2	CHC-C1C	3.13	1.46	1.39
45	18	310	KC2	CHC-C1C	3.13	1.46	1.39
34	0	318	SQD	O48-C23	3.12	1.42	1.33
31	4	315	CLA	C4D-ND	-3.12	1.33	1.37
42	14	313	KC1	C4D-CHA	3.12	1.48	1.45
31	B	615	CLA	C3B-C2B	-3.12	1.36	1.40
31	d	401	CLA	CMB-C2B	-3.12	1.45	1.51
43	4	302	A86	C13-C11	-3.12	1.43	1.49
42	1	314	KC1	C4D-CHA	3.12	1.48	1.45
31	8	312	CLA	MG-ND	-3.12	1.99	2.05
34	A	411	SQD	O48-C23	3.12	1.42	1.33
31	15	312	CLA	C1D-ND	3.12	1.41	1.37
31	13	308	CLA	CHC-C1C	3.11	1.42	1.35
31	B	608	CLA	CMB-C2B	-3.11	1.45	1.51
45	11	311	KC2	CHC-C1C	3.11	1.46	1.39
31	10	307	CLA	C1D-ND	3.11	1.41	1.37
31	P	602	CLA	CHC-C1C	3.11	1.42	1.35
31	1	313	CLA	CMD-C2D	-3.11	1.44	1.50
45	18	308	KC2	CHC-C1C	3.11	1.46	1.39
39	C	518	DGD	O1G-C1G	-3.11	1.38	1.45
31	16	313	CLA	C4D-ND	-3.11	1.33	1.37
31	16	309	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	14	305	A86	O1-C20	-3.11	1.41	1.46
31	1	321	CLA	C1D-ND	3.11	1.41	1.37
31	P	604	CLA	CHC-C1C	3.11	1.42	1.35
45	18	308	KC2	CHB-C4A	3.11	1.46	1.39
31	c	512	CLA	CMD-C2D	-3.10	1.44	1.50
41	E	101	HEM	CAB-C3B	3.10	1.55	1.47
45	8	310	KC2	CHC-C1C	3.10	1.46	1.39
43	7	301	A86	O1-C20	-3.10	1.41	1.46
43	1	306	A86	C32-C31	-3.10	1.49	1.54
31	5	307	CLA	C1D-ND	3.10	1.41	1.37
43	5	305	A86	O1-C20	-3.10	1.41	1.46
43	8	304	A86	O1-C15	-3.10	1.40	1.45
31	A	403	CLA	CMD-C2D	-3.10	1.44	1.50
31	a	403	CLA	CMD-C2D	-3.10	1.44	1.50
31	10	316	CLA	CHC-C1C	3.10	1.42	1.35
31	19	308	CLA	C4D-ND	-3.10	1.33	1.37
45	9	309	KC2	CHC-C1C	3.10	1.46	1.39
45	16	312	KC2	CHC-C1C	3.10	1.46	1.39
43	17	316	A86	C17-C18	-3.10	1.47	1.52
31	8	307	CLA	C3B-C2B	-3.09	1.36	1.40
34	i	101	SQD	O48-C23	3.09	1.42	1.33
45	8	308	KC2	CHB-C4A	3.09	1.46	1.39
31	B	616	CLA	C1D-ND	3.09	1.41	1.37
31	14	312	CLA	MG-ND	-3.09	1.99	2.05
39	c	518	DGD	O1G-C1G	-3.09	1.38	1.45
31	14	312	CLA	CHC-C1C	3.09	1.42	1.35
31	19	310	CLA	CHC-C1C	3.09	1.42	1.35
45	5	310	KC2	C4D-CHA	3.09	1.48	1.45
31	p	602	CLA	CHC-C1C	3.09	1.42	1.35
31	12	313	CLA	C3B-C2B	-3.09	1.36	1.40
43	9	305	A86	C30-C29	-3.08	1.26	1.32
31	0	314	CLA	CHC-C1C	3.08	1.42	1.35
43	13	303	A86	C30-C29	-3.08	1.26	1.32
31	p	604	CLA	CHC-C1C	3.08	1.42	1.35
31	14	315	CLA	C4D-ND	-3.08	1.33	1.37
32	a	405	PHO	CAC-C3C	-3.08	1.46	1.52
42	4	313	KC1	CHC-C1C	3.08	1.46	1.39
43	3	302	A86	O1-C20	-3.08	1.41	1.46
45	8	308	KC2	C4D-CHA	3.08	1.48	1.45
31	17	313	CLA	C4D-ND	-3.08	1.33	1.37
31	1	313	CLA	CMB-C2B	-3.08	1.45	1.51
41	e	101	HEM	CAB-C3B	3.08	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	12	307	CLA	CHC-C1C	3.08	1.42	1.35
41	e	101	HEM	FE-ND	3.08	2.12	1.96
42	18	313	KC1	CHC-C1C	3.08	1.46	1.39
31	18	309	CLA	C1D-ND	3.08	1.41	1.37
31	P	606	CLA	C1B-NB	3.08	1.38	1.35
31	11	315	CLA	C4D-ND	-3.08	1.33	1.37
35	D	406	PL9	C7-C8	-3.08	1.46	1.50
31	9	310	CLA	CHC-C1C	3.08	1.42	1.35
41	E	101	HEM	FE-ND	3.08	2.12	1.96
31	10	317	CLA	CMB-C2B	-3.08	1.45	1.51
45	12	311	KC2	C4D-CHA	3.08	1.48	1.45
42	14	313	KC1	CHC-C1C	3.08	1.46	1.39
31	12	310	CLA	C4D-ND	-3.07	1.33	1.37
38	0	317	LMG	C4-C3	3.07	1.60	1.52
31	8	311	CLA	CMD-C2D	-3.07	1.44	1.50
31	19	312	CLA	CHC-C1C	3.07	1.42	1.35
32	A	405	PHO	CAC-C3C	-3.07	1.46	1.52
43	1	304	A86	O1-C20	-3.07	1.41	1.46
45	4	310	KC2	C1A-CHA	3.07	1.48	1.40
31	11	307	CLA	C1D-ND	3.07	1.41	1.37
31	14	315	CLA	CHC-C1C	3.07	1.42	1.35
31	3	310	CLA	C4D-ND	-3.07	1.33	1.37
31	r	101	CLA	C4D-ND	-3.07	1.33	1.37
31	9	312	CLA	CHC-C1C	3.07	1.42	1.35
31	12	316	CLA	CHC-C1C	3.07	1.42	1.35
45	15	308	KC2	C3C-C4C	3.07	1.51	1.44
42	12	314	KC1	C4D-CHA	3.06	1.48	1.45
31	15	311	CLA	MG-ND	-3.06	1.99	2.05
43	17	302	A86	O1-C20	-3.06	1.41	1.46
43	17	316	A86	C13-C11	-3.06	1.43	1.49
31	b	614	CLA	C1D-ND	3.06	1.41	1.37
33	A	407	BCR	C1-C6	-3.06	1.49	1.53
31	9	313	CLA	C4D-ND	-3.06	1.33	1.37
31	7	310	CLA	CHC-C1C	3.06	1.42	1.35
45	14	310	KC2	C1A-CHA	3.06	1.48	1.40
31	11	312	CLA	C1D-ND	3.06	1.41	1.37
31	C	509	CLA	CHC-C1C	3.06	1.42	1.35
31	c	509	CLA	CHC-C1C	3.06	1.42	1.35
31	3	310	CLA	CHC-C1C	3.06	1.42	1.35
31	14	311	CLA	CHC-C1C	3.06	1.42	1.35
31	p	602	CLA	CMB-C2B	-3.06	1.45	1.51
31	C	503	CLA	C1D-ND	3.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	307	CLA	C1D-ND	3.06	1.41	1.37
31	p	606	CLA	C1B-NB	3.05	1.37	1.35
31	9	311	CLA	C4D-ND	-3.05	1.33	1.37
43	11	305	A86	C13-C11	-3.05	1.43	1.49
43	4	303	A86	O1-C20	-3.05	1.41	1.46
31	12	313	CLA	CMD-C2D	-3.05	1.44	1.50
31	17	312	CLA	CHC-C1C	3.05	1.42	1.35
31	6	313	CLA	CHC-C1C	3.05	1.42	1.35
43	4	304	A86	C30-C29	-3.05	1.26	1.32
33	b	620	BCR	C30-C25	-3.05	1.49	1.53
31	b	617	CLA	C1D-ND	3.05	1.41	1.37
31	D	401	CLA	CMB-C2B	-3.05	1.45	1.51
31	16	313	CLA	CHC-C1C	3.05	1.42	1.35
43	6	307	A86	C40-C32	-3.05	1.47	1.53
31	c	512	CLA	MG-ND	-3.05	1.99	2.05
31	P	610	CLA	CHC-C1C	3.04	1.42	1.35
31	p	610	CLA	CHC-C1C	3.04	1.42	1.35
33	C	516	BCR	C1-C6	-3.04	1.49	1.53
31	C	503	CLA	C1C-NC	-3.04	1.33	1.37
42	8	313	KC1	CHB-C4A	3.04	1.46	1.39
31	R	101	CLA	C4D-ND	-3.04	1.33	1.37
38	J	101	LMG	O7-C8	-3.04	1.39	1.46
31	0	312	CLA	CHC-C1C	3.04	1.42	1.35
31	11	316	CLA	C4D-ND	-3.04	1.33	1.37
31	18	307	CLA	CHC-C1C	3.04	1.42	1.35
43	7	303	A86	C30-C29	-3.03	1.26	1.32
31	c	503	CLA	C1C-NC	-3.03	1.33	1.37
31	A	403	CLA	CMB-C2B	-3.03	1.45	1.51
41	V	201	HEM	CAB-C3B	3.03	1.55	1.47
43	11	302	A86	O1-C15	-3.03	1.40	1.45
43	p	611	A86	C13-C11	-3.03	1.43	1.49
42	18	313	KC1	C3D-C2D	3.03	1.44	1.39
38	m	101	LMG	O8-C9	-3.03	1.38	1.45
38	j	101	LMG	O7-C8	-3.03	1.39	1.46
43	14	305	A86	C13-C11	-3.02	1.43	1.49
38	D	403	LMG	C4-C3	3.02	1.60	1.52
31	7	312	CLA	CHC-C1C	3.02	1.42	1.35
31	0	307	CLA	CHC-C1C	3.02	1.42	1.35
34	L	102	SQD	O47-C7	3.02	1.42	1.34
41	v	201	HEM	CAB-C3B	3.02	1.55	1.47
34	10	320	SQD	O48-C23	3.02	1.42	1.33
33	a	407	BCR	C1-C6	-3.02	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	406	PL9	C7-C8	-3.02	1.46	1.50
33	c	516	BCR	C1-C6	-3.02	1.49	1.53
42	2	313	KC1	C1A-CHA	3.02	1.48	1.40
31	2	311	CLA	C4D-ND	-3.02	1.33	1.37
31	14	307	CLA	CHC-C1C	3.02	1.42	1.35
31	17	310	CLA	CHC-C1C	3.02	1.42	1.35
31	14	306	CLA	MG-ND	-3.02	1.99	2.05
45	1	309	KC2	C3C-C4C	3.02	1.50	1.44
31	15	313	CLA	CHC-C1C	3.02	1.42	1.35
31	15	313	CLA	C4D-ND	-3.02	1.33	1.37
42	0	315	KC1	CHC-C1C	3.02	1.46	1.39
31	0	316	CLA	CHC-C1C	3.02	1.42	1.35
31	b	604	CLA	CMD-C2D	-3.02	1.44	1.50
31	b	616	CLA	C1D-ND	3.02	1.41	1.37
31	a	403	CLA	CMB-C2B	-3.02	1.45	1.51
31	3	313	CLA	CMD-C2D	-3.02	1.44	1.50
31	13	310	CLA	CHC-C1C	3.01	1.42	1.35
31	b	602	CLA	C1D-ND	3.01	1.41	1.37
31	10	314	CLA	C4D-ND	-3.01	1.33	1.37
31	c	514	CLA	CHC-C1C	3.01	1.42	1.35
43	P	611	A86	C13-C11	-3.01	1.43	1.49
31	10	309	CLA	C1D-ND	3.01	1.41	1.37
42	8	313	KC1	C4D-CHA	3.01	1.48	1.45
31	10	314	CLA	CHC-C1C	3.01	1.42	1.35
31	B	603	CLA	CMD-C2D	-3.01	1.44	1.50
42	3	314	KC1	C4D-CHA	3.01	1.48	1.45
43	2	302	A86	O1-C15	-3.01	1.40	1.45
43	12	304	A86	C13-C11	-3.01	1.43	1.49
31	A	406	CLA	CHC-C1C	3.01	1.42	1.35
31	4	307	CLA	CHC-C1C	3.01	1.42	1.35
31	10	312	CLA	CHC-C1C	3.01	1.42	1.35
31	C	506	CLA	CHC-C1C	3.01	1.42	1.35
31	B	601	CLA	C1D-ND	3.01	1.41	1.37
35	D	406	PL9	C16-C14	-3.00	1.45	1.51
35	d	406	PL9	C16-C14	-3.00	1.45	1.51
31	b	613	CLA	CMD-C2D	-3.00	1.44	1.50
31	19	313	CLA	C4D-ND	-3.00	1.33	1.37
31	C	514	CLA	CHC-C1C	3.00	1.42	1.35
31	8	307	CLA	CHC-C1C	3.00	1.42	1.35
31	D	404	CLA	CMD-C2D	-3.00	1.44	1.50
43	16	305	A86	C30-C29	-3.00	1.27	1.32
31	c	506	CLA	CHC-C1C	3.00	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	619	BCR	C30-C25	-3.00	1.49	1.53
43	11	302	A86	C30-C29	-3.00	1.27	1.32
43	10	302	A86	C30-C29	-3.00	1.27	1.32
39	c	520	DGD	O1G-C1G	-3.00	1.38	1.45
31	12	310	CLA	CHC-C1C	3.00	1.42	1.35
43	3	305	A86	C30-C29	-3.00	1.27	1.32
31	B	614	CLA	C1D-ND	2.99	1.41	1.37
31	C	512	CLA	MG-ND	-2.99	1.99	2.05
45	0	310	KC2	CHC-C1C	2.99	1.46	1.39
45	2	310	KC2	CHC-C1C	2.99	1.46	1.39
31	d	404	CLA	CMD-C2D	-2.99	1.44	1.50
31	2	309	CLA	C4D-ND	-2.99	1.33	1.37
31	C	508	CLA	CMB-C2B	-2.99	1.45	1.51
31	2	312	CLA	MG-ND	-2.99	1.99	2.05
31	b	603	CLA	CMB-C2B	-2.99	1.45	1.51
31	2	311	CLA	CHC-C1C	2.99	1.42	1.35
31	4	311	CLA	CHC-C1C	2.99	1.42	1.35
31	0	313	CLA	CHC-C1C	2.99	1.42	1.35
31	16	309	CLA	C1D-ND	2.99	1.41	1.37
45	10	310	KC2	CHC-C1C	2.99	1.46	1.39
43	5	305	A86	C33-C34	2.99	1.57	1.51
43	19	305	A86	C30-C29	-2.99	1.27	1.32
31	c	502	CLA	CMD-C2D	-2.99	1.44	1.50
31	B	612	CLA	CMD-C2D	-2.99	1.44	1.50
31	14	311	CLA	CMD-C2D	-2.98	1.44	1.50
31	3	312	CLA	CHC-C1C	2.98	1.42	1.35
31	P	602	CLA	CMB-C2B	-2.98	1.45	1.51
35	d	406	PL9	C53-C6	-2.98	1.44	1.50
31	D	405	CLA	CHC-C1C	2.98	1.42	1.35
31	5	314	CLA	C4D-ND	-2.98	1.33	1.37
31	4	315	CLA	CHC-C1C	2.98	1.42	1.35
31	1	321	CLA	MG-ND	-2.98	1.99	2.05
43	18	303	A86	O1-C20	-2.98	1.41	1.46
31	a	406	CLA	CHC-C1C	2.98	1.42	1.35
45	5	308	KC2	C3C-C4C	2.98	1.50	1.44
44	p	612	DD6	O1-C20	-2.98	1.41	1.46
31	p	610	CLA	C1D-ND	2.98	1.41	1.37
42	10	315	KC1	CHC-C1C	2.98	1.46	1.39
45	0	310	KC2	C1B-NB	-2.98	1.34	1.37
31	b	615	CLA	C1D-ND	2.98	1.41	1.37
31	10	314	CLA	CMD-C2D	-2.98	1.44	1.50
31	B	609	CLA	C1D-ND	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	607	CLA	CMD-C2D	-2.98	1.44	1.50
43	5	304	A86	C30-C29	-2.97	1.27	1.32
38	d	403	LMG	C4-C3	2.97	1.59	1.52
34	l	101	SQD	O47-C7	2.97	1.42	1.34
39	C	520	DGD	O1G-C1G	-2.97	1.38	1.45
31	10	311	CLA	CHC-C1C	2.97	1.42	1.35
31	12	308	CLA	CMB-C2B	-2.97	1.45	1.51
43	12	301	A86	O1-C15	-2.97	1.40	1.45
31	c	508	CLA	CMB-C2B	-2.97	1.45	1.51
43	19	302	A86	C30-C29	-2.97	1.27	1.32
31	B	602	CLA	CMB-C2B	-2.97	1.45	1.51
31	18	311	CLA	CMD-C2D	-2.97	1.44	1.50
31	11	312	CLA	CMB-C2B	-2.97	1.45	1.51
31	17	315	CLA	C4D-ND	-2.97	1.33	1.37
31	0	311	CLA	CHC-C1C	2.97	1.42	1.35
43	4	301	A86	C30-C29	-2.97	1.27	1.32
31	0	307	CLA	C1D-ND	2.96	1.41	1.37
45	10	310	KC2	C1B-NB	-2.96	1.34	1.37
31	c	502	CLA	C1D-ND	2.96	1.41	1.37
31	c	503	CLA	C1D-ND	2.96	1.41	1.37
43	15	302	A86	C40-C32	-2.96	1.47	1.53
31	2	314	CLA	CHC-C1C	2.96	1.42	1.35
31	b	603	CLA	CMC-C2C	-2.96	1.44	1.50
43	15	305	A86	C30-C29	-2.96	1.27	1.32
35	D	406	PL9	C53-C6	-2.96	1.44	1.50
31	d	405	CLA	CHC-C1C	2.96	1.42	1.35
31	11	307	CLA	CHC-C1C	2.96	1.42	1.35
31	D	405	CLA	C1D-ND	2.95	1.41	1.37
43	2	304	A86	C40-C32	-2.95	1.47	1.53
31	2	315	CLA	C3C-C2C	2.95	1.43	1.36
31	4	309	CLA	CHC-C1C	2.95	1.42	1.35
31	14	309	CLA	CHC-C1C	2.95	1.42	1.35
31	1	313	CLA	MG-ND	-2.95	1.99	2.05
31	P	603	CLA	CMD-C2D	-2.95	1.44	1.50
31	18	307	CLA	CMD-C2D	-2.95	1.44	1.50
31	12	313	CLA	CMB-C2B	-2.95	1.45	1.51
31	15	307	CLA	CMB-C2B	-2.95	1.45	1.51
43	12	306	A86	C41-C32	-2.95	1.48	1.53
45	5	310	KC2	C1B-NB	-2.94	1.34	1.37
34	b	601	SQD	O48-C23	2.94	1.41	1.33
34	B	623	SQD	O48-C23	2.94	1.41	1.33
31	C	502	CLA	CMD-C2D	-2.94	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	315	CLA	C4D-ND	-2.94	1.33	1.37
31	10	313	CLA	CHC-C1C	2.94	1.42	1.35
31	B	602	CLA	CMC-C2C	-2.94	1.44	1.50
43	5	301	A86	C13-C11	-2.94	1.44	1.49
31	c	508	CLA	C3B-C2B	-2.94	1.36	1.40
31	C	505	CLA	C1D-ND	2.94	1.41	1.37
31	5	307	CLA	CHC-C1C	2.93	1.42	1.35
31	18	307	CLA	C3B-C2B	-2.93	1.36	1.40
31	B	614	CLA	CHC-C1C	2.93	1.42	1.35
31	P	603	CLA	CHC-C1C	2.93	1.42	1.35
31	19	307	CLA	CHC-C1C	2.93	1.42	1.35
31	13	307	CLA	C4D-ND	-2.93	1.33	1.37
45	15	310	KC2	CHC-C1C	2.93	1.45	1.39
45	5	310	KC2	CHC-C1C	2.93	1.45	1.39
31	B	616	CLA	CMB-C2B	-2.93	1.45	1.51
31	P	610	CLA	C1D-ND	2.93	1.41	1.37
45	5	308	KC2	C1B-NB	-2.93	1.34	1.37
31	B	601	CLA	CHC-C1C	2.93	1.42	1.35
43	15	301	A86	C13-C11	-2.93	1.44	1.49
31	B	615	CLA	CMC-C2C	-2.93	1.44	1.50
43	9	304	A86	C30-C29	-2.93	1.27	1.32
31	P	601	CLA	C1D-ND	2.93	1.41	1.37
31	d	405	CLA	C1D-ND	2.93	1.41	1.37
33	c	516	BCR	C30-C25	-2.93	1.49	1.53
43	6	302	A86	O1-C20	-2.93	1.42	1.46
31	C	507	CLA	C1D-ND	2.93	1.41	1.37
31	c	506	CLA	C1D-ND	2.93	1.41	1.37
31	c	507	CLA	C1D-ND	2.93	1.41	1.37
42	8	313	KC1	CHC-C1C	2.92	1.45	1.39
31	19	313	CLA	C1D-ND	2.92	1.41	1.37
31	C	510	CLA	C1D-ND	2.92	1.41	1.37
31	c	510	CLA	C1D-ND	2.92	1.41	1.37
35	A	409	PL9	C6-C1	-2.92	1.43	1.48
43	5	305	A86	C13-C11	-2.92	1.44	1.49
31	2	309	CLA	CHC-C1C	2.92	1.42	1.35
43	9	306	A86	C40-C32	-2.92	1.48	1.53
31	B	615	CLA	C1D-ND	2.92	1.41	1.37
43	18	301	A86	C13-C11	-2.92	1.44	1.49
43	3	304	A86	O1-C20	-2.92	1.42	1.46
31	11	310	CLA	CHC-C1C	2.92	1.42	1.35
31	6	316	CLA	C4D-ND	-2.92	1.33	1.37
33	C	516	BCR	C30-C25	-2.92	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	8	308	KC2	C1B-NB	-2.92	1.34	1.37
45	18	310	KC2	C1B-NB	-2.92	1.34	1.37
31	d	404	CLA	CMB-C2B	-2.92	1.45	1.51
43	16	303	A86	O1-C20	-2.92	1.42	1.46
43	8	301	A86	C33-C34	2.92	1.57	1.51
31	R	101	CLA	CHC-C1C	2.92	1.42	1.35
34	A	408	SQD	O48-C23	2.92	1.41	1.33
31	12	315	CLA	C4D-ND	-2.92	1.33	1.37
31	b	610	CLA	C1D-ND	2.92	1.41	1.37
31	b	602	CLA	CHC-C1C	2.92	1.42	1.35
31	p	603	CLA	CMD-C2D	-2.91	1.44	1.50
31	p	603	CLA	CHC-C1C	2.91	1.42	1.35
31	r	101	CLA	CHC-C1C	2.91	1.42	1.35
31	13	316	CLA	CHC-C1C	2.91	1.42	1.35
43	8	303	A86	C13-C11	-2.91	1.44	1.49
31	C	508	CLA	C3B-C2B	-2.91	1.36	1.40
33	f	101	BCR	C1-C6	-2.91	1.49	1.53
33	Y	101	BCR	C33-C5	-2.91	1.46	1.50
42	6	315	KC1	C1B-NB	-2.91	1.34	1.37
31	a	403	CLA	CHC-C1C	2.91	1.42	1.35
31	7	315	CLA	CHC-C1C	2.91	1.42	1.35
31	7	313	CLA	MG-ND	-2.91	2.00	2.05
31	A	403	CLA	CHC-C1C	2.91	1.42	1.35
31	D	404	CLA	CMB-C2B	-2.91	1.45	1.51
31	a	404	CLA	CMB-C2B	-2.91	1.45	1.51
31	b	617	CLA	CMB-C2B	-2.91	1.45	1.51
31	10	313	CLA	C4D-ND	-2.91	1.33	1.37
31	19	315	CLA	C4D-ND	-2.91	1.33	1.37
31	2	314	CLA	C4D-ND	-2.90	1.33	1.37
31	10	307	CLA	CHC-C1C	2.90	1.42	1.35
43	p	613	A86	C30-C29	-2.90	1.27	1.32
31	3	315	CLA	CHC-C1C	2.90	1.42	1.35
43	14	305	A86	C30-C29	-2.90	1.27	1.32
31	15	307	CLA	CHC-C1C	2.90	1.42	1.35
34	a	408	SQD	O48-C23	2.90	1.41	1.33
31	b	614	CLA	CHC-C1C	2.90	1.42	1.35
43	9	306	A86	C30-C29	-2.90	1.27	1.32
43	16	303	A86	C13-C11	-2.90	1.44	1.49
43	10	304	A86	O1-C15	-2.90	1.40	1.45
31	5	306	CLA	CHC-C1C	2.90	1.42	1.35
31	0	313	CLA	C4D-ND	-2.89	1.33	1.37
35	d	406	PL9	C52-C5	-2.89	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	409	PL9	C6-C1	-2.89	1.43	1.48
31	C	502	CLA	C1D-ND	2.89	1.41	1.37
31	C	506	CLA	C1D-ND	2.89	1.41	1.37
31	b	615	CLA	CHC-C1C	2.89	1.42	1.35
43	0	304	A86	O1-C15	-2.89	1.40	1.45
31	A	404	CLA	CMB-C2B	-2.89	1.45	1.51
38	15	315	LMG	O1-C7	-2.89	1.38	1.43
31	B	603	CLA	C1D-ND	2.89	1.41	1.37
31	c	505	CLA	C1D-ND	2.89	1.41	1.37
43	18	304	A86	O1-C15	-2.89	1.40	1.45
35	D	406	PL9	C52-C5	-2.89	1.44	1.50
31	5	314	CLA	CHC-C1C	2.89	1.42	1.35
31	b	610	CLA	CHC-C1C	2.88	1.42	1.35
31	9	313	CLA	C1D-ND	2.88	1.41	1.37
31	B	606	CLA	CMD-C2D	-2.88	1.44	1.50
31	13	316	CLA	C4D-ND	-2.88	1.33	1.37
31	15	309	CLA	CHC-C1C	2.88	1.42	1.35
43	P	613	A86	C30-C29	-2.88	1.27	1.32
31	W	202	CLA	CHC-C1C	2.88	1.42	1.35
31	18	307	CLA	CMC-C2C	-2.88	1.44	1.50
31	17	313	CLA	MG-ND	-2.88	2.00	2.05
31	B	613	CLA	CHC-C1C	2.88	1.42	1.35
31	13	308	CLA	CMB-C2B	-2.88	1.45	1.51
31	B	609	CLA	CMB-C2B	-2.88	1.45	1.51
31	11	313	CLA	CMB-C2B	-2.88	1.45	1.51
31	7	307	CLA	C4D-ND	-2.88	1.33	1.37
39	B	621	DGD	O1G-C1G	-2.88	1.38	1.45
34	l	101	SQD	O48-C23	2.88	1.41	1.33
31	b	606	CLA	C1D-ND	2.88	1.41	1.37
31	C	512	CLA	CMB-C2B	-2.87	1.45	1.51
43	11	305	A86	C40-C32	-2.87	1.48	1.53
42	7	314	KC1	C4D-CHA	2.87	1.48	1.45
39	C	518	DGD	O5D-C6D	-2.87	1.38	1.43
39	c	518	DGD	O5D-C6D	-2.87	1.38	1.43
31	9	307	CLA	CHC-C1C	2.87	1.42	1.35
31	b	610	CLA	CMB-C2B	-2.87	1.45	1.51
43	9	301	A86	O1-C15	-2.87	1.40	1.45
42	16	301	KC1	C4D-CHA	2.87	1.48	1.45
31	B	605	CLA	C1D-ND	2.87	1.41	1.37
43	9	303	A86	C30-C29	-2.87	1.27	1.32
33	h	101	BCR	C1-C6	-2.87	1.49	1.53
43	14	301	A86	C13-C11	-2.87	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	19	301	A86	O1-C15	-2.87	1.40	1.45
31	1	310	CLA	CHC-C1C	2.87	1.42	1.35
31	b	604	CLA	C1D-ND	2.87	1.41	1.37
31	8	307	CLA	CMB-C2B	-2.87	1.45	1.51
31	b	607	CLA	C3B-C2B	-2.87	1.36	1.40
43	3	306	A86	C30-C29	-2.87	1.27	1.32
31	12	308	CLA	C1D-ND	2.86	1.41	1.37
43	17	302	A86	C13-C11	-2.86	1.44	1.49
31	14	312	CLA	C3B-C2B	-2.86	1.36	1.40
31	6	314	CLA	CHC-C1C	2.86	1.42	1.35
31	5	309	CLA	CHC-C1C	2.86	1.42	1.35
38	1	301	LMG	C4-C3	2.86	1.59	1.52
45	17	311	KC2	C1A-CHA	2.86	1.48	1.40
45	8	310	KC2	C1B-NB	-2.86	1.34	1.37
31	C	504	CLA	CHC-C1C	2.86	1.42	1.35
33	y	101	BCR	C33-C5	-2.86	1.46	1.50
45	1	311	KC2	C1B-NB	-2.86	1.34	1.37
38	11	301	LMG	C4-C3	2.86	1.59	1.52
43	17	302	A86	C40-C32	-2.86	1.48	1.53
31	B	609	CLA	CHC-C1C	2.86	1.42	1.35
31	2	307	CLA	CMD-C2D	-2.86	1.44	1.50
31	w	203	CLA	CHC-C1C	2.86	1.42	1.35
31	c	512	CLA	CMB-C2B	-2.86	1.45	1.51
36	L	101	LHG	O7-C5	-2.85	1.39	1.46
31	5	312	CLA	C3B-C2B	-2.85	1.36	1.40
31	4	307	CLA	CMB-C2B	-2.85	1.45	1.51
31	12	312	CLA	CHC-C1C	2.85	1.42	1.35
45	15	310	KC2	C4D-CHA	2.85	1.48	1.45
31	12	316	CLA	C4D-ND	-2.85	1.33	1.37
33	F	101	BCR	C1-C6	-2.85	1.49	1.53
34	L	102	SQD	O48-C23	2.85	1.41	1.33
31	17	315	CLA	CHC-C1C	2.85	1.42	1.35
31	p	601	CLA	C1D-ND	2.85	1.41	1.37
45	15	310	KC2	C1B-NB	-2.85	1.34	1.37
31	p	601	CLA	CHC-C1C	2.85	1.42	1.35
31	c	510	CLA	CHC-C1C	2.85	1.42	1.35
31	b	607	CLA	CMB-C2B	-2.85	1.45	1.51
31	16	311	CLA	CHC-C1C	2.84	1.42	1.35
31	17	312	CLA	CMD-C2D	-2.84	1.44	1.50
31	B	606	CLA	CMB-C2B	-2.84	1.45	1.51
45	18	308	KC2	C1B-NB	-2.84	1.34	1.37
31	c	504	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	306	CLA	CHC-C1C	2.84	1.42	1.35
31	P	601	CLA	CHC-C1C	2.84	1.42	1.35
31	A	403	CLA	C1D-ND	2.84	1.41	1.37
31	19	311	CLA	C4D-ND	-2.84	1.33	1.37
36	l	102	LHG	O7-C5	-2.84	1.39	1.46
31	18	311	CLA	CHC-C1C	2.84	1.42	1.35
31	8	314	CLA	CHC-C1C	2.84	1.42	1.35
42	10	315	KC1	C1A-CHA	2.84	1.48	1.40
43	13	306	A86	O1-C15	-2.84	1.40	1.45
43	8	303	A86	C26-C27	-2.84	1.32	1.35
35	D	406	PL9	C46-C44	-2.84	1.45	1.51
35	d	406	PL9	C46-C44	-2.84	1.45	1.51
31	10	311	CLA	C1D-ND	2.84	1.41	1.37
31	p	605	CLA	CHC-C1C	2.83	1.42	1.35
31	2	306	CLA	CHC-C1C	2.83	1.42	1.35
31	7	312	CLA	CMD-C2D	-2.83	1.44	1.50
31	12	312	CLA	C4D-ND	-2.83	1.33	1.37
43	13	305	A86	C30-C29	-2.83	1.27	1.32
42	16	301	KC1	C1B-NB	-2.83	1.34	1.37
43	7	301	A86	C13-C11	-2.83	1.44	1.49
43	15	301	A86	C32-C31	-2.83	1.49	1.54
43	15	304	A86	C35-C34	2.83	1.56	1.51
31	18	309	CLA	CHC-C1C	2.83	1.42	1.35
33	H	101	BCR	C1-C6	-2.83	1.49	1.53
43	17	305	A86	C30-C29	-2.83	1.27	1.32
42	16	315	KC1	C1B-NB	-2.82	1.34	1.37
31	C	510	CLA	CHC-C1C	2.82	1.42	1.35
31	p	606	CLA	CHC-C1C	2.82	1.42	1.35
31	B	616	CLA	C3B-C2B	-2.82	1.36	1.40
39	C	518	DGD	O4D-C4D	-2.82	1.36	1.43
33	B	617	BCR	C30-C25	-2.82	1.49	1.53
31	0	311	CLA	C1D-ND	2.82	1.41	1.37
45	12	309	KC2	C1B-NB	-2.82	1.34	1.37
31	8	307	CLA	CMC-C2C	-2.82	1.44	1.50
31	8	309	CLA	CHC-C1C	2.82	1.42	1.35
43	0	305	A86	C30-C29	-2.82	1.27	1.32
31	13	315	CLA	C4D-ND	-2.82	1.33	1.37
45	4	310	KC2	C1B-NB	-2.82	1.34	1.37
31	4	315	CLA	CMB-C2B	-2.82	1.45	1.51
31	8	311	CLA	CHC-C1C	2.82	1.42	1.35
31	8	311	CLA	C4D-ND	-2.82	1.33	1.37
31	8	312	CLA	C3B-CAB	-2.82	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	511	CLA	CHC-C1C	2.82	1.42	1.35
31	c	511	CLA	CHC-C1C	2.82	1.42	1.35
43	7	302	A86	C32-C31	-2.81	1.49	1.54
43	13	303	A86	O1-C20	-2.81	1.42	1.46
31	b	617	CLA	C3B-C2B	-2.81	1.36	1.40
33	b	618	BCR	C30-C25	-2.81	1.49	1.53
31	P	605	CLA	CHC-C1C	2.81	1.42	1.35
31	17	308	CLA	CMD-C2D	-2.81	1.44	1.50
38	N	101	LMG	O2-C2	-2.81	1.36	1.43
34	A	411	SQD	O47-C7	2.81	1.42	1.34
34	i	101	SQD	O47-C7	2.81	1.42	1.34
43	2	303	A86	C30-C29	-2.81	1.27	1.32
31	c	514	CLA	C1D-ND	2.81	1.41	1.37
31	9	310	CLA	C4D-ND	-2.81	1.33	1.37
43	1	306	A86	O1-C15	-2.81	1.40	1.45
31	7	308	CLA	CMD-C2D	-2.81	1.44	1.50
31	8	307	CLA	CMD-C2D	-2.81	1.44	1.50
31	p	606	CLA	C4D-ND	-2.80	1.33	1.37
35	D	406	PL9	C11-C9	-2.80	1.45	1.51
35	d	406	PL9	C11-C9	-2.80	1.45	1.51
31	a	403	CLA	C1D-ND	2.80	1.41	1.37
31	P	606	CLA	CHC-C1C	2.80	1.42	1.35
31	4	311	CLA	CMD-C2D	-2.80	1.44	1.50
43	7	306	A86	C19-C20	2.80	1.56	1.52
31	C	506	CLA	CMD-C2D	-2.80	1.44	1.50
31	c	506	CLA	CMD-C2D	-2.80	1.44	1.50
43	1	303	A86	C13-C11	-2.80	1.44	1.49
42	16	315	KC1	C1D-CHD	2.80	1.48	1.41
31	B	603	CLA	CAC-C3C	-2.79	1.43	1.51
42	p	609	KC1	CHC-C1C	2.79	1.45	1.39
31	0	313	CLA	C3B-C2B	-2.79	1.36	1.40
31	11	307	CLA	C4D-ND	-2.79	1.33	1.37
31	16	316	CLA	C4D-ND	-2.79	1.33	1.37
31	b	611	CLA	CMB-C2B	-2.79	1.45	1.51
43	4	306	A86	C13-C11	-2.79	1.44	1.49
43	4	301	A86	O1-C20	-2.79	1.42	1.46
31	11	308	CLA	C1D-ND	2.79	1.41	1.37
31	9	312	CLA	C4D-ND	-2.79	1.33	1.37
31	B	606	CLA	C3B-C2B	-2.79	1.36	1.40
43	1	319	A86	C30-C29	-2.79	1.27	1.32
31	19	310	CLA	C4D-ND	-2.79	1.33	1.37
31	6	311	CLA	CHC-C1C	2.78	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	505	CLA	CMB-C2B	-2.78	1.45	1.51
31	c	505	CLA	CMB-C2B	-2.78	1.45	1.51
31	d	401	CLA	C1D-ND	2.78	1.41	1.37
31	6	316	CLA	CHC-C1C	2.78	1.42	1.35
31	12	315	CLA	CHC-C1C	2.78	1.42	1.35
45	1	309	KC2	C1B-NB	-2.78	1.34	1.37
31	b	613	CLA	CHC-C1C	2.78	1.42	1.35
31	P	606	CLA	C4D-ND	-2.78	1.33	1.37
31	6	313	CLA	CMD-C2D	-2.78	1.44	1.50
42	P	609	KC1	CHC-C1C	2.78	1.45	1.39
31	2	311	CLA	CMD-C2D	-2.77	1.44	1.50
31	W	202	CLA	CMB-C2B	-2.77	1.45	1.51
31	1	312	CLA	CMB-C2B	-2.77	1.45	1.51
31	5	307	CLA	CMB-C2B	-2.77	1.45	1.51
31	B	614	CLA	CMB-C2B	-2.77	1.45	1.51
31	B	606	CLA	CHC-C1C	2.77	1.42	1.35
31	B	608	CLA	CMD-C2D	-2.77	1.44	1.50
31	1	307	CLA	CHC-C1C	2.77	1.42	1.35
31	3	312	CLA	CMD-C2D	-2.77	1.44	1.50
31	B	604	CLA	CAC-C3C	-2.77	1.44	1.51
39	c	518	DGD	O2G-C2G	-2.77	1.39	1.46
31	11	313	CLA	C3B-C2B	-2.77	1.36	1.40
35	D	406	PL9	C36-C34	-2.77	1.45	1.51
35	d	406	PL9	C36-C34	-2.77	1.45	1.51
39	C	518	DGD	O2G-C2G	-2.77	1.39	1.46
31	C	502	CLA	CHC-C1C	2.77	1.42	1.35
31	b	609	CLA	CHC-C1C	2.77	1.42	1.35
31	16	314	CLA	C1D-ND	2.77	1.41	1.37
31	C	513	CLA	CHC-C1C	2.77	1.42	1.35
31	a	404	CLA	CHC-C1C	2.77	1.42	1.35
31	c	513	CLA	CHC-C1C	2.77	1.42	1.35
43	10	305	A86	C30-C29	-2.77	1.27	1.32
31	B	612	CLA	CHC-C1C	2.77	1.42	1.35
31	10	313	CLA	CMB-C2B	-2.77	1.45	1.51
43	11	302	A86	C32-C31	2.77	1.59	1.54
39	c	518	DGD	O4D-C4D	-2.77	1.36	1.43
39	w	204	DGD	O2G-C2G	-2.76	1.39	1.46
31	b	615	CLA	CMB-C2B	-2.76	1.45	1.51
31	1	316	CLA	CHC-C1C	2.76	1.42	1.35
31	b	605	CLA	CAC-C3C	-2.76	1.44	1.51
43	p	611	A86	C35-C34	2.76	1.56	1.51
38	k	101	LMG	O6-C5	-2.76	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	12	311	KC2	C1B-NB	-2.76	1.34	1.37
31	13	312	CLA	CHC-C1C	2.76	1.42	1.35
31	B	615	CLA	CMB-C2B	-2.76	1.45	1.51
31	6	309	CLA	C1D-ND	2.76	1.41	1.37
38	F	102	LMG	O7-C8	-2.76	1.39	1.46
38	K	101	LMG	O6-C5	-2.76	1.37	1.44
38	11	317	LMG	C4-C5	2.75	1.58	1.53
31	b	604	CLA	CAC-C3C	-2.75	1.44	1.51
31	19	307	CLA	C4D-ND	-2.75	1.33	1.37
31	b	612	CLA	CHC-C1C	2.75	1.42	1.35
43	6	302	A86	C13-C11	-2.75	1.44	1.49
31	B	608	CLA	CHC-C1C	2.75	1.42	1.35
31	Z	101	CLA	CHC-C1C	2.75	1.42	1.35
31	w	203	CLA	CMB-C2B	-2.75	1.45	1.51
31	0	309	CLA	C1D-ND	2.75	1.41	1.37
32	D	402	PHO	CAC-C3C	-2.75	1.47	1.52
42	18	313	KC1	C1D-CHD	2.75	1.48	1.41
31	A	404	CLA	CHC-C1C	2.75	1.42	1.35
43	11	320	A86	O1-C20	-2.75	1.42	1.46
31	C	507	CLA	CHC-C1C	2.75	1.42	1.35
31	c	507	CLA	CHC-C1C	2.75	1.42	1.35
45	14	310	KC2	C1B-NB	-2.75	1.34	1.37
39	W	203	DGD	O2G-C2G	-2.75	1.39	1.46
31	1	308	CLA	CMB-C2B	-2.75	1.45	1.51
31	B	616	CLA	CMC-C2C	-2.74	1.45	1.50
31	16	316	CLA	CHC-C1C	2.74	1.42	1.35
43	12	306	A86	C13-C11	-2.74	1.44	1.49
31	z	101	CLA	CHC-C1C	2.74	1.42	1.35
31	C	514	CLA	C1D-ND	2.74	1.41	1.37
31	18	312	CLA	C3B-CAB	-2.74	1.42	1.47
43	17	302	A86	C37-C36	-2.74	1.48	1.52
31	P	608	CLA	CHC-C1C	2.74	1.42	1.35
31	B	610	CLA	CMB-C2B	-2.74	1.45	1.51
31	D	401	CLA	C1D-ND	2.74	1.41	1.37
43	11	320	A86	C30-C29	-2.74	1.27	1.32
31	17	307	CLA	C4D-ND	-2.74	1.33	1.37
43	8	304	A86	C33-C34	2.74	1.56	1.51
42	6	315	KC1	C4D-CHA	2.74	1.48	1.45
31	p	608	CLA	CHC-C1C	2.74	1.42	1.35
43	0	302	A86	C17-C16	2.74	1.58	1.54
43	17	301	A86	C32-C31	-2.74	1.50	1.54
45	2	310	KC2	C1B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	16	305	A86	C13-C11	-2.74	1.44	1.49
43	5	303	A86	C30-C29	-2.73	1.27	1.32
32	d	402	PHO	CAC-C3C	-2.73	1.47	1.52
31	b	616	CLA	CMB-C2B	-2.73	1.46	1.51
31	14	307	CLA	C1D-ND	2.73	1.41	1.37
31	4	311	CLA	C4D-ND	-2.73	1.33	1.37
31	9	315	CLA	C4D-ND	-2.73	1.33	1.37
45	14	308	KC2	C1B-NB	-2.73	1.34	1.37
31	c	502	CLA	CHC-C1C	2.73	1.42	1.35
45	3	311	KC2	C1A-CHA	2.73	1.47	1.40
31	A	406	CLA	C1D-ND	2.73	1.41	1.37
43	10	306	A86	C13-C11	-2.73	1.44	1.49
38	n	701	LMG	O2-C2	-2.73	1.36	1.43
39	W	203	DGD	C1E-C2E	2.73	1.60	1.52
43	6	304	A86	C13-C11	-2.73	1.44	1.49
43	P	611	A86	C35-C34	2.73	1.56	1.51
34	10	320	SQD	O47-C7	2.73	1.42	1.34
31	b	609	CLA	CMD-C2D	-2.73	1.45	1.50
39	C	518	DGD	O2D-C2D	-2.73	1.36	1.43
31	18	314	CLA	CHC-C1C	2.73	1.42	1.35
31	18	314	CLA	CMB-C2B	-2.73	1.46	1.51
34	B	623	SQD	O47-C7	2.73	1.42	1.34
39	c	518	DGD	O2D-C2D	-2.73	1.36	1.43
31	9	307	CLA	C4D-ND	-2.72	1.33	1.37
31	11	308	CLA	CMB-C2B	-2.72	1.46	1.51
31	d	405	CLA	CMB-C2B	-2.72	1.46	1.51
31	C	511	CLA	CMD-C2D	-2.72	1.45	1.50
34	b	601	SQD	O47-C7	2.72	1.42	1.34
38	Z	102	LMG	C4-C5	2.72	1.58	1.53
31	19	312	CLA	C4D-ND	-2.72	1.33	1.37
31	B	611	CLA	CHC-C1C	2.72	1.41	1.35
31	b	606	CLA	CMB-C2B	-2.72	1.46	1.51
34	0	318	SQD	O47-C7	2.72	1.42	1.34
42	8	313	KC1	C1D-CHD	2.72	1.48	1.41
38	f	102	LMG	O7-C8	-2.72	1.39	1.46
31	B	604	CLA	MG-ND	-2.72	2.00	2.05
31	b	605	CLA	MG-ND	-2.72	2.00	2.05
31	8	314	CLA	CMB-C2B	-2.72	1.46	1.51
45	3	309	KC2	C1A-CHA	2.72	1.47	1.40
39	C	519	DGD	O4E-C4E	-2.72	1.36	1.43
31	1	321	CLA	CHC-C1C	2.71	1.41	1.35
39	w	204	DGD	C1E-C2E	2.71	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	513	CLA	C1D-ND	2.71	1.41	1.37
45	3	309	KC2	C3C-C4C	2.71	1.50	1.44
43	3	301	A86	O1-C20	-2.71	1.42	1.46
31	b	607	CLA	CHC-C1C	2.71	1.41	1.35
31	c	510	CLA	CMB-C2B	-2.71	1.46	1.51
31	b	616	CLA	CHC-C1C	2.71	1.41	1.35
31	6	314	CLA	C1D-ND	2.71	1.41	1.37
43	0	306	A86	C13-C11	-2.71	1.44	1.49
31	D	405	CLA	CMB-C2B	-2.71	1.46	1.51
31	B	615	CLA	CHC-C1C	2.70	1.41	1.35
43	1	305	A86	O1-C20	-2.70	1.42	1.46
31	p	606	CLA	MG-NA	-2.70	1.99	2.06
43	19	304	A86	C30-C29	-2.70	1.27	1.32
43	12	306	A86	C30-C29	-2.70	1.27	1.32
31	B	606	CLA	C3B-CAB	-2.70	1.42	1.47
31	3	308	CLA	C1D-ND	2.70	1.41	1.37
31	15	311	CLA	CMD-C2D	-2.70	1.45	1.50
45	11	311	KC2	C1B-NB	-2.70	1.34	1.37
43	9	304	A86	O1-C15	-2.70	1.41	1.45
31	P	606	CLA	MG-NA	-2.70	1.99	2.06
31	14	312	CLA	C1D-ND	2.70	1.41	1.37
31	B	607	CLA	CHC-C1C	2.70	1.41	1.35
31	b	608	CLA	CHC-C1C	2.70	1.41	1.35
31	14	311	CLA	C4D-ND	-2.70	1.34	1.37
31	P	602	CLA	C1D-ND	2.69	1.41	1.37
31	p	607	CLA	CMB-C2B	-2.69	1.46	1.51
31	C	507	CLA	C3B-C2B	-2.69	1.36	1.40
31	c	507	CLA	C3B-C2B	-2.69	1.36	1.40
45	4	308	KC2	C1B-NB	-2.69	1.34	1.37
31	b	602	CLA	C3B-CAB	-2.69	1.42	1.47
42	11	314	KC1	C4D-CHA	2.69	1.48	1.45
31	18	306	CLA	C3B-C2B	-2.69	1.36	1.40
31	P	603	CLA	CMB-C2B	-2.69	1.46	1.51
31	Z	101	CLA	CMB-C2B	-2.69	1.46	1.51
31	14	307	CLA	CMB-C2B	-2.69	1.46	1.51
43	14	303	A86	C30-C29	-2.69	1.27	1.32
31	b	602	CLA	C3B-C2B	-2.69	1.36	1.40
33	c	517	BCR	C30-C25	-2.69	1.50	1.53
39	W	203	DGD	O5D-C1E	2.69	1.44	1.40
39	w	204	DGD	O5D-C1E	2.69	1.44	1.40
43	6	305	A86	C14-C13	2.69	1.54	1.51
31	6	309	CLA	CMD-C2D	-2.69	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	0	302	A86	C30-C29	-2.69	1.27	1.32
45	13	309	KC2	C1A-CHA	2.68	1.47	1.40
31	c	511	CLA	CMD-C2D	-2.68	1.45	1.50
31	15	312	CLA	C1A-CHA	-2.68	1.32	1.43
34	A	408	SQD	O47-C7	2.68	1.41	1.34
34	a	408	SQD	O47-C7	2.68	1.41	1.34
31	14	306	CLA	C1B-NB	-2.68	1.32	1.35
45	18	310	KC2	C1A-CHA	2.68	1.47	1.40
43	8	302	A86	C13-C11	-2.68	1.44	1.49
43	15	301	A86	O3-C36	-2.68	1.38	1.43
43	11	319	A86	C30-C29	-2.68	1.27	1.32
31	6	308	CLA	CHC-C1C	2.68	1.41	1.35
31	10	313	CLA	C3B-C2B	-2.68	1.36	1.40
31	13	307	CLA	CHC-C1C	2.68	1.41	1.35
43	6	302	A86	C33-C34	2.68	1.56	1.51
42	17	314	KC1	C1A-CHA	2.68	1.47	1.40
39	c	519	DGD	O4E-C4E	-2.68	1.36	1.43
43	1	302	A86	C30-C29	-2.68	1.27	1.32
31	C	510	CLA	CMB-C2B	-2.68	1.46	1.51
43	12	304	A86	C30-C29	-2.67	1.27	1.32
31	b	607	CLA	C3B-CAB	-2.67	1.42	1.47
33	h	101	BCR	C30-C25	-2.67	1.50	1.53
31	c	505	CLA	C3B-C2B	-2.67	1.36	1.40
39	b	622	DGD	O1G-C1G	-2.67	1.39	1.45
42	3	314	KC1	C1A-CHA	2.67	1.47	1.40
31	10	308	CLA	C4D-ND	-2.67	1.34	1.37
31	a	406	CLA	C1D-ND	2.67	1.41	1.37
43	3	301	A86	C5-C6	-2.67	1.32	1.35
31	12	315	CLA	CMB-C2B	-2.67	1.46	1.51
31	0	308	CLA	C4D-ND	-2.67	1.34	1.37
31	6	308	CLA	C4D-ND	-2.67	1.34	1.37
31	10	317	CLA	CHC-C1C	2.67	1.41	1.35
31	R	101	CLA	CMB-C2B	-2.67	1.46	1.51
31	b	617	CLA	CMC-C2C	-2.67	1.45	1.50
31	c	513	CLA	C1D-ND	2.67	1.41	1.37
31	P	606	CLA	CMB-C2B	-2.67	1.46	1.51
31	C	505	CLA	C3B-C2B	-2.66	1.36	1.40
42	7	314	KC1	C1B-NB	-2.66	1.34	1.37
33	H	101	BCR	C30-C25	-2.66	1.50	1.53
31	11	313	CLA	MG-ND	-2.66	2.00	2.05
45	2	310	KC2	C1A-CHA	2.66	1.47	1.40
31	3	313	CLA	MG-ND	-2.66	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	605	CLA	CMB-C2B	-2.66	1.46	1.51
43	4	305	A86	C37-C36	2.66	1.57	1.52
43	12	302	A86	C13-C11	-2.66	1.44	1.49
31	z	101	CLA	CMB-C2B	-2.66	1.46	1.51
31	3	316	CLA	CMB-C2B	-2.66	1.46	1.51
31	C	512	CLA	CHC-C1C	2.66	1.41	1.35
31	p	606	CLA	C1C-NC	-2.66	1.33	1.37
31	0	312	CLA	CMD-C2D	-2.66	1.45	1.50
39	c	520	DGD	O2G-C2G	-2.65	1.40	1.46
43	18	304	A86	C33-C34	2.65	1.56	1.51
31	P	607	CLA	CMB-C2B	-2.65	1.46	1.51
31	11	315	CLA	CMB-C2B	-2.65	1.46	1.51
31	8	311	CLA	C3B-C2B	-2.65	1.36	1.40
43	19	304	A86	O1-C15	-2.65	1.41	1.45
42	16	301	KC1	C1A-CHA	2.65	1.47	1.40
31	P	606	CLA	C3B-CAB	-2.65	1.42	1.47
31	p	606	CLA	C3B-CAB	-2.65	1.42	1.47
31	b	614	CLA	CMB-C2B	-2.65	1.46	1.51
31	18	306	CLA	CHC-C1C	2.65	1.41	1.35
31	P	608	CLA	CMB-C2B	-2.65	1.46	1.51
42	0	315	KC1	C1B-NB	-2.65	1.34	1.37
43	17	302	A86	O3-C36	2.65	1.47	1.43
31	8	311	CLA	CMB-C2B	-2.65	1.46	1.51
31	18	311	CLA	CMB-C2B	-2.65	1.46	1.51
31	17	308	CLA	C1D-ND	2.64	1.41	1.37
31	8	306	CLA	CHC-C1C	2.64	1.41	1.35
39	C	520	DGD	O2G-C2G	-2.64	1.40	1.46
45	17	309	KC2	C3C-C4C	2.64	1.50	1.44
31	b	604	CLA	C3B-C2B	-2.64	1.36	1.40
31	1	312	CLA	CMD-C2D	-2.64	1.45	1.50
31	c	502	CLA	CMB-C2B	-2.64	1.46	1.51
45	18	308	KC2	C3C-C4C	2.64	1.50	1.44
43	13	301	A86	C33-C34	2.64	1.56	1.51
43	11	306	A86	C14-C15	2.64	1.57	1.52
31	16	314	CLA	C3D-C2D	-2.64	1.31	1.39
31	r	101	CLA	CMB-C2B	-2.64	1.46	1.51
39	C	520	DGD	O2E-C2E	-2.64	1.36	1.43
31	B	601	CLA	C3B-CAB	-2.64	1.42	1.47
31	c	508	CLA	CHC-C1C	2.64	1.41	1.35
43	11	304	A86	C13-C11	-2.64	1.44	1.49
31	2	315	CLA	CMC-C2C	-2.64	1.45	1.50
31	D	401	CLA	CHC-C1C	2.64	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	5	313	KC1	C1B-NB	-2.64	1.34	1.37
31	D	404	CLA	CMC-C2C	-2.64	1.45	1.50
31	P	606	CLA	C1C-NC	-2.64	1.33	1.37
31	W	202	CLA	CMC-C2C	-2.64	1.45	1.50
36	B	622	LHG	O7-C5	-2.64	1.40	1.46
36	b	623	LHG	O7-C5	-2.64	1.40	1.46
45	7	311	KC2	C1A-CHA	2.63	1.47	1.40
31	p	606	CLA	CMB-C2B	-2.63	1.46	1.51
31	C	508	CLA	CHC-C1C	2.63	1.41	1.35
43	4	305	A86	C40-C32	-2.63	1.48	1.53
31	p	603	CLA	CMB-C2B	-2.63	1.46	1.51
31	c	512	CLA	CHC-C1C	2.63	1.41	1.35
31	11	312	CLA	CHC-C1C	2.63	1.41	1.35
31	11	313	CLA	C3B-CAB	-2.63	1.42	1.47
43	18	301	A86	C30-C29	-2.63	1.27	1.32
38	c	522	LMG	C4-C5	2.63	1.58	1.53
33	c	515	BCR	C1-C6	-2.63	1.50	1.53
31	p	608	CLA	CMB-C2B	-2.63	1.46	1.51
45	4	308	KC2	C1A-CHA	2.62	1.47	1.40
31	p	602	CLA	C1D-ND	2.62	1.41	1.37
43	17	302	A86	C33-C34	2.62	1.56	1.51
31	C	502	CLA	CMB-C2B	-2.62	1.46	1.51
31	w	203	CLA	CMC-C2C	-2.62	1.45	1.50
43	4	305	A86	C13-C11	-2.62	1.44	1.49
31	4	314	CLA	CMB-C2B	-2.62	1.46	1.51
31	0	312	CLA	CMB-C2B	-2.62	1.46	1.51
31	z	103	CLA	C3B-C2B	-2.62	1.36	1.40
31	P	601	CLA	CMB-C2B	-2.62	1.46	1.51
31	b	605	CLA	CMD-C2D	-2.62	1.45	1.50
31	6	308	CLA	CMB-C2B	-2.62	1.46	1.51
31	B	605	CLA	CMD-C2D	-2.62	1.45	1.50
31	13	312	CLA	C4D-ND	-2.62	1.34	1.37
31	6	309	CLA	CMB-C2B	-2.62	1.46	1.51
31	16	309	CLA	CMB-C2B	-2.62	1.46	1.51
31	A	406	CLA	CMB-C2B	-2.62	1.46	1.51
33	C	517	BCR	C30-C25	-2.62	1.50	1.53
38	J	101	LMG	C4-C5	2.62	1.58	1.53
32	A	405	PHO	CMD-C2D	-2.62	1.45	1.51
31	p	601	CLA	CMB-C2B	-2.61	1.46	1.51
31	10	312	CLA	CMD-C2D	-2.61	1.45	1.50
45	2	308	KC2	C1D-CHD	2.61	1.48	1.41
31	3	308	CLA	C3B-C2B	-2.61	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	613	CLA	CMB-C2B	-2.61	1.46	1.51
36	d	407	LHG	O7-C5	-2.61	1.40	1.46
43	18	305	A86	C13-C11	-2.61	1.44	1.49
31	B	603	CLA	C3B-C2B	-2.61	1.36	1.40
31	z	103	CLA	CHC-C1C	2.61	1.41	1.35
36	D	407	LHG	O7-C5	-2.61	1.40	1.46
31	B	612	CLA	MG-ND	-2.61	2.00	2.05
31	d	401	CLA	CHC-C1C	2.61	1.41	1.35
31	18	311	CLA	MG-ND	-2.61	2.00	2.05
31	c	505	CLA	CMD-C2D	-2.61	1.45	1.50
38	1	317	LMG	C4-C5	2.61	1.58	1.53
45	8	308	KC2	C3C-C4C	2.61	1.50	1.44
31	11	312	CLA	C3B-C2B	-2.61	1.36	1.40
43	5	318	A86	C30-C29	-2.61	1.27	1.32
31	3	307	CLA	CMB-C2B	-2.61	1.46	1.51
45	13	311	KC2	C1D-CHD	2.61	1.48	1.41
31	11	312	CLA	CMD-C2D	-2.61	1.45	1.50
43	12	301	A86	C33-C34	2.60	1.56	1.51
31	13	315	CLA	CMB-C2B	-2.60	1.46	1.51
43	19	303	A86	C30-C29	-2.60	1.27	1.32
39	c	520	DGD	O2E-C2E	-2.60	1.36	1.43
31	14	314	CLA	CMB-C2B	-2.60	1.46	1.51
31	b	609	CLA	C1D-ND	2.60	1.41	1.37
43	3	301	A86	C40-C32	-2.60	1.48	1.53
45	7	309	KC2	C3C-C4C	2.60	1.50	1.44
43	18	304	A86	C13-C11	-2.60	1.44	1.49
31	B	604	CLA	CMD-C2D	-2.60	1.45	1.50
31	5	312	CLA	MG-ND	-2.60	2.00	2.05
31	d	404	CLA	CMC-C2C	-2.60	1.45	1.50
38	j	101	LMG	C4-C5	2.60	1.58	1.53
31	a	406	CLA	CMB-C2B	-2.59	1.46	1.51
31	16	308	CLA	C4D-ND	-2.59	1.34	1.37
38	k	101	LMG	O8-C9	-2.59	1.39	1.45
31	B	601	CLA	C3B-C2B	-2.59	1.36	1.40
32	a	405	PHO	CMD-C2D	-2.59	1.45	1.51
31	C	504	CLA	CMB-C2B	-2.59	1.46	1.51
31	c	504	CLA	CMB-C2B	-2.59	1.46	1.51
43	16	306	A86	C14-C13	2.59	1.54	1.51
38	5	316	LMG	C4-C3	2.59	1.58	1.52
31	b	613	CLA	MG-ND	-2.59	2.00	2.05
31	1	321	CLA	CMB-C2B	-2.59	1.46	1.51
31	C	505	CLA	CMD-C2D	-2.58	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	10	313	CLA	CMD-C2D	-2.58	1.45	1.50
42	9	314	KC1	C1A-CHA	2.58	1.47	1.40
43	8	304	A86	C13-C11	-2.58	1.44	1.49
31	P	606	CLA	CMD-C2D	-2.58	1.45	1.50
31	p	606	CLA	CMD-C2D	-2.58	1.45	1.50
45	14	308	KC2	C1A-CHA	2.58	1.47	1.40
31	B	612	CLA	CMB-C2B	-2.58	1.46	1.51
31	b	613	CLA	CMB-C2B	-2.58	1.46	1.51
31	2	307	CLA	CMB-C2B	-2.58	1.46	1.51
31	1	313	CLA	C3B-CAB	-2.58	1.42	1.47
31	C	512	CLA	C3B-CAB	-2.58	1.42	1.47
31	c	512	CLA	C3B-CAB	-2.58	1.42	1.47
39	C	519	DGD	O1G-C1G	-2.58	1.39	1.45
39	c	519	DGD	O1G-C1G	-2.58	1.39	1.45
45	16	310	KC2	C1B-NB	-2.58	1.34	1.37
45	2	308	KC2	C3C-C4C	2.58	1.50	1.44
38	K	101	LMG	O8-C9	-2.58	1.39	1.45
31	5	311	CLA	CMD-C2D	-2.58	1.45	1.50
31	b	606	CLA	CMD-C2D	-2.57	1.45	1.50
31	d	404	CLA	C3B-C2B	-2.57	1.36	1.40
42	3	314	KC1	C1B-NB	-2.57	1.34	1.37
31	6	314	CLA	C3B-C2B	-2.57	1.36	1.40
43	1	319	A86	C13-C11	-2.57	1.44	1.49
31	B	608	CLA	C1D-ND	2.57	1.40	1.37
31	13	313	CLA	MG-ND	-2.57	2.00	2.05
45	16	310	KC2	C3C-C4C	2.57	1.50	1.44
31	1	312	CLA	CHC-C1C	2.57	1.41	1.35
31	b	606	CLA	CHC-C1C	2.57	1.41	1.35
45	19	309	KC2	C1B-NB	-2.57	1.34	1.37
31	b	607	CLA	CMC-C2C	-2.57	1.45	1.50
31	B	605	CLA	CHC-C1C	2.57	1.41	1.35
31	14	315	CLA	CMB-C2B	-2.57	1.46	1.51
31	15	309	CLA	CMB-C2B	-2.56	1.46	1.51
45	12	309	KC2	C1A-CHA	2.56	1.47	1.40
31	C	513	CLA	CMB-C2B	-2.56	1.46	1.51
31	b	612	CLA	C1D-ND	2.56	1.40	1.37
31	18	307	CLA	MG-ND	-2.56	2.00	2.05
31	14	306	CLA	CMB-C2B	-2.56	1.46	1.51
31	3	313	CLA	C1D-ND	2.56	1.40	1.37
31	18	311	CLA	C3B-C2B	-2.56	1.36	1.40
31	16	308	CLA	CMB-C2B	-2.56	1.46	1.51
31	13	307	CLA	CMB-C2B	-2.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	19	301	A86	C33-C34	2.56	1.56	1.51
45	10	310	KC2	C4B-NB	-2.56	1.34	1.37
43	16	303	A86	C33-C34	2.56	1.56	1.51
31	P	607	CLA	C3B-C2B	-2.56	1.36	1.40
31	11	316	CLA	CMB-C2B	-2.56	1.46	1.51
45	2	310	KC2	C1D-CHD	2.56	1.48	1.41
43	17	303	A86	C19-C20	2.56	1.55	1.52
43	13	302	A86	C13-C11	-2.55	1.44	1.49
42	6	315	KC1	C4C-C3C	2.55	1.49	1.45
31	a	406	CLA	CMD-C2D	-2.55	1.45	1.50
43	3	305	A86	O4-C34	-2.55	1.40	1.46
31	10	308	CLA	CHC-C1C	2.55	1.41	1.35
31	4	312	CLA	CMD-C2D	-2.55	1.45	1.50
33	Y	101	BCR	C38-C26	-2.55	1.46	1.50
31	p	604	CLA	CMB-C2B	-2.55	1.46	1.51
43	13	306	A86	C13-C11	-2.55	1.44	1.49
43	16	306	A86	C33-C34	2.55	1.56	1.51
31	4	307	CLA	C1D-ND	2.55	1.40	1.37
31	P	604	CLA	CMB-C2B	-2.55	1.46	1.51
45	6	310	KC2	C1B-NB	-2.55	1.34	1.37
31	p	607	CLA	C1D-ND	2.55	1.40	1.37
31	B	601	CLA	CMC-C2C	-2.55	1.45	1.50
31	b	602	CLA	CMC-C2C	-2.55	1.45	1.50
31	15	307	CLA	CMD-C2D	-2.55	1.45	1.50
45	16	310	KC2	C1A-CHA	2.55	1.47	1.40
43	2	304	A86	O1-C15	-2.54	1.41	1.45
31	b	602	CLA	CMB-C2B	-2.54	1.46	1.51
45	3	309	KC2	C1B-NB	-2.54	1.34	1.37
31	10	311	CLA	CMB-C2B	-2.54	1.46	1.51
31	D	401	CLA	CMD-C2D	-2.54	1.45	1.50
31	0	308	CLA	CHC-C1C	2.54	1.41	1.35
38	c	521	LMG	C4-C5	2.54	1.58	1.53
31	P	610	CLA	CMB-C2B	-2.54	1.46	1.51
31	5	312	CLA	CMD-C2D	-2.54	1.45	1.50
31	0	311	CLA	CMB-C2B	-2.54	1.46	1.51
45	3	309	KC2	C1D-CHD	2.54	1.48	1.41
31	17	308	CLA	CMB-C2B	-2.54	1.46	1.51
31	7	308	CLA	CMB-C2B	-2.54	1.46	1.51
31	10	312	CLA	CMB-C2B	-2.54	1.46	1.51
31	d	401	CLA	CMD-C2D	-2.53	1.45	1.50
45	7	309	KC2	C1D-CHD	2.53	1.48	1.41
31	17	308	CLA	C3B-C2B	-2.53	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	515	BCR	C1-C6	-2.53	1.50	1.53
31	A	406	CLA	CMD-C2D	-2.53	1.45	1.50
45	17	309	KC2	C1D-CHD	2.53	1.48	1.41
31	b	605	CLA	C1D-ND	2.53	1.40	1.37
34	a	408	SQD	O2-C2	-2.53	1.37	1.43
31	B	601	CLA	CMB-C2B	-2.53	1.46	1.51
43	9	306	A86	C41-C32	2.53	1.58	1.53
43	3	301	A86	C26-C27	-2.53	1.32	1.35
31	5	309	CLA	CMB-C2B	-2.53	1.46	1.51
31	1	316	CLA	C3B-C2B	-2.53	1.36	1.40
43	10	302	A86	C13-C11	-2.53	1.44	1.49
43	15	305	A86	O1-C20	-2.53	1.42	1.46
38	15	315	LMG	O8-C9	-2.53	1.39	1.45
31	0	314	CLA	CMB-C2B	-2.53	1.46	1.51
45	6	312	KC2	C1D-CHD	2.52	1.48	1.41
31	C	509	CLA	MG-ND	-2.52	2.00	2.05
31	c	509	CLA	MG-ND	-2.52	2.00	2.05
31	10	307	CLA	MG-ND	-2.52	2.00	2.05
31	C	511	CLA	CMB-C2B	-2.52	1.46	1.51
31	c	511	CLA	CMB-C2B	-2.52	1.46	1.51
31	p	610	CLA	CMB-C2B	-2.52	1.46	1.51
34	A	408	SQD	O2-C2	-2.52	1.37	1.43
38	15	315	LMG	C4-C3	2.52	1.58	1.52
31	1	313	CLA	C3B-C2B	-2.52	1.36	1.40
39	C	518	DGD	O3G-C3G	-2.52	1.39	1.43
39	h	102	DGD	C3G-C2G	2.52	1.58	1.50
31	2	314	CLA	CMB-C2B	-2.52	1.46	1.51
42	5	313	KC1	C4D-CHA	2.52	1.48	1.45
31	B	611	CLA	C1D-ND	2.52	1.40	1.37
43	15	305	A86	C14-C13	2.52	1.54	1.51
31	c	510	CLA	CMC-C2C	-2.52	1.45	1.50
45	6	310	KC2	C1A-CHA	2.52	1.47	1.40
31	7	308	CLA	C1D-ND	2.52	1.40	1.37
31	3	308	CLA	CMB-C2B	-2.52	1.46	1.51
31	D	404	CLA	C3B-C2B	-2.52	1.36	1.40
43	2	303	A86	C13-C11	-2.52	1.44	1.49
43	10	318	A86	C32-C31	-2.52	1.50	1.54
31	14	312	CLA	CMD-C2D	-2.52	1.45	1.50
31	p	607	CLA	C3B-C2B	-2.52	1.36	1.40
31	12	316	CLA	CMB-C2B	-2.51	1.46	1.51
43	4	301	A86	C13-C11	-2.51	1.44	1.49
43	19	304	A86	C13-C11	-2.51	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	315	CLA	CMB-C2B	-2.51	1.46	1.51
43	10	304	A86	C30-C29	-2.51	1.27	1.32
31	3	315	CLA	CMB-C2B	-2.51	1.46	1.51
31	c	513	CLA	CMB-C2B	-2.51	1.46	1.51
42	19	314	KC1	C1A-CHA	2.51	1.47	1.40
31	8	307	CLA	C1D-ND	2.51	1.40	1.37
39	H	102	DGD	C3G-C2G	2.51	1.58	1.50
43	3	303	A86	C13-C11	-2.51	1.44	1.49
45	1	311	KC2	C1A-CHA	2.51	1.47	1.40
45	2	308	KC2	C1A-CHA	2.51	1.47	1.40
31	C	514	CLA	CMB-C2B	-2.51	1.46	1.51
31	6	316	CLA	CMB-C2B	-2.51	1.46	1.51
31	C	509	CLA	CMD-C2D	-2.51	1.45	1.50
31	c	508	CLA	C3B-CAB	-2.51	1.42	1.47
43	3	302	A86	C13-C11	-2.51	1.44	1.49
42	16	315	KC1	C4C-C3C	2.51	1.49	1.45
43	5	304	A86	C32-C31	-2.51	1.50	1.54
43	18	303	A86	C13-C11	-2.51	1.44	1.49
31	13	313	CLA	CMB-C2B	-2.51	1.46	1.51
31	B	606	CLA	CMC-C2C	-2.51	1.45	1.50
43	11	303	A86	C13-C11	-2.51	1.44	1.49
42	13	314	KC1	C1D-CHD	2.51	1.48	1.41
42	p	609	KC1	C4B-NB	-2.51	1.34	1.37
43	14	304	A86	C35-C34	2.50	1.56	1.51
31	C	514	CLA	CMC-C2C	-2.50	1.45	1.50
43	12	303	A86	C13-C11	-2.50	1.44	1.49
31	11	315	CLA	CHC-C1C	2.50	1.41	1.35
31	16	308	CLA	CHC-C1C	2.50	1.41	1.35
45	11	309	KC2	C4D-CHA	2.50	1.48	1.45
31	4	315	CLA	C1D-ND	2.50	1.40	1.37
43	9	303	A86	C13-C11	-2.50	1.44	1.49
31	B	602	CLA	CHC-C1C	2.50	1.41	1.35
31	b	603	CLA	CHC-C1C	2.50	1.41	1.35
31	7	307	CLA	CMB-C2B	-2.50	1.46	1.51
31	7	307	CLA	CHC-C1C	2.50	1.41	1.35
31	P	608	CLA	CMC-C2C	-2.50	1.45	1.50
42	4	313	KC1	OBD-CAD	2.50	1.25	1.22
31	C	505	CLA	CHC-C1C	2.50	1.41	1.35
45	2	310	KC2	C3C-C4C	2.50	1.49	1.44
33	y	101	BCR	C38-C26	-2.50	1.46	1.50
43	13	301	A86	C13-C11	-2.50	1.44	1.49
31	B	610	CLA	C3B-C2B	-2.50	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	5	310	KC2	C1D-CHD	2.50	1.47	1.41
31	P	607	CLA	C1D-ND	2.50	1.40	1.37
31	B	610	CLA	CHC-C1C	2.49	1.41	1.35
31	B	616	CLA	CHC-C1C	2.49	1.41	1.35
45	16	310	KC2	C1D-CHD	2.49	1.47	1.41
45	13	311	KC2	C1A-CHA	2.49	1.47	1.40
43	8	301	A86	C2-C1	-2.49	1.32	1.35
31	12	307	CLA	C4D-ND	-2.49	1.34	1.37
43	15	304	A86	O1-C20	-2.49	1.42	1.46
31	11	307	CLA	MG-ND	-2.49	2.00	2.05
42	P	609	KC1	C4B-NB	-2.49	1.34	1.37
42	17	314	KC1	C1B-NB	-2.49	1.34	1.37
42	16	315	KC1	C4A-C3A	2.49	1.49	1.44
38	C	522	LMG	C4-C5	2.49	1.58	1.53
31	c	514	CLA	CMC-C2C	-2.49	1.45	1.50
31	14	306	CLA	C1D-ND	2.49	1.40	1.37
43	12	304	A86	O1-C15	-2.49	1.41	1.45
43	3	302	A86	C33-C34	2.49	1.56	1.51
36	P	615	LHG	O7-C5	-2.49	1.40	1.46
39	c	518	DGD	O3G-C3G	-2.49	1.39	1.43
31	11	310	CLA	CMB-C2B	-2.49	1.46	1.51
45	16	312	KC2	C1A-CHA	2.48	1.47	1.40
31	17	312	CLA	CMB-C2B	-2.48	1.46	1.51
43	7	301	A86	C33-C34	2.48	1.56	1.51
31	p	603	CLA	C1D-ND	2.48	1.40	1.37
31	P	607	CLA	CMD-C2D	-2.48	1.45	1.50
31	P	602	CLA	MG-ND	-2.48	2.00	2.05
31	C	508	CLA	C3B-CAB	-2.48	1.42	1.47
31	C	510	CLA	CMC-C2C	-2.48	1.45	1.50
43	8	302	A86	C17-C18	-2.48	1.48	1.52
31	10	314	CLA	CMB-C2B	-2.48	1.46	1.51
45	0	310	KC2	C1A-CHA	2.48	1.47	1.40
43	9	304	A86	C13-C11	-2.48	1.44	1.49
31	4	307	CLA	CMD-C2D	-2.48	1.45	1.50
31	10	307	CLA	C3B-C2B	-2.48	1.36	1.40
31	c	505	CLA	CAC-C3C	-2.48	1.44	1.51
31	C	506	CLA	CMB-C2B	-2.48	1.46	1.51
31	7	312	CLA	CMB-C2B	-2.48	1.46	1.51
43	18	305	A86	C32-C31	-2.48	1.50	1.54
45	0	310	KC2	C4B-NB	-2.48	1.34	1.37
38	1	301	LMG	O7-C8	-2.48	1.40	1.46
31	c	509	CLA	CMD-C2D	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	14	304	A86	C13-C11	-2.48	1.44	1.49
45	17	309	KC2	C1A-CHA	2.48	1.47	1.40
31	b	611	CLA	CHC-C1C	2.48	1.41	1.35
35	D	406	PL9	C31-C29	-2.48	1.46	1.51
35	d	406	PL9	C31-C29	-2.48	1.46	1.51
31	5	311	CLA	C1D-ND	2.48	1.40	1.37
42	13	314	KC1	C1B-NB	-2.48	1.34	1.37
45	7	309	KC2	C1A-CHA	2.48	1.47	1.40
31	P	605	CLA	CMB-C2B	-2.48	1.46	1.51
31	1	307	CLA	CMB-C2B	-2.48	1.46	1.51
31	c	512	CLA	C3B-C2B	-2.48	1.36	1.40
31	5	307	CLA	CMD-C2D	-2.48	1.45	1.50
45	12	311	KC2	C1A-CHA	2.48	1.47	1.40
45	6	310	KC2	C1D-CHD	2.48	1.47	1.41
31	b	617	CLA	CHC-C1C	2.48	1.41	1.35
45	15	310	KC2	C4B-NB	-2.48	1.34	1.37
31	5	311	CLA	MG-ND	-2.48	2.00	2.05
45	16	312	KC2	C1D-CHD	2.48	1.47	1.41
31	p	605	CLA	CMB-C2B	-2.47	1.46	1.51
42	8	313	KC1	C1A-CHA	2.47	1.47	1.40
42	13	314	KC1	C4D-CHA	2.47	1.48	1.45
31	c	503	CLA	CMD-C2D	-2.47	1.45	1.50
31	16	309	CLA	C3B-C2B	-2.47	1.36	1.40
31	5	306	CLA	CMB-C2B	-2.47	1.46	1.51
31	17	315	CLA	CMB-C2B	-2.47	1.46	1.51
45	15	310	KC2	C1D-CHD	2.47	1.47	1.41
43	16	304	A86	C13-C11	-2.47	1.44	1.49
31	5	314	CLA	CMB-C2B	-2.47	1.46	1.51
45	1	309	KC2	C1D-CHD	2.47	1.47	1.41
38	11	301	LMG	O7-C8	-2.47	1.40	1.46
31	0	308	CLA	CMB-C2B	-2.47	1.46	1.51
31	1	310	CLA	CMB-C2B	-2.47	1.46	1.51
45	19	309	KC2	C1D-CHD	2.47	1.47	1.41
43	5	302	A86	C13-C11	-2.47	1.45	1.49
31	b	611	CLA	C3B-C2B	-2.47	1.36	1.40
31	2	306	CLA	C4D-ND	-2.47	1.34	1.37
31	18	306	CLA	CMB-C2B	-2.47	1.46	1.51
42	7	314	KC1	C1D-CHD	2.47	1.47	1.41
31	c	514	CLA	CMB-C2B	-2.47	1.46	1.51
31	15	313	CLA	CMB-C2B	-2.47	1.46	1.51
31	p	608	CLA	CMC-C2C	-2.47	1.45	1.50
31	17	307	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	6	301	A86	C13-C11	-2.47	1.45	1.49
31	C	502	CLA	MG-ND	-2.47	2.00	2.05
31	c	502	CLA	MG-ND	-2.47	2.00	2.05
45	5	310	KC2	C4B-NB	-2.47	1.34	1.37
45	6	310	KC2	C3C-C4C	2.46	1.49	1.44
31	17	307	CLA	CHC-C1C	2.46	1.41	1.35
45	12	311	KC2	C1D-CHD	2.46	1.47	1.41
31	c	506	CLA	CMB-C2B	-2.46	1.46	1.51
31	B	612	CLA	CMC-C2C	-2.46	1.45	1.50
45	12	309	KC2	C1D-CHD	2.46	1.47	1.41
39	w	204	DGD	O4D-C4D	-2.46	1.37	1.43
45	9	309	KC2	C1B-NB	-2.46	1.34	1.37
39	W	203	DGD	O4D-C4D	-2.46	1.37	1.43
43	5	305	A86	C32-C31	-2.46	1.50	1.54
39	11	318	DGD	C4E-C3E	2.46	1.58	1.52
31	4	307	CLA	CMC-C2C	-2.46	1.45	1.50
31	P	603	CLA	C1D-ND	2.46	1.40	1.37
43	p	611	A86	C37-C36	2.46	1.56	1.52
45	5	308	KC2	C1D-CHD	2.46	1.47	1.41
31	3	312	CLA	CMB-C2B	-2.46	1.46	1.51
31	P	610	CLA	CMD-C2D	-2.46	1.45	1.50
31	b	613	CLA	CMC-C2C	-2.46	1.45	1.50
31	p	602	CLA	MG-ND	-2.46	2.00	2.05
31	11	315	CLA	C3C-C2C	2.46	1.41	1.36
45	15	308	KC2	C1D-CHD	2.46	1.47	1.41
45	11	311	KC2	C1A-CHA	2.46	1.47	1.40
42	3	314	KC1	C4A-C3A	2.46	1.49	1.44
42	7	314	KC1	C1A-CHA	2.46	1.47	1.40
39	c	520	DGD	O6D-C5D	-2.46	1.38	1.44
43	3	301	A86	C2-C1	-2.46	1.32	1.35
31	15	306	CLA	CMB-C2B	-2.45	1.46	1.51
45	17	311	KC2	C1D-CHD	2.45	1.47	1.41
43	0	302	A86	C21-C20	-2.45	1.48	1.51
45	13	309	KC2	C1B-NB	-2.45	1.34	1.37
31	3	312	CLA	C4D-ND	-2.45	1.34	1.37
31	p	610	CLA	CMD-C2D	-2.45	1.45	1.50
45	6	312	KC2	C1A-CHA	2.45	1.47	1.40
43	7	302	A86	C26-C27	-2.45	1.32	1.35
31	13	310	CLA	CMB-C2B	-2.45	1.46	1.51
43	6	301	A86	C30-C29	-2.45	1.27	1.32
45	18	308	KC2	C4B-NB	-2.45	1.34	1.37
43	10	301	A86	C33-C34	2.45	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	607	CLA	CMD-C2D	-2.45	1.45	1.50
45	8	310	KC2	C1A-CHA	2.45	1.47	1.40
31	8	311	CLA	MG-ND	-2.45	2.00	2.05
31	16	314	CLA	C3B-C2B	-2.45	1.37	1.40
31	d	404	CLA	MG-ND	-2.45	2.00	2.05
31	15	311	CLA	C4B-CHC	-2.45	1.34	1.41
31	C	508	CLA	C1D-ND	2.45	1.40	1.37
31	c	508	CLA	C1D-ND	2.45	1.40	1.37
42	3	314	KC1	C1D-CHD	2.45	1.47	1.41
31	c	505	CLA	CHC-C1C	2.45	1.41	1.35
43	17	303	A86	C32-C31	-2.45	1.50	1.54
31	C	505	CLA	CAC-C3C	-2.44	1.44	1.51
31	10	308	CLA	CMB-C2B	-2.44	1.46	1.51
45	4	308	KC2	C1D-CHD	2.44	1.47	1.41
39	H	102	DGD	O1G-C1G	-2.44	1.39	1.45
31	17	308	CLA	MG-ND	-2.44	2.00	2.05
31	13	312	CLA	CMB-C2B	-2.44	1.46	1.51
43	P	611	A86	C37-C36	2.44	1.56	1.52
31	16	313	CLA	CMB-C2B	-2.44	1.46	1.51
31	C	508	CLA	CMC-C2C	-2.44	1.45	1.50
43	11	319	A86	O1-C20	-2.44	1.42	1.46
45	18	308	KC2	C1D-CHD	2.44	1.47	1.41
38	N	101	LMG	C7-C8	2.44	1.58	1.50
42	17	314	KC1	C1D-CHD	2.44	1.47	1.41
31	B	604	CLA	C1D-ND	2.44	1.40	1.37
31	0	316	CLA	CMB-C2B	-2.44	1.46	1.51
31	C	503	CLA	CMD-C2D	-2.43	1.45	1.50
31	7	308	CLA	MG-ND	-2.43	2.01	2.05
31	6	314	CLA	C3B-CAB	-2.43	1.43	1.47
32	D	402	PHO	CMC-C2C	-2.43	1.45	1.51
43	12	304	A86	O4-C34	-2.43	1.40	1.46
31	10	317	CLA	C3B-C2B	-2.43	1.37	1.40
31	A	404	CLA	CMD-C2D	-2.43	1.45	1.50
31	a	404	CLA	CMD-C2D	-2.43	1.45	1.50
36	p	615	LHG	O7-C5	-2.43	1.40	1.46
43	5	301	A86	C30-C29	-2.43	1.27	1.32
31	3	308	CLA	CMC-C2C	-2.43	1.45	1.50
31	18	312	CLA	CMD-C2D	-2.43	1.45	1.50
31	5	307	CLA	MG-ND	-2.43	2.01	2.05
42	0	315	KC1	C4D-CHA	2.43	1.48	1.45
31	17	313	CLA	C3B-C2B	-2.43	1.37	1.40
31	5	311	CLA	CHC-C1C	2.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	0	306	A86	O3-C36	2.43	1.47	1.43
31	14	315	CLA	C1D-ND	2.43	1.40	1.37
31	17	308	CLA	C3B-CAB	-2.43	1.43	1.47
31	C	503	CLA	CAC-C3C	-2.43	1.44	1.51
31	4	315	CLA	C3B-C2B	-2.43	1.37	1.40
31	10	313	CLA	CMC-C2C	-2.43	1.45	1.50
31	B	604	CLA	CMC-C2C	-2.43	1.45	1.50
31	1	315	CLA	CMB-C2B	-2.43	1.46	1.51
31	C	512	CLA	C3B-C2B	-2.42	1.37	1.40
31	p	608	CLA	CMD-C2D	-2.42	1.45	1.50
31	13	313	CLA	C1D-ND	2.42	1.40	1.37
42	13	314	KC1	C4B-NB	-2.42	1.34	1.37
43	19	303	A86	C13-C11	-2.42	1.45	1.49
31	14	307	CLA	CMD-C2D	-2.42	1.45	1.50
31	2	315	CLA	CMB-C2B	-2.42	1.46	1.51
31	p	603	CLA	MG-ND	-2.42	2.01	2.05
45	16	312	KC2	C1B-NB	-2.42	1.34	1.37
45	18	308	KC2	C1A-CHA	2.42	1.47	1.40
31	18	309	CLA	CMB-C2B	-2.42	1.46	1.51
31	C	510	CLA	CMD-C2D	-2.42	1.45	1.50
31	16	316	CLA	CMB-C2B	-2.42	1.46	1.51
45	9	309	KC2	C1D-CHD	2.41	1.47	1.41
31	15	312	CLA	C3B-CAB	-2.41	1.43	1.47
43	15	304	A86	C13-C11	-2.41	1.45	1.49
43	8	303	A86	C2-C1	-2.41	1.32	1.35
31	c	508	CLA	CMC-C2C	-2.41	1.45	1.50
31	14	307	CLA	CMC-C2C	-2.41	1.45	1.50
31	8	309	CLA	CMB-C2B	-2.41	1.46	1.51
31	7	308	CLA	C3B-C2B	-2.41	1.37	1.40
31	c	503	CLA	CAC-C3C	-2.41	1.44	1.51
45	19	309	KC2	C4A-C3A	2.41	1.49	1.44
31	6	313	CLA	CMB-C2B	-2.41	1.46	1.51
38	M	101	LMG	O8-C9	-2.41	1.39	1.45
45	13	311	KC2	C1B-NB	-2.41	1.34	1.37
31	12	313	CLA	MG-ND	-2.41	2.01	2.05
31	P	603	CLA	MG-ND	-2.41	2.01	2.05
39	h	102	DGD	O2D-C2D	-2.41	1.37	1.43
45	15	308	KC2	C1A-CHA	2.41	1.47	1.40
43	0	306	A86	C28-C27	-2.41	1.45	1.50
31	2	307	CLA	C3B-C2B	-2.41	1.37	1.40
43	10	301	A86	C13-C11	-2.41	1.45	1.49
31	b	604	CLA	C4B-CHC	-2.41	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	10	304	A86	C13-C11	-2.41	1.45	1.49
43	11	306	A86	C13-C11	-2.41	1.45	1.49
31	2	311	CLA	CMB-C2B	-2.41	1.46	1.51
43	0	304	A86	C13-C11	-2.40	1.45	1.49
31	B	603	CLA	C3B-CAB	-2.40	1.43	1.47
31	D	404	CLA	MG-ND	-2.40	2.01	2.05
43	7	306	A86	C13-C11	-2.40	1.45	1.49
31	7	308	CLA	C3B-CAB	-2.40	1.43	1.47
43	4	303	A86	C13-C11	-2.40	1.45	1.49
31	b	606	CLA	CMC-C2C	-2.40	1.45	1.50
39	c	519	DGD	O5D-C6D	-2.40	1.39	1.43
31	0	309	CLA	CMB-C2B	-2.40	1.46	1.51
31	b	605	CLA	CMC-C2C	-2.40	1.45	1.50
31	3	308	CLA	CMD-C2D	-2.40	1.45	1.50
31	1	315	CLA	CHC-C1C	2.40	1.41	1.35
39	C	520	DGD	O6D-C5D	-2.40	1.38	1.44
31	b	604	CLA	C3B-CAB	-2.40	1.43	1.47
45	8	308	KC2	C1D-CHD	2.40	1.47	1.41
31	c	510	CLA	CMD-C2D	-2.40	1.45	1.50
31	0	309	CLA	CMD-C2D	-2.40	1.45	1.50
31	B	603	CLA	C4B-CHC	-2.39	1.34	1.41
32	d	402	PHO	CMC-C2C	-2.39	1.45	1.51
43	16	306	A86	C14-C15	2.39	1.57	1.52
31	11	308	CLA	CMC-C2C	-2.39	1.45	1.50
33	C	516	BCR	C38-C26	-2.39	1.47	1.50
33	c	516	BCR	C38-C26	-2.39	1.47	1.50
45	14	308	KC2	C1D-CHD	2.39	1.47	1.41
31	10	316	CLA	CMB-C2B	-2.39	1.46	1.51
31	13	316	CLA	CMB-C2B	-2.39	1.46	1.51
45	17	311	KC2	C1B-NB	-2.39	1.34	1.37
31	1	312	CLA	C3B-C2B	-2.39	1.37	1.40
38	10	319	LMG	C7-C8	2.39	1.58	1.50
31	1	312	CLA	MG-ND	-2.39	2.01	2.05
43	10	318	A86	C30-C29	-2.39	1.28	1.32
33	b	620	BCR	C38-C26	-2.39	1.47	1.50
31	5	312	CLA	CMA-C3A	-2.39	1.48	1.53
43	4	302	A86	C33-C34	2.39	1.56	1.51
39	1	318	DGD	C4E-C3E	2.39	1.58	1.52
38	1	301	LMG	C3-C2	2.39	1.58	1.52
31	B	602	CLA	C4B-CHC	-2.39	1.34	1.41
31	15	307	CLA	MG-ND	-2.39	2.01	2.05
42	1	314	KC1	C1D-CHD	2.39	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	8	301	A86	C13-C11	-2.39	1.45	1.49
39	h	102	DGD	O1G-C1G	-2.39	1.39	1.45
31	b	604	CLA	CHC-C1C	2.38	1.41	1.35
31	12	312	CLA	CMB-C2B	-2.38	1.46	1.51
43	p	611	A86	C30-C29	-2.38	1.28	1.32
31	3	316	CLA	CHC-C1C	2.38	1.41	1.35
45	8	308	KC2	C1A-CHA	2.38	1.46	1.40
43	10	303	A86	C5-C6	-2.38	1.32	1.35
45	5	308	KC2	C1A-CHA	2.38	1.46	1.40
31	3	307	CLA	CHC-C1C	2.38	1.41	1.35
31	8	306	CLA	C3B-C2B	-2.38	1.37	1.40
43	4	306	A86	C33-C34	2.38	1.56	1.51
31	12	308	CLA	CMD-C2D	-2.38	1.45	1.50
31	8	307	CLA	C3B-CAB	-2.38	1.43	1.47
43	P	611	A86	C30-C29	-2.38	1.28	1.32
31	B	610	CLA	CMC-C2C	-2.38	1.45	1.50
31	A	403	CLA	CMC-C2C	-2.38	1.45	1.50
31	B	616	CLA	CMD-C2D	-2.38	1.45	1.50
31	P	608	CLA	CMD-C2D	-2.38	1.45	1.50
31	z	103	CLA	CMD-C2D	-2.38	1.45	1.50
31	a	403	CLA	CMC-C2C	-2.38	1.45	1.50
38	W	201	LMG	O1-C1	2.38	1.44	1.40
43	7	302	A86	C2-C1	-2.38	1.32	1.35
31	11	307	CLA	CMD-C2D	-2.38	1.45	1.50
45	2	308	KC2	C1B-NB	-2.38	1.34	1.37
38	w	201	LMG	O1-C1	2.38	1.44	1.40
31	15	312	CLA	CMA-C3A	-2.38	1.48	1.53
39	H	102	DGD	O2D-C2D	-2.37	1.37	1.43
43	5	303	A86	C13-C11	-2.37	1.45	1.49
31	B	614	CLA	CMD-C2D	-2.37	1.45	1.50
43	15	305	A86	C32-C31	-2.37	1.50	1.54
31	0	313	CLA	CMC-C2C	-2.37	1.45	1.50
42	0	315	KC1	C1D-CHD	2.37	1.47	1.41
42	18	313	KC1	C4B-NB	-2.37	1.34	1.37
31	15	313	CLA	CMD-C2D	-2.37	1.45	1.50
42	14	313	KC1	OBD-CAD	2.37	1.25	1.22
31	C	504	CLA	MG-ND	-2.37	2.01	2.05
43	10	318	A86	C17-C18	-2.37	1.48	1.52
31	C	507	CLA	CMC-C2C	-2.37	1.45	1.50
31	13	308	CLA	CMC-C2C	-2.37	1.45	1.50
45	9	309	KC2	C1A-CHA	2.37	1.46	1.40
42	19	314	KC1	C1D-CHD	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	617	CLA	CMD-C2D	-2.36	1.45	1.50
31	11	313	CLA	CMD-C2D	-2.36	1.45	1.50
39	C	519	DGD	O5D-C6D	-2.36	1.39	1.43
31	b	615	CLA	CMD-C2D	-2.36	1.45	1.50
45	7	311	KC2	C1D-CHD	2.36	1.47	1.41
31	B	609	CLA	CMD-C2D	-2.36	1.45	1.50
45	8	308	KC2	C4B-NB	-2.36	1.34	1.37
43	p	611	A86	C5-C6	-2.36	1.32	1.35
38	d	403	LMG	C3-C2	2.36	1.58	1.52
31	10	317	CLA	CMD-C2D	-2.36	1.45	1.50
43	0	301	A86	C33-C34	2.36	1.56	1.51
31	b	611	CLA	CMC-C2C	-2.36	1.45	1.50
31	b	611	CLA	CMD-C2D	-2.36	1.45	1.50
31	a	403	CLA	MG-ND	-2.36	2.01	2.05
31	4	314	CLA	C3B-C2B	-2.36	1.37	1.40
42	13	314	KC1	C1A-CHA	2.36	1.46	1.40
38	1	317	LMG	C9-C8	2.36	1.57	1.50
42	P	609	KC1	C1A-CHA	2.36	1.46	1.40
43	2	302	A86	C33-C34	2.36	1.56	1.51
31	b	603	CLA	C4B-CHC	-2.36	1.34	1.41
45	8	310	KC2	C1D-CHD	2.36	1.47	1.41
42	5	313	KC1	C1A-CHA	2.36	1.46	1.40
31	p	607	CLA	CMC-C2C	-2.36	1.45	1.50
31	16	309	CLA	CMD-C2D	-2.36	1.45	1.50
31	z	101	CLA	CMD-C2D	-2.36	1.45	1.50
35	A	409	PL9	C10-C9	-2.35	1.44	1.50
42	5	313	KC1	C1D-CHD	2.35	1.47	1.41
43	6	306	A86	C33-C34	2.35	1.56	1.51
31	D	405	CLA	CMD-C2D	-2.35	1.45	1.50
43	5	318	A86	C13-C11	-2.35	1.45	1.49
42	6	315	KC1	C3D-C2D	2.35	1.43	1.39
31	C	513	CLA	CMC-C2C	-2.35	1.45	1.50
31	B	603	CLA	CHC-C1C	2.35	1.41	1.35
45	0	310	KC2	C4D-CHA	2.35	1.48	1.45
42	p	609	KC1	C1A-CHA	2.35	1.46	1.40
31	w	203	CLA	CMD-C2D	-2.35	1.45	1.50
31	8	307	CLA	MG-ND	-2.35	2.01	2.05
45	15	310	KC2	C3C-C4C	2.35	1.49	1.44
31	b	612	CLA	MG-ND	-2.35	2.01	2.05
42	16	315	KC1	C4D-CHA	2.35	1.48	1.45
31	c	507	CLA	MG-ND	-2.35	2.01	2.05
43	0	304	A86	C30-C29	-2.35	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	16	311	CLA	CMB-C2B	-2.35	1.46	1.51
43	6	305	A86	C14-C15	2.35	1.57	1.52
43	3	305	A86	C13-C11	-2.35	1.45	1.49
38	D	408	LMG	O8-C9	-2.35	1.39	1.45
31	b	610	CLA	CMD-C2D	-2.35	1.45	1.50
31	B	613	CLA	CMC-C2C	-2.35	1.45	1.50
31	11	307	CLA	CMB-C2B	-2.35	1.46	1.51
31	0	307	CLA	MG-ND	-2.35	2.01	2.05
45	7	309	KC2	C1B-NB	-2.35	1.34	1.37
43	17	306	A86	C33-C34	2.35	1.56	1.51
43	0	301	A86	C13-C11	-2.35	1.45	1.49
31	B	605	CLA	CMC-C2C	-2.35	1.45	1.50
43	7	306	A86	C30-C29	-2.34	1.28	1.32
45	6	312	KC2	C1B-NB	-2.34	1.34	1.37
32	A	405	PHO	CMC-C2C	-2.34	1.46	1.51
32	a	405	PHO	CMC-C2C	-2.34	1.46	1.51
42	9	314	KC1	C1D-CHD	2.34	1.47	1.41
31	c	507	CLA	CMC-C2C	-2.34	1.45	1.50
31	P	601	CLA	MG-ND	-2.34	2.01	2.05
45	10	310	KC2	C1A-CHA	2.34	1.46	1.40
38	11	301	LMG	C3-C2	2.34	1.58	1.52
43	16	302	A86	C13-C11	-2.34	1.45	1.49
31	A	403	CLA	MG-ND	-2.34	2.01	2.05
31	3	308	CLA	C3B-CAB	-2.34	1.43	1.47
43	11	306	A86	C14-C13	2.34	1.54	1.51
31	b	614	CLA	CMC-C2C	-2.34	1.45	1.50
33	B	619	BCR	C38-C26	-2.34	1.47	1.50
35	d	406	PL9	C26-C24	-2.34	1.46	1.51
31	2	309	CLA	CMB-C2B	-2.34	1.46	1.51
31	P	607	CLA	CMC-C2C	-2.34	1.45	1.50
45	19	309	KC2	C1A-CHA	2.34	1.46	1.40
31	w	203	CLA	C3B-C2B	-2.34	1.37	1.40
31	B	610	CLA	CMD-C2D	-2.34	1.45	1.50
31	d	405	CLA	CMD-C2D	-2.34	1.45	1.50
31	13	313	CLA	CMC-C2C	-2.34	1.45	1.50
45	9	309	KC2	C4A-C3A	2.33	1.49	1.44
31	6	311	CLA	CMB-C2B	-2.33	1.46	1.51
43	5	304	A86	O1-C20	-2.33	1.42	1.46
38	5	316	LMG	O8-C9	-2.33	1.39	1.45
31	12	310	CLA	CMB-C2B	-2.33	1.46	1.51
45	3	311	KC2	C1D-CHD	2.33	1.47	1.41
31	p	601	CLA	MG-ND	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	c	519	DGD	O3D-C3D	-2.33	1.37	1.43
31	b	612	CLA	C3B-C2B	-2.33	1.37	1.40
31	C	508	CLA	MG-ND	-2.33	2.01	2.05
31	5	311	CLA	C3B-C2B	-2.33	1.37	1.40
38	D	403	LMG	C3-C2	2.33	1.58	1.52
31	b	608	CLA	CMC-C2C	-2.33	1.45	1.50
45	12	311	KC2	C3C-C4C	2.33	1.49	1.44
35	a	409	PL9	C10-C9	-2.33	1.44	1.50
45	18	310	KC2	C1D-CHD	2.33	1.47	1.41
31	1	310	CLA	C3B-CAB	-2.33	1.43	1.47
31	c	512	CLA	CMC-C2C	-2.33	1.45	1.50
31	c	513	CLA	CMC-C2C	-2.33	1.45	1.50
39	B	621	DGD	O4D-C4D	-2.33	1.37	1.43
45	13	309	KC2	C1D-CHD	2.33	1.47	1.41
42	10	315	KC1	C4B-NB	-2.33	1.34	1.37
31	4	311	CLA	CMB-C2B	-2.33	1.46	1.51
31	P	602	CLA	CMC-C2C	-2.33	1.45	1.50
38	D	403	LMG	O1-C7	-2.33	1.39	1.43
38	K	101	LMG	O4-C4	-2.33	1.37	1.43
38	k	101	LMG	O4-C4	-2.33	1.37	1.43
45	1	309	KC2	C1A-CHA	2.32	1.46	1.40
31	1	307	CLA	MG-ND	-2.32	2.01	2.05
31	C	514	CLA	CMD-C2D	-2.32	1.45	1.50
31	4	309	CLA	CMB-C2B	-2.32	1.46	1.51
43	11	304	A86	C5-C6	-2.32	1.32	1.35
31	C	507	CLA	MG-ND	-2.32	2.01	2.05
31	7	313	CLA	CAA-C2A	-2.32	1.49	1.54
31	14	311	CLA	CMB-C2B	-2.32	1.46	1.51
31	7	313	CLA	C3B-C2B	-2.32	1.37	1.40
31	W	202	CLA	CMD-C2D	-2.32	1.45	1.50
38	W	201	LMG	O8-C9	-2.32	1.39	1.45
31	B	611	CLA	C3B-C2B	-2.32	1.37	1.40
42	19	314	KC1	C4A-C3A	2.32	1.49	1.44
31	2	312	CLA	C1D-ND	2.32	1.40	1.37
31	r	101	CLA	CMD-C2D	-2.32	1.45	1.50
38	1	317	LMG	C7-C8	2.31	1.57	1.50
31	Z	101	CLA	CMD-C2D	-2.31	1.45	1.50
31	6	309	CLA	C3B-C2B	-2.31	1.37	1.40
45	6	312	KC2	C4A-C3A	2.31	1.49	1.44
42	2	313	KC1	C1B-NB	-2.31	1.34	1.37
38	11	317	LMG	C7-C8	2.31	1.57	1.50
39	C	519	DGD	O3D-C3D	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	310	CLA	CMB-C2B	-2.31	1.46	1.51
31	p	602	CLA	CMC-C2C	-2.31	1.45	1.50
43	6	305	A86	C33-C34	2.31	1.55	1.51
31	B	611	CLA	MG-ND	-2.31	2.01	2.05
35	D	406	PL9	C41-C39	-2.31	1.46	1.51
31	0	308	CLA	CMD-C2D	-2.31	1.45	1.50
31	p	602	CLA	C3B-CAB	-2.31	1.43	1.47
43	8	305	A86	C30-C29	-2.31	1.28	1.32
31	9	308	CLA	CMB-C2B	-2.31	1.46	1.51
31	C	513	CLA	MG-ND	-2.31	2.01	2.05
43	7	301	A86	C30-C29	-2.31	1.28	1.32
45	5	310	KC2	C3C-C4C	2.31	1.49	1.44
31	C	512	CLA	CMC-C2C	-2.31	1.45	1.50
31	c	504	CLA	MG-ND	-2.31	2.01	2.05
43	6	307	A86	C5-C6	-2.31	1.32	1.35
38	W	201	LMG	O7-C8	-2.30	1.40	1.46
31	b	615	CLA	MG-ND	-2.30	2.01	2.05
31	b	610	CLA	C3B-C2B	-2.30	1.37	1.40
31	R	101	CLA	CMD-C2D	-2.30	1.45	1.50
31	c	514	CLA	CMD-C2D	-2.30	1.45	1.50
43	4	305	A86	C41-C32	-2.30	1.49	1.53
31	15	311	CLA	CHC-C1C	2.30	1.40	1.35
31	B	602	CLA	MG-ND	-2.30	2.01	2.05
31	P	602	CLA	C3B-C2B	-2.30	1.37	1.40
43	0	303	A86	C5-C6	-2.30	1.32	1.35
31	19	308	CLA	CMB-C2B	-2.30	1.46	1.51
45	2	310	KC2	C4B-NB	-2.30	1.35	1.37
42	6	315	KC1	C4A-C3A	2.30	1.49	1.44
31	4	314	CLA	C3B-CAB	-2.30	1.43	1.47
31	16	314	CLA	C3B-CAB	-2.30	1.43	1.47
43	P	611	A86	C5-C6	-2.30	1.32	1.35
32	a	405	PHO	CBD-CGD	-2.30	1.49	1.52
38	w	201	LMG	O7-C8	-2.30	1.40	1.46
31	c	508	CLA	MG-ND	-2.30	2.01	2.05
31	p	608	CLA	C3B-C2B	-2.30	1.37	1.40
45	17	311	KC2	C3C-C4C	2.30	1.49	1.44
31	14	315	CLA	C3B-C2B	-2.30	1.37	1.40
31	C	502	CLA	CMC-C2C	-2.30	1.45	1.50
31	c	513	CLA	CMD-C2D	-2.30	1.45	1.50
31	10	308	CLA	CMD-C2D	-2.30	1.45	1.50
43	15	303	A86	C13-C11	-2.29	1.45	1.49
43	2	301	A86	C2-C1	-2.29	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	622	DGD	C4E-C3E	2.29	1.58	1.52
31	C	503	CLA	MG-ND	-2.29	2.01	2.05
31	0	311	CLA	MG-ND	-2.29	2.01	2.05
35	d	406	PL9	C20-C19	-2.29	1.44	1.50
43	12	306	A86	C2-C1	-2.29	1.32	1.35
31	c	513	CLA	MG-ND	-2.29	2.01	2.05
43	0	305	A86	C13-C11	-2.29	1.45	1.49
31	11	308	CLA	CMD-C2D	-2.29	1.45	1.50
31	16	309	CLA	C3B-CAB	-2.29	1.43	1.47
38	d	408	LMG	O8-C9	-2.29	1.39	1.45
43	18	302	A86	O1-C20	-2.29	1.42	1.46
34	10	320	SQD	O2-C2	-2.29	1.37	1.43
35	d	406	PL9	C41-C39	-2.29	1.46	1.51
31	C	513	CLA	CMD-C2D	-2.29	1.46	1.50
31	B	607	CLA	CMC-C2C	-2.29	1.46	1.50
31	b	603	CLA	MG-ND	-2.28	2.01	2.05
33	B	618	BCR	C1-C6	-2.28	1.50	1.53
43	19	306	A86	C13-C11	-2.28	1.45	1.49
31	B	609	CLA	C3B-C2B	-2.28	1.37	1.40
45	5	308	KC2	C4A-C3A	2.28	1.49	1.44
31	13	308	CLA	CMD-C2D	-2.28	1.46	1.50
38	w	201	LMG	O8-C9	-2.28	1.39	1.45
43	15	302	A86	C13-C11	-2.28	1.45	1.49
43	1	305	A86	C32-C31	-2.28	1.50	1.54
43	7	305	A86	C33-C34	2.28	1.55	1.51
31	5	311	CLA	C1A-CHA	-2.28	1.33	1.43
43	15	301	A86	C40-C32	2.28	1.58	1.53
31	B	601	CLA	CMD-C2D	-2.28	1.46	1.50
43	1	320	A86	C41-C32	-2.28	1.49	1.53
31	C	508	CLA	CMD-C2D	-2.28	1.46	1.50
31	c	508	CLA	CMD-C2D	-2.28	1.46	1.50
31	10	307	CLA	C3B-CAB	-2.28	1.43	1.47
38	c	521	LMG	C3-C2	2.28	1.58	1.52
31	10	311	CLA	MG-ND	-2.28	2.01	2.05
31	10	309	CLA	CMB-C2B	-2.28	1.46	1.51
42	9	314	KC1	C4C-C3C	2.28	1.49	1.45
32	A	405	PHO	CMB-C2B	-2.28	1.46	1.51
43	12	306	A86	C26-C27	-2.28	1.32	1.35
31	b	606	CLA	C3B-CAB	-2.28	1.43	1.47
31	P	610	CLA	CMC-C2C	-2.28	1.46	1.50
31	a	404	CLA	MG-ND	-2.28	2.01	2.05
42	9	314	KC1	C4A-C3A	2.28	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	623	SQD	O2-C2	-2.27	1.37	1.43
43	19	305	A86	C14-C13	2.27	1.54	1.51
31	P	602	CLA	C3B-CAB	-2.27	1.43	1.47
43	p	611	A86	C26-C27	-2.27	1.32	1.35
42	14	313	KC1	C1D-CHD	2.27	1.47	1.41
31	p	601	CLA	CMD-C2D	-2.27	1.46	1.50
35	D	406	PL9	C26-C24	-2.27	1.46	1.51
31	18	314	CLA	C3B-C2B	-2.27	1.37	1.40
45	11	311	KC2	C3C-C4C	2.27	1.49	1.44
31	B	614	CLA	MG-ND	-2.27	2.01	2.05
31	b	602	CLA	CMD-C2D	-2.27	1.46	1.50
31	14	314	CLA	C3B-CAB	-2.27	1.43	1.47
31	B	613	CLA	CMD-C2D	-2.27	1.46	1.50
31	p	610	CLA	CMC-C2C	-2.27	1.46	1.50
31	B	605	CLA	C3B-CAB	-2.27	1.43	1.47
31	b	615	CLA	CMC-C2C	-2.27	1.46	1.50
31	b	614	CLA	CMD-C2D	-2.27	1.46	1.50
45	4	310	KC2	C1D-CHD	2.27	1.47	1.41
31	P	607	CLA	MG-ND	-2.27	2.01	2.05
31	c	505	CLA	CMC-C2C	-2.27	1.46	1.50
45	3	311	KC2	C1B-NB	-2.27	1.35	1.37
31	c	506	CLA	CMC-C2C	-2.27	1.46	1.50
31	W	202	CLA	C3B-C2B	-2.27	1.37	1.40
31	c	503	CLA	MG-ND	-2.27	2.01	2.05
31	9	312	CLA	CMB-C2B	-2.27	1.46	1.51
31	C	511	CLA	CMC-C2C	-2.27	1.46	1.50
31	18	307	CLA	C1D-ND	2.27	1.40	1.37
31	9	307	CLA	CMB-C2B	-2.27	1.46	1.51
33	b	619	BCR	C1-C6	-2.26	1.50	1.53
31	D	401	CLA	MG-ND	-2.26	2.01	2.05
34	l	101	SQD	O2-C2	-2.26	1.37	1.43
34	i	101	SQD	O2-C2	-2.26	1.37	1.43
31	c	511	CLA	CMC-C2C	-2.26	1.46	1.50
45	3	309	KC2	C4B-NB	-2.26	1.35	1.37
43	1	306	A86	C13-C11	-2.26	1.45	1.49
45	16	312	KC2	C4A-C3A	2.26	1.48	1.44
34	10	320	SQD	O4-C4	-2.26	1.37	1.43
31	9	313	CLA	CMB-C2B	-2.26	1.46	1.51
31	C	504	CLA	CMD-C2D	-2.26	1.46	1.50
31	c	504	CLA	CMD-C2D	-2.26	1.46	1.50
39	c	518	DGD	O2E-C2E	-2.26	1.37	1.43
45	13	311	KC2	C3C-C4C	2.26	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	16	303	A86	C26-C27	-2.26	1.32	1.35
31	13	308	CLA	MG-ND	-2.26	2.01	2.05
39	c	520	DGD	O4D-C4D	-2.26	1.37	1.43
31	18	314	CLA	CMD-C2D	-2.26	1.46	1.50
31	w	203	CLA	MG-ND	-2.26	2.01	2.05
42	14	313	KC1	C4B-NB	-2.26	1.35	1.37
43	4	305	A86	C26-C27	-2.26	1.32	1.35
39	c	520	DGD	O3D-C3D	-2.26	1.37	1.43
34	b	601	SQD	O2-C2	-2.26	1.37	1.43
38	C	522	LMG	C3-C2	2.26	1.58	1.52
38	w	201	LMG	O4-C4	-2.26	1.37	1.43
31	c	502	CLA	CMC-C2C	-2.25	1.46	1.50
39	C	520	DGD	O4D-C4D	-2.25	1.37	1.43
43	17	316	A86	C40-C32	-2.25	1.49	1.53
42	1	314	KC1	C4B-NB	-2.25	1.35	1.37
39	C	519	DGD	O2E-C2E	-2.25	1.37	1.43
31	12	307	CLA	CMB-C2B	-2.25	1.47	1.51
31	0	313	CLA	CMD-C2D	-2.25	1.46	1.50
43	1	302	A86	O1-C20	-2.25	1.43	1.46
43	13	305	A86	C13-C11	-2.25	1.45	1.49
45	2	308	KC2	C4A-C3A	2.25	1.48	1.44
39	C	520	DGD	O3D-C3D	-2.25	1.37	1.43
31	b	616	CLA	CMD-C2D	-2.25	1.46	1.50
45	17	309	KC2	C1B-NB	-2.25	1.35	1.37
31	C	505	CLA	CMC-C2C	-2.25	1.46	1.50
43	3	304	A86	O3-C36	-2.25	1.39	1.43
44	P	612	DD6	O1-C20	-2.25	1.43	1.46
45	13	311	KC2	C4A-C3A	2.25	1.48	1.44
31	B	608	CLA	MG-ND	-2.25	2.01	2.05
32	D	402	PHO	CMD-C2D	-2.25	1.46	1.51
31	p	607	CLA	MG-ND	-2.25	2.01	2.05
42	16	315	KC1	C1A-CHA	2.25	1.46	1.40
31	6	309	CLA	MG-ND	-2.25	2.01	2.05
31	19	307	CLA	CMB-C2B	-2.25	1.47	1.51
31	2	307	CLA	MG-ND	-2.25	2.01	2.05
32	d	402	PHO	CMD-C2D	-2.25	1.46	1.51
31	14	314	CLA	C3B-C2B	-2.25	1.37	1.40
43	P	611	A86	C26-C27	-2.25	1.32	1.35
43	2	304	A86	C26-C27	-2.25	1.32	1.35
43	4	305	A86	C2-C1	-2.25	1.32	1.35
39	c	519	DGD	O2E-C2E	-2.25	1.37	1.43
31	P	601	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	17	309	KC2	C4A-C3A	2.24	1.48	1.44
38	15	314	LMG	C7-C8	2.24	1.57	1.50
31	C	509	CLA	C1D-ND	2.24	1.40	1.37
31	c	509	CLA	C1D-ND	2.24	1.40	1.37
31	11	312	CLA	MG-ND	-2.24	2.01	2.05
35	D	406	PL9	C20-C19	-2.24	1.44	1.50
31	p	601	CLA	C3B-C2B	-2.24	1.37	1.40
43	11	305	A86	O1-C20	-2.24	1.43	1.46
31	15	311	CLA	C1A-CHA	-2.24	1.33	1.43
39	C	518	DGD	O2E-C2E	-2.24	1.37	1.43
31	14	312	CLA	C3B-CAB	-2.24	1.43	1.47
31	d	401	CLA	MG-ND	-2.24	2.01	2.05
43	4	303	A86	C19-C20	2.24	1.55	1.52
31	8	311	CLA	CMC-C2C	-2.24	1.46	1.50
31	4	307	CLA	MG-ND	-2.24	2.01	2.05
31	5	311	CLA	C4B-CHC	-2.24	1.34	1.41
42	4	313	KC1	C1D-CHD	2.24	1.47	1.41
34	A	411	SQD	O2-C2	-2.24	1.37	1.43
31	19	312	CLA	CMB-C2B	-2.24	1.47	1.51
43	11	302	A86	O3-C36	2.24	1.47	1.43
43	10	318	A86	C33-C34	2.24	1.55	1.51
43	10	318	A86	C37-C36	-2.24	1.49	1.52
43	9	305	A86	C14-C13	2.24	1.54	1.51
31	0	314	CLA	CMD-C2D	-2.24	1.46	1.50
43	13	304	A86	C32-C31	-2.24	1.50	1.54
42	2	313	KC1	C4C-C3C	2.24	1.48	1.45
31	B	611	CLA	CMD-C2D	-2.24	1.46	1.50
42	4	313	KC1	C1B-NB	-2.24	1.35	1.37
43	2	301	A86	C13-C11	-2.24	1.45	1.49
31	p	602	CLA	C3B-C2B	-2.24	1.37	1.40
31	8	314	CLA	C3B-C2B	-2.24	1.37	1.40
39	11	318	DGD	C3G-C2G	2.24	1.57	1.50
31	19	310	CLA	CMB-C2B	-2.23	1.47	1.51
31	C	504	CLA	CMC-C2C	-2.23	1.46	1.50
31	c	504	CLA	CMC-C2C	-2.23	1.46	1.50
45	1	309	KC2	C4B-NB	-2.23	1.35	1.37
38	b	621	LMG	O3-C3	-2.23	1.37	1.43
31	19	313	CLA	CMB-C2B	-2.23	1.47	1.51
31	0	314	CLA	CMC-C2C	-2.23	1.46	1.50
43	4	303	A86	C32-C31	-2.23	1.50	1.54
42	18	313	KC1	C4A-C3A	2.23	1.48	1.44
42	11	314	KC1	C4B-NB	-2.23	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	610	CLA	MG-ND	-2.23	2.01	2.05
43	11	306	A86	C32-C31	-2.23	1.50	1.54
31	7	313	CLA	CMC-C2C	-2.23	1.46	1.50
31	W	202	CLA	MG-ND	-2.23	2.01	2.05
31	1	315	CLA	CMD-C2D	-2.23	1.46	1.50
43	4	304	A86	C13-C11	-2.23	1.45	1.49
31	8	314	CLA	CMD-C2D	-2.23	1.46	1.50
31	9	310	CLA	CMB-C2B	-2.23	1.47	1.51
43	8	305	A86	C32-C31	-2.23	1.50	1.54
31	A	404	CLA	MG-ND	-2.23	2.01	2.05
31	18	311	CLA	C3B-CAB	-2.23	1.43	1.47
31	4	314	CLA	CMD-C2D	-2.23	1.46	1.50
43	8	303	A86	C32-C31	-2.23	1.50	1.54
42	12	314	KC1	C4B-NB	-2.23	1.35	1.37
43	17	304	A86	C13-C11	-2.23	1.45	1.49
31	a	406	CLA	MG-ND	-2.22	2.01	2.05
31	A	406	CLA	CMC-C2C	-2.22	1.46	1.50
34	0	318	SQD	O2-C2	-2.22	1.37	1.43
43	14	303	A86	C13-C11	-2.22	1.45	1.49
31	b	616	CLA	C3B-CAB	-2.22	1.43	1.47
42	4	313	KC1	C4B-NB	-2.22	1.35	1.37
38	B	620	LMG	O3-C3	-2.22	1.37	1.43
31	A	406	CLA	MG-ND	-2.22	2.01	2.05
31	D	404	CLA	CAA-C2A	-2.22	1.50	1.54
31	B	607	CLA	CMD-C2D	-2.22	1.46	1.50
31	14	309	CLA	CMB-C2B	-2.22	1.47	1.51
31	10	308	CLA	CMC-C2C	-2.22	1.46	1.50
32	a	405	PHO	CMB-C2B	-2.22	1.46	1.51
42	12	314	KC1	C4C-C3C	2.22	1.48	1.45
31	13	313	CLA	C3B-C2B	-2.22	1.37	1.40
34	L	102	SQD	O2-C2	-2.22	1.37	1.43
38	W	201	LMG	O4-C4	-2.22	1.37	1.43
31	p	610	CLA	MG-ND	-2.22	2.01	2.05
31	P	601	CLA	CMC-C2C	-2.22	1.46	1.50
31	2	307	CLA	CMC-C2C	-2.22	1.46	1.50
32	A	405	PHO	CBD-CGD	-2.22	1.49	1.52
41	V	201	HEM	CAA-C2A	2.22	1.55	1.52
45	11	309	KC2	C1D-CHD	2.22	1.47	1.41
31	B	614	CLA	CMC-C2C	-2.22	1.46	1.50
31	15	311	CLA	C1D-ND	2.22	1.40	1.37
43	14	302	A86	C13-C11	-2.22	1.45	1.49
42	16	301	KC1	C1D-CHD	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	17	314	KC1	C4A-C3A	2.22	1.48	1.44
31	5	314	CLA	CMD-C2D	-2.22	1.46	1.50
43	1	320	A86	C13-C11	-2.22	1.45	1.49
31	2	307	CLA	C3B-CAB	-2.22	1.43	1.47
31	B	615	CLA	CMD-C2D	-2.22	1.46	1.50
45	18	310	KC2	C4B-NB	-2.21	1.35	1.37
31	12	313	CLA	CMC-C2C	-2.21	1.46	1.50
43	6	307	A86	C4-C3	-2.21	1.30	1.36
43	17	301	A86	C13-C11	-2.21	1.45	1.49
31	18	312	CLA	CMC-C2C	-2.21	1.46	1.50
43	11	319	A86	C13-C11	-2.21	1.45	1.49
31	12	308	CLA	CMC-C2C	-2.21	1.46	1.50
34	A	408	SQD	O3-C3	-2.21	1.37	1.43
31	P	608	CLA	C3B-C2B	-2.21	1.37	1.40
45	7	311	KC2	C3C-C4C	2.21	1.49	1.44
45	7	309	KC2	C4A-C3A	2.21	1.48	1.44
39	c	518	DGD	O3G-C1D	-2.21	1.36	1.40
31	18	311	CLA	CMC-C2C	-2.21	1.46	1.50
39	1	318	DGD	O1G-C1G	-2.21	1.40	1.45
31	B	615	CLA	C3B-CAB	-2.21	1.43	1.47
44	p	612	DD6	C13-C14	2.21	1.37	1.32
43	3	301	A86	C4-C3	-2.21	1.30	1.36
31	10	314	CLA	CMC-C2C	-2.21	1.46	1.50
43	17	316	A86	C2-C1	-2.21	1.32	1.35
45	5	310	KC2	C1A-CHA	2.21	1.46	1.40
31	19	315	CLA	CMB-C2B	-2.21	1.47	1.51
31	0	316	CLA	CMD-C2D	-2.21	1.46	1.50
31	17	310	CLA	CMB-C2B	-2.21	1.47	1.51
31	C	506	CLA	CMC-C2C	-2.21	1.46	1.50
31	9	308	CLA	CMD-C2D	-2.21	1.46	1.50
42	2	313	KC1	C1D-CHD	2.21	1.47	1.41
31	13	310	CLA	C3B-CAB	-2.21	1.43	1.47
34	0	318	SQD	O4-C4	-2.21	1.37	1.43
45	5	308	KC2	C4B-NB	-2.21	1.35	1.37
43	0	306	A86	C41-C32	-2.20	1.49	1.53
31	b	609	CLA	MG-ND	-2.20	2.01	2.05
31	d	404	CLA	CAA-C2A	-2.20	1.50	1.54
31	a	406	CLA	CMC-C2C	-2.20	1.46	1.50
31	b	603	CLA	CMD-C2D	-2.20	1.46	1.50
38	n	701	LMG	C7-C8	2.20	1.57	1.50
43	18	302	A86	C32-C31	-2.20	1.50	1.54
43	1	304	A86	C5-C6	-2.20	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	101	LMG	O4-C4	-2.20	1.37	1.43
38	j	101	LMG	O4-C4	-2.20	1.37	1.43
31	16	313	CLA	MG-ND	-2.20	2.01	2.05
43	0	304	A86	C32-C31	-2.20	1.50	1.54
31	D	404	CLA	C3B-CAB	-2.20	1.43	1.47
31	d	404	CLA	C3B-CAB	-2.20	1.43	1.47
43	17	303	A86	C13-C11	-2.20	1.45	1.49
31	B	608	CLA	C3B-C2B	-2.20	1.37	1.40
31	z	103	CLA	MG-ND	-2.20	2.01	2.05
31	2	312	CLA	CMC-C2C	-2.20	1.46	1.50
31	P	601	CLA	C3B-C2B	-2.20	1.37	1.40
31	b	612	CLA	CMD-C2D	-2.20	1.46	1.50
31	p	607	CLA	C3B-CAB	-2.20	1.43	1.47
31	D	401	CLA	C4B-CHC	-2.20	1.34	1.41
31	P	605	CLA	CMD-C2D	-2.20	1.46	1.50
31	11	313	CLA	C1D-ND	2.20	1.40	1.37
31	r	101	CLA	C3B-C2B	-2.20	1.37	1.40
31	P	605	CLA	CMC-C2C	-2.20	1.46	1.50
31	10	316	CLA	CMC-C2C	-2.20	1.46	1.50
43	5	302	A86	C40-C32	-2.19	1.49	1.53
31	z	101	CLA	C3B-C2B	-2.19	1.37	1.40
31	D	404	CLA	CHD-C1D	-2.19	1.34	1.38
31	d	404	CLA	CHD-C1D	-2.19	1.34	1.38
45	14	310	KC2	C1D-CHD	2.19	1.47	1.41
43	1	306	A86	C19-C20	2.19	1.55	1.52
44	P	612	DD6	C36-C31	-2.19	1.32	1.34
34	a	408	SQD	O3-C3	-2.19	1.37	1.43
31	0	316	CLA	CMC-C2C	-2.19	1.46	1.50
31	4	312	CLA	C3B-C2B	-2.19	1.37	1.40
31	0	309	CLA	CMC-C2C	-2.19	1.46	1.50
31	10	317	CLA	MG-ND	-2.19	2.01	2.05
43	12	305	A86	C13-C11	-2.19	1.45	1.49
31	p	601	CLA	CMC-C2C	-2.19	1.46	1.50
31	0	308	CLA	CMC-C2C	-2.19	1.46	1.50
31	1	312	CLA	CMC-C2C	-2.19	1.46	1.50
31	1	313	CLA	CMC-C2C	-2.19	1.46	1.50
31	b	602	CLA	MG-ND	-2.19	2.01	2.05
43	1	304	A86	C13-C11	-2.19	1.45	1.49
31	a	406	CLA	C3B-CAB	-2.19	1.43	1.47
31	b	608	CLA	CMD-C2D	-2.19	1.46	1.50
31	r	101	CLA	MG-ND	-2.19	2.01	2.05
31	12	312	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	19	305	A86	C14-C15	2.19	1.57	1.52
43	12	306	A86	C35-C34	2.19	1.55	1.51
39	C	520	DGD	O3E-C3E	-2.19	1.37	1.43
31	p	605	CLA	CMC-C2C	-2.19	1.46	1.50
31	R	101	CLA	MG-ND	-2.19	2.01	2.05
31	b	603	CLA	CAA-C2A	-2.18	1.50	1.54
42	7	314	KC1	C4B-NB	-2.18	1.35	1.37
44	p	612	DD6	C36-C31	-2.18	1.32	1.34
31	10	316	CLA	CMD-C2D	-2.18	1.46	1.50
31	A	406	CLA	C3B-CAB	-2.18	1.43	1.47
31	7	310	CLA	CMB-C2B	-2.18	1.47	1.51
31	B	602	CLA	CMD-C2D	-2.18	1.46	1.50
31	b	609	CLA	C3B-C2B	-2.18	1.37	1.40
38	D	403	LMG	O6-C1	2.18	1.47	1.41
31	11	310	CLA	C3B-CAB	-2.18	1.43	1.47
31	2	311	CLA	MG-ND	-2.18	2.01	2.05
43	10	305	A86	C13-C11	-2.18	1.45	1.49
43	19	302	A86	C13-C11	-2.18	1.45	1.49
31	4	312	CLA	CMC-C2C	-2.18	1.46	1.50
31	16	314	CLA	C1A-CHA	-2.18	1.34	1.43
31	p	605	CLA	CMD-C2D	-2.18	1.46	1.50
33	H	101	BCR	C33-C5	-2.18	1.47	1.50
31	10	309	CLA	CMC-C2C	-2.18	1.46	1.50
43	19	303	A86	C35-C34	2.18	1.55	1.51
38	p	614	LMG	O7-C8	-2.18	1.41	1.46
31	10	311	CLA	CMD-C2D	-2.18	1.46	1.50
43	16	305	A86	C5-C6	-2.18	1.32	1.35
41	v	201	HEM	CAA-C2A	2.18	1.55	1.52
31	13	312	CLA	CMD-C2D	-2.18	1.46	1.50
31	B	601	CLA	MG-ND	-2.18	2.01	2.05
43	17	301	A86	C30-C29	-2.18	1.28	1.32
43	1	320	A86	C35-C34	2.18	1.55	1.51
31	19	315	CLA	CMC-C2C	-2.17	1.46	1.50
39	c	520	DGD	O3E-C3E	-2.17	1.37	1.43
43	7	304	A86	C13-C11	-2.17	1.45	1.49
45	7	311	KC2	C1B-NB	-2.17	1.35	1.37
31	9	315	CLA	CMB-C2B	-2.17	1.47	1.51
31	R	101	CLA	C3B-C2B	-2.17	1.37	1.40
42	18	313	KC1	C4D-CHA	2.17	1.47	1.45
31	B	605	CLA	C4B-CHC	-2.17	1.35	1.41
31	d	405	CLA	C3B-C2B	-2.17	1.37	1.40
31	19	312	CLA	MG-ND	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	307	CLA	CMC-C2C	-2.17	1.46	1.50
31	a	404	CLA	CMC-C2C	-2.17	1.46	1.50
43	9	306	A86	C13-C11	-2.17	1.45	1.49
43	7	305	A86	C32-C31	-2.17	1.50	1.54
42	1	314	KC1	C4A-C3A	2.17	1.48	1.44
31	0	311	CLA	CMD-C2D	-2.17	1.46	1.50
35	d	406	PL9	C35-C34	-2.17	1.45	1.50
31	10	314	CLA	MG-ND	-2.17	2.01	2.05
31	b	607	CLA	MG-ND	-2.17	2.01	2.05
31	b	616	CLA	C4B-CHC	-2.17	1.35	1.41
43	8	301	A86	C5-C6	-2.17	1.32	1.35
43	3	304	A86	C13-C11	-2.17	1.45	1.49
31	1	321	CLA	CMC-C2C	-2.17	1.46	1.50
42	11	314	KC1	C4A-C3A	2.17	1.48	1.44
31	P	604	CLA	CMD-C2D	-2.17	1.46	1.50
31	12	315	CLA	CMD-C2D	-2.17	1.46	1.50
31	0	313	CLA	MG-ND	-2.17	2.01	2.05
31	c	505	CLA	C3B-CAB	-2.17	1.43	1.47
31	D	405	CLA	C3B-C2B	-2.17	1.37	1.40
38	10	319	LMG	C3-C2	2.17	1.57	1.52
42	14	313	KC1	C1B-NB	-2.17	1.35	1.37
31	14	314	CLA	CMD-C2D	-2.17	1.46	1.50
31	C	505	CLA	C4B-CHC	-2.17	1.35	1.41
38	d	403	LMG	O6-C1	2.16	1.47	1.41
43	14	305	A86	C17-C18	-2.16	1.49	1.52
31	6	309	CLA	C3B-CAB	-2.16	1.43	1.47
31	c	507	CLA	C3B-CAB	-2.16	1.43	1.47
31	10	316	CLA	C3B-CAB	-2.16	1.43	1.47
31	d	401	CLA	C4B-CHC	-2.16	1.35	1.41
39	c	518	DGD	O4E-C4E	-2.16	1.37	1.43
33	h	101	BCR	C33-C5	-2.16	1.47	1.50
31	16	313	CLA	C3B-CAB	-2.16	1.43	1.47
31	2	307	CLA	C1D-ND	2.16	1.40	1.37
39	C	518	DGD	O4E-C4E	-2.16	1.37	1.43
31	C	507	CLA	C3B-CAB	-2.16	1.43	1.47
31	P	607	CLA	C3B-CAB	-2.16	1.43	1.47
31	C	505	CLA	MG-ND	-2.16	2.01	2.05
31	c	505	CLA	MG-ND	-2.16	2.01	2.05
39	C	518	DGD	O6D-C5D	-2.16	1.39	1.44
31	C	507	CLA	CMD-C2D	-2.16	1.46	1.50
43	9	301	A86	C33-C34	2.16	1.55	1.51
43	1	306	A86	O1-C20	-2.16	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	18	307	CLA	C3B-CAB	-2.16	1.43	1.47
38	d	403	LMG	C7-C8	2.16	1.57	1.50
43	13	304	A86	O4-C34	-2.16	1.41	1.46
43	14	305	A86	C5-C6	-2.16	1.32	1.35
42	11	314	KC1	C1A-CHA	2.16	1.46	1.40
31	13	315	CLA	CMD-C2D	-2.16	1.46	1.50
39	b	622	DGD	C6E-C5E	2.16	1.59	1.51
31	0	309	CLA	MG-ND	-2.15	2.01	2.05
39	C	518	DGD	O3G-C1D	-2.15	1.36	1.40
31	12	307	CLA	CMD-C2D	-2.15	1.46	1.50
39	C	520	DGD	O2D-C2D	-2.15	1.37	1.43
31	B	606	CLA	MG-ND	-2.15	2.01	2.05
43	P	611	A86	C2-C1	-2.15	1.32	1.35
39	C	519	DGD	O3G-C3G	-2.15	1.39	1.43
31	5	312	CLA	C3B-CAB	-2.15	1.43	1.47
31	1	308	CLA	CMD-C2D	-2.15	1.46	1.50
31	14	314	CLA	CMC-C2C	-2.15	1.46	1.50
43	9	305	A86	C14-C15	2.15	1.56	1.52
39	C	519	DGD	O6E-C5E	-2.15	1.39	1.44
39	c	519	DGD	O6E-C5E	-2.15	1.39	1.44
43	1	303	A86	C17-C18	-2.15	1.49	1.52
31	12	308	CLA	MG-ND	-2.15	2.01	2.05
43	2	305	A86	C32-C31	-2.15	1.50	1.54
31	10	313	CLA	MG-ND	-2.15	2.01	2.05
31	15	306	CLA	C1B-NB	2.15	1.37	1.35
35	D	406	PL9	C35-C34	-2.15	1.45	1.50
45	4	310	KC2	C4B-NB	-2.15	1.35	1.37
38	B	620	LMG	C4-C5	2.15	1.57	1.53
31	z	101	CLA	MG-ND	-2.15	2.01	2.05
45	13	309	KC2	C4A-C3A	2.15	1.48	1.44
31	A	404	CLA	CMC-C2C	-2.15	1.46	1.50
43	16	305	A86	C2-C1	-2.15	1.32	1.35
31	b	617	CLA	MG-ND	-2.15	2.01	2.05
31	1	312	CLA	O2D-CED	-2.15	1.40	1.45
31	p	604	CLA	CMD-C2D	-2.15	1.46	1.50
31	B	616	CLA	MG-ND	-2.15	2.01	2.05
31	d	405	CLA	CMC-C2C	-2.15	1.46	1.50
42	14	313	KC1	C4C-C3C	2.15	1.48	1.45
31	18	306	CLA	MG-ND	-2.15	2.01	2.05
45	3	311	KC2	C4A-C3A	2.15	1.48	1.44
31	5	312	CLA	C1D-ND	2.15	1.40	1.37
42	0	315	KC1	C4B-NB	-2.15	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	8	310	KC2	C3C-C4C	2.15	1.49	1.44
31	15	312	CLA	MG-ND	-2.15	2.01	2.05
31	C	505	CLA	C3B-CAB	-2.15	1.43	1.47
34	A	408	SQD	O4-C4	-2.15	1.37	1.43
31	B	611	CLA	CAC-C3C	-2.15	1.45	1.51
31	8	306	CLA	MG-ND	-2.14	2.01	2.05
31	C	510	CLA	MG-ND	-2.14	2.01	2.05
31	c	505	CLA	C4B-CHC	-2.14	1.35	1.41
42	11	314	KC1	C1D-CHD	2.14	1.46	1.41
45	0	310	KC2	C4A-C3A	2.14	1.48	1.44
43	14	302	A86	C32-C31	-2.14	1.51	1.54
38	5	315	LMG	C1-C2	2.14	1.58	1.52
31	18	309	CLA	CMD-C2D	-2.14	1.46	1.50
31	6	313	CLA	C3B-CAB	-2.14	1.43	1.47
39	1	318	DGD	C4E-C5E	2.14	1.57	1.53
31	b	608	CLA	C3B-CAB	-2.14	1.43	1.47
31	4	312	CLA	C3B-CAB	-2.14	1.43	1.47
31	0	311	CLA	CMC-C2C	-2.14	1.46	1.50
31	11	315	CLA	C4C-C3C	2.14	1.48	1.45
31	14	307	CLA	MG-ND	-2.14	2.01	2.05
31	8	312	CLA	CMC-C2C	-2.14	1.46	1.50
42	19	314	KC1	C1C-C2C	2.14	1.48	1.44
31	Z	101	CLA	MG-ND	-2.14	2.01	2.05
31	4	309	CLA	CMC-C2C	-2.14	1.46	1.50
31	c	511	CLA	MG-ND	-2.14	2.01	2.05
38	P	614	LMG	O7-C8	-2.14	1.41	1.46
31	17	313	CLA	C1D-ND	2.14	1.40	1.37
39	c	520	DGD	O2D-C2D	-2.13	1.37	1.43
31	1	310	CLA	CMC-C2C	-2.13	1.46	1.50
31	11	308	CLA	MG-ND	-2.13	2.01	2.05
31	14	309	CLA	CMC-C2C	-2.13	1.46	1.50
31	P	604	CLA	CMC-C2C	-2.13	1.46	1.50
31	8	309	CLA	CMD-C2D	-2.13	1.46	1.50
31	18	309	CLA	CMC-C2C	-2.13	1.46	1.50
45	15	308	KC2	C4B-NB	-2.13	1.35	1.37
31	5	309	CLA	CMD-C2D	-2.13	1.46	1.50
31	C	503	CLA	CMC-C2C	-2.13	1.46	1.50
42	12	314	KC1	C1D-CHD	2.13	1.46	1.41
45	8	310	KC2	C4B-NB	-2.13	1.35	1.37
31	p	604	CLA	CMC-C2C	-2.13	1.46	1.50
31	B	613	CLA	MG-ND	-2.13	2.01	2.05
31	b	610	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	405	CLA	CMC-C2C	-2.13	1.46	1.50
43	7	302	A86	C13-C11	-2.13	1.45	1.49
39	c	518	DGD	O6D-C5D	-2.13	1.39	1.44
31	c	507	CLA	CMD-C2D	-2.13	1.46	1.50
43	6	305	A86	C32-C31	-2.13	1.51	1.54
31	3	313	CLA	CMC-C2C	-2.13	1.46	1.50
31	0	314	CLA	MG-ND	-2.13	2.01	2.05
31	2	306	CLA	CMB-C2B	-2.13	1.47	1.51
31	15	306	CLA	CMD-C2D	-2.13	1.46	1.50
31	19	313	CLA	CMC-C2C	-2.13	1.46	1.50
34	A	411	SQD	O4-C4	-2.13	1.38	1.43
39	h	102	DGD	O4D-C4D	-2.13	1.38	1.43
42	11	314	KC1	C4C-C3C	2.13	1.48	1.45
31	15	309	CLA	CMD-C2D	-2.13	1.46	1.50
34	i	101	SQD	O4-C4	-2.13	1.38	1.43
31	B	615	CLA	C4B-CHC	-2.13	1.35	1.41
31	b	612	CLA	C4B-CHC	-2.13	1.35	1.41
34	a	408	SQD	O4-C4	-2.13	1.38	1.43
31	14	306	CLA	CMC-C2C	-2.13	1.46	1.50
42	11	314	KC1	O2A-CGA	-2.13	1.24	1.30
38	5	315	LMG	C9-C8	2.13	1.57	1.50
33	B	618	BCR	C30-C25	-2.13	1.50	1.53
36	8	316	LHG	P-O6	2.13	1.67	1.59
45	3	311	KC2	C3C-C4C	2.13	1.49	1.44
45	15	310	KC2	C1A-CHA	2.13	1.46	1.40
31	9	312	CLA	MG-ND	-2.13	2.01	2.05
39	C	519	DGD	O6D-C5D	-2.13	1.39	1.44
43	17	301	A86	C26-C27	-2.12	1.33	1.35
31	5	309	CLA	C3B-CAB	-2.12	1.43	1.47
43	17	305	A86	C14-C13	2.12	1.53	1.51
39	b	622	DGD	C3G-C2G	2.12	1.57	1.50
31	11	313	CLA	CMC-C2C	-2.12	1.46	1.50
43	14	301	A86	C8-C6	2.12	1.50	1.45
31	z	101	CLA	CMC-C2C	-2.12	1.46	1.50
31	16	314	CLA	CMC-C2C	-2.12	1.46	1.50
43	5	303	A86	C17-C18	-2.12	1.49	1.52
42	p	609	KC1	C1D-CHD	2.12	1.46	1.41
31	b	610	CLA	CMC-C2C	-2.12	1.46	1.50
43	17	316	A86	C35-C34	2.12	1.55	1.51
31	B	612	CLA	CMA-C3A	-2.12	1.48	1.53
43	9	302	A86	C13-C11	-2.12	1.45	1.49
45	10	310	KC2	C1D-CHD	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	16	316	CLA	CMD-C2D	-2.12	1.46	1.50
31	B	607	CLA	C3B-CAB	-2.12	1.43	1.47
43	8	305	A86	C33-C34	2.12	1.55	1.51
36	A	410	LHG	O8-C6	-2.12	1.40	1.45
36	a	410	LHG	O8-C6	-2.12	1.40	1.45
34	i	101	SQD	O3-C3	-2.12	1.38	1.43
31	C	511	CLA	MG-ND	-2.12	2.01	2.05
31	B	616	CLA	C4B-CHC	-2.12	1.35	1.41
31	Z	101	CLA	CMC-C2C	-2.12	1.46	1.50
38	w	201	LMG	C7-C8	2.12	1.57	1.50
31	B	609	CLA	CMC-C2C	-2.12	1.46	1.50
39	W	203	DGD	C4D-C3D	2.12	1.57	1.52
31	17	315	CLA	CMD-C2D	-2.11	1.46	1.50
43	5	305	A86	C5-C6	-2.11	1.33	1.35
31	D	401	CLA	C3B-C2B	-2.11	1.37	1.40
34	A	411	SQD	O3-C3	-2.11	1.38	1.43
31	17	313	CLA	CMC-C2C	-2.11	1.46	1.50
31	19	308	CLA	CMD-C2D	-2.11	1.46	1.50
45	14	310	KC2	C4B-NB	-2.11	1.35	1.37
45	17	311	KC2	C4B-NB	-2.11	1.35	1.37
31	B	611	CLA	C4B-CHC	-2.11	1.35	1.41
31	18	306	CLA	CMD-C2D	-2.11	1.46	1.50
38	f	102	LMG	O4-C4	-2.11	1.38	1.43
31	6	313	CLA	MG-ND	-2.11	2.01	2.05
34	l	101	SQD	O3-C3	-2.11	1.38	1.43
31	b	617	CLA	C4B-CHC	-2.11	1.35	1.41
31	D	401	CLA	CAC-C3C	-2.11	1.45	1.51
31	8	306	CLA	CMC-C2C	-2.11	1.46	1.50
42	9	314	KC1	C3B-C4B	2.11	1.49	1.46
42	P	609	KC1	C1D-CHD	2.11	1.46	1.41
38	B	620	LMG	O4-C4	-2.11	1.38	1.43
38	f	102	LMG	O3-C3	-2.11	1.38	1.43
31	11	312	CLA	CMC-C2C	-2.11	1.46	1.50
45	6	312	KC2	C3C-C4C	2.11	1.49	1.44
45	16	312	KC2	C3C-C4C	2.11	1.49	1.44
31	c	510	CLA	MG-ND	-2.11	2.01	2.05
39	H	102	DGD	O4D-C4D	-2.11	1.38	1.43
31	15	309	CLA	MG-ND	-2.11	2.01	2.05
31	b	613	CLA	CMA-C3A	-2.10	1.48	1.53
38	W	201	LMG	C7-C8	2.10	1.57	1.50
43	7	304	A86	C14-C13	2.10	1.53	1.51
31	b	612	CLA	CAC-C3C	-2.10	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	606	CLA	C4B-CHC	-2.10	1.35	1.41
34	L	102	SQD	O3-C3	-2.10	1.38	1.43
31	8	306	CLA	CMD-C2D	-2.10	1.46	1.50
31	11	310	CLA	CMC-C2C	-2.10	1.46	1.50
31	b	607	CLA	C4B-CHC	-2.10	1.35	1.41
31	B	606	CLA	CAC-C3C	-2.10	1.45	1.51
43	0	303	A86	C37-C36	-2.10	1.49	1.52
36	C	521	LHG	O7-C5	-2.10	1.41	1.46
36	w	202	LHG	O7-C5	-2.10	1.41	1.46
45	11	309	KC2	C1A-CHA	2.10	1.46	1.40
31	Z	101	CLA	C3B-C2B	-2.10	1.37	1.40
34	L	102	SQD	O4-C4	-2.10	1.38	1.43
31	b	611	CLA	MG-ND	-2.10	2.01	2.05
31	10	309	CLA	CMD-C2D	-2.10	1.46	1.50
39	c	519	DGD	O3G-C3G	-2.10	1.39	1.43
43	p	613	A86	C13-C11	-2.10	1.45	1.49
42	7	314	KC1	C1B-C2B	2.10	1.49	1.45
33	c	516	BCR	C27-C26	-2.10	1.46	1.51
31	15	307	CLA	CMC-C2C	-2.10	1.46	1.50
42	19	314	KC1	C3B-C4B	2.10	1.49	1.46
31	5	309	CLA	MG-ND	-2.10	2.01	2.05
31	P	603	CLA	CMC-C2C	-2.10	1.46	1.50
31	1	308	CLA	CMC-C2C	-2.10	1.46	1.50
42	14	313	KC1	C4A-C3A	2.10	1.48	1.44
31	1	310	CLA	CMD-C2D	-2.10	1.46	1.50
42	11	314	KC1	C1B-NB	-2.10	1.35	1.37
31	2	311	CLA	C3B-C2B	-2.09	1.37	1.40
31	B	602	CLA	C3B-C2B	-2.09	1.37	1.40
31	c	503	CLA	CMC-C2C	-2.09	1.46	1.50
31	p	604	CLA	MG-ND	-2.09	2.01	2.05
43	15	303	A86	C17-C18	-2.09	1.49	1.52
42	19	314	KC1	C4C-C3C	2.09	1.48	1.45
43	8	303	A86	C5-C6	-2.09	1.33	1.35
39	c	519	DGD	O6D-C5D	-2.09	1.39	1.44
31	8	309	CLA	CMC-C2C	-2.09	1.46	1.50
31	11	316	CLA	CMC-C2C	-2.09	1.46	1.50
45	5	308	KC2	O2A-CGA	-2.09	1.24	1.30
45	8	308	KC2	O2A-CGA	-2.09	1.24	1.30
45	16	310	KC2	C4B-NB	-2.09	1.35	1.37
32	a	405	PHO	C1C-NC	-2.09	1.32	1.38
42	4	313	KC1	C4C-C3C	2.09	1.48	1.45
31	a	404	CLA	C3B-C2B	-2.09	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	14	304	A86	C32-C31	-2.09	1.51	1.54
38	b	621	LMG	O4-C4	-2.09	1.38	1.43
45	10	310	KC2	C4A-C3A	2.09	1.48	1.44
42	4	313	KC1	O2A-CGA	-2.09	1.24	1.30
31	9	313	CLA	CMC-C2C	-2.09	1.46	1.50
31	12	312	CLA	MG-ND	-2.09	2.01	2.05
34	l	101	SQD	O4-C4	-2.09	1.38	1.43
38	F	102	LMG	O3-C3	-2.09	1.38	1.43
31	d	401	CLA	CAC-C3C	-2.09	1.45	1.51
38	5	315	LMG	O7-C8	-2.09	1.41	1.46
39	w	204	DGD	C4D-C3D	2.09	1.57	1.52
31	0	307	CLA	CMC-C2C	-2.09	1.46	1.50
45	5	310	KC2	O2A-CGA	-2.09	1.24	1.30
31	4	315	CLA	CMC-C2C	-2.09	1.46	1.50
43	7	303	A86	C13-C11	-2.09	1.45	1.49
31	6	311	CLA	CMD-C2D	-2.09	1.46	1.50
31	6	316	CLA	CMD-C2D	-2.09	1.46	1.50
31	p	603	CLA	CMC-C2C	-2.09	1.46	1.50
31	12	310	CLA	CMC-C2C	-2.09	1.46	1.50
45	15	310	KC2	O2A-CGA	-2.09	1.24	1.30
31	8	311	CLA	C3B-CAB	-2.08	1.43	1.47
31	b	609	CLA	CMC-C2C	-2.08	1.46	1.50
36	18	316	LHG	P-O6	2.08	1.67	1.59
43	12	302	A86	C32-C31	2.08	1.58	1.54
31	14	306	CLA	CMD-C2D	-2.08	1.46	1.50
45	4	308	KC2	C4B-NB	-2.08	1.35	1.37
43	4	305	A86	C5-C6	-2.08	1.33	1.35
31	B	604	CLA	CMA-C3A	-2.08	1.48	1.53
31	2	309	CLA	CMC-C2C	-2.08	1.46	1.50
39	B	621	DGD	C4E-C3E	2.08	1.57	1.52
43	6	305	A86	C40-C32	-2.08	1.49	1.53
34	B	623	SQD	O3-C3	-2.08	1.38	1.43
38	N	101	LMG	O4-C4	-2.08	1.38	1.43
38	15	314	LMG	C9-C8	2.08	1.57	1.50
31	4	314	CLA	CMC-C2C	-2.08	1.46	1.50
31	14	312	CLA	CMC-C2C	-2.08	1.46	1.50
31	19	313	CLA	CMD-C2D	-2.08	1.46	1.50
31	4	311	CLA	MG-ND	-2.08	2.01	2.05
31	z	103	CLA	CMC-C2C	-2.08	1.46	1.50
31	1	316	CLA	CMC-C2C	-2.08	1.46	1.50
32	A	405	PHO	C1C-NC	-2.08	1.32	1.38
34	b	601	SQD	O3-C3	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	11	318	DGD	O2G-C2G	-2.08	1.41	1.46
31	11	310	CLA	CMD-C2D	-2.08	1.46	1.50
33	b	619	BCR	C30-C25	-2.08	1.50	1.53
31	B	602	CLA	CAA-C2A	-2.08	1.50	1.54
31	5	312	CLA	CMC-C2C	-2.07	1.46	1.50
31	9	315	CLA	CMC-C2C	-2.07	1.46	1.50
31	18	312	CLA	OBD-CAD	-2.07	1.18	1.22
34	10	320	SQD	O3-C3	-2.07	1.38	1.43
43	16	307	A86	C33-C34	2.07	1.55	1.51
31	3	308	CLA	MG-ND	-2.07	2.01	2.05
31	D	405	CLA	C3B-CAB	-2.07	1.43	1.47
35	A	409	PL9	C53-C6	-2.07	1.46	1.50
31	b	614	CLA	MG-ND	-2.07	2.01	2.05
45	18	310	KC2	C3C-C4C	2.07	1.49	1.44
33	C	516	BCR	C27-C26	-2.07	1.46	1.51
38	n	701	LMG	O4-C4	-2.07	1.38	1.43
32	D	402	PHO	CMB-C2B	-2.07	1.46	1.51
31	c	506	CLA	MG-ND	-2.07	2.01	2.05
31	b	603	CLA	C3B-C2B	-2.07	1.37	1.40
31	13	313	CLA	CMA-C3A	-2.07	1.48	1.53
39	B	621	DGD	O2D-C2D	-2.07	1.38	1.43
43	0	303	A86	C32-C31	-2.07	1.51	1.54
43	p	611	A86	C2-C1	-2.07	1.33	1.35
43	14	305	A86	C33-C34	2.07	1.55	1.51
42	18	313	KC1	C1A-CHA	2.07	1.46	1.40
31	11	316	CLA	CMD-C2D	-2.07	1.46	1.50
31	19	308	CLA	CMC-C2C	-2.07	1.46	1.50
31	0	316	CLA	C3B-CAB	-2.07	1.43	1.47
31	14	315	CLA	C3B-CAB	-2.07	1.43	1.47
42	19	314	KC1	C1B-NB	-2.07	1.35	1.37
31	16	309	CLA	CMC-C2C	-2.07	1.46	1.50
39	W	203	DGD	O1G-C1G	-2.07	1.40	1.45
38	Z	102	LMG	O1-C1	2.07	1.43	1.40
31	B	608	CLA	CMC-C2C	-2.07	1.46	1.50
43	P	613	A86	C13-C11	-2.07	1.45	1.49
31	d	401	CLA	C3B-CAB	-2.07	1.43	1.47
38	w	201	LMG	O2-C2	-2.07	1.38	1.43
43	10	303	A86	C37-C36	-2.07	1.49	1.52
42	8	313	KC1	O2A-CGA	-2.07	1.24	1.30
38	n	701	LMG	C4-C5	2.07	1.57	1.53
31	14	311	CLA	MG-ND	-2.07	2.01	2.05
31	0	307	CLA	C3B-C2B	-2.07	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	13	315	CLA	C3B-C2B	-2.07	1.37	1.40
34	b	601	SQD	O4-C4	-2.06	1.38	1.43
35	a	409	PL9	C53-C6	-2.06	1.46	1.50
31	B	609	CLA	MG-ND	-2.06	2.01	2.05
38	N	101	LMG	C4-C5	2.06	1.57	1.53
42	0	315	KC1	C1A-CHA	2.06	1.46	1.40
45	12	311	KC2	C4A-C3A	2.06	1.48	1.44
45	18	308	KC2	O2A-CGA	-2.06	1.24	1.30
31	A	404	CLA	C3B-C2B	-2.06	1.37	1.40
31	13	316	CLA	CMD-C2D	-2.06	1.46	1.50
31	4	315	CLA	CMA-C3A	-2.06	1.48	1.53
31	A	404	CLA	C3B-CAB	-2.06	1.43	1.47
39	w	204	DGD	O1G-C1G	-2.06	1.40	1.45
45	7	311	KC2	C4A-C3A	2.06	1.48	1.44
31	1	321	CLA	CMD-C2D	-2.06	1.46	1.50
36	l	102	LHG	P-O6	2.06	1.67	1.59
34	B	623	SQD	O4-C4	-2.06	1.38	1.43
31	10	317	CLA	CMC-C2C	-2.06	1.46	1.50
45	7	311	KC2	C4B-NB	-2.06	1.35	1.37
31	P	604	CLA	MG-ND	-2.06	2.01	2.05
31	10	311	CLA	CMC-C2C	-2.06	1.46	1.50
31	12	312	CLA	CMC-C2C	-2.06	1.46	1.50
38	c	522	LMG	C1-C2	2.06	1.58	1.52
38	15	314	LMG	O4-C4	-2.06	1.38	1.43
31	14	309	CLA	CMD-C2D	-2.06	1.46	1.50
43	17	305	A86	C14-C15	2.06	1.56	1.52
45	6	310	KC2	C4B-NB	-2.06	1.35	1.37
31	14	315	CLA	CMC-C2C	-2.06	1.46	1.50
31	7	312	CLA	CMC-C2C	-2.06	1.46	1.50
31	9	313	CLA	CMD-C2D	-2.06	1.46	1.50
45	11	311	KC2	C1D-CHD	2.05	1.46	1.41
36	4	317	LHG	P-O6	2.05	1.67	1.59
45	0	310	KC2	C1D-CHD	2.05	1.46	1.41
34	0	318	SQD	O3-C3	-2.05	1.38	1.43
31	13	313	CLA	C1A-CHA	-2.05	1.34	1.43
31	9	308	CLA	CMC-C2C	-2.05	1.46	1.50
31	14	311	CLA	C3C-C2C	2.05	1.41	1.36
31	b	605	CLA	CMA-C3A	-2.05	1.48	1.53
38	F	102	LMG	O4-C4	-2.05	1.38	1.43
45	15	310	KC2	C4A-C3A	2.05	1.48	1.44
38	W	201	LMG	O2-C2	-2.05	1.38	1.43
31	P	603	CLA	C3B-CAB	-2.05	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	622	DGD	O4D-C4D	-2.05	1.38	1.43
31	7	315	CLA	CMD-C2D	-2.05	1.46	1.50
43	10	318	A86	C23-C16	-2.05	1.49	1.53
31	B	606	CLA	C4B-CHC	-2.05	1.35	1.41
31	5	306	CLA	CMD-C2D	-2.05	1.46	1.50
42	6	315	KC1	CMD-C2D	-2.05	1.47	1.51
45	15	308	KC2	C4A-C3A	2.05	1.48	1.44
31	1	307	CLA	CMD-C2D	-2.05	1.46	1.50
31	d	401	CLA	C3B-C2B	-2.05	1.37	1.40
31	16	309	CLA	MG-ND	-2.05	2.01	2.05
31	18	312	CLA	MG-ND	-2.05	2.01	2.05
31	2	315	CLA	C3D-C4D	2.05	1.48	1.44
38	5	315	LMG	O4-C4	-2.05	1.38	1.43
31	b	607	CLA	CAC-C3C	-2.05	1.45	1.51
31	4	309	CLA	CMD-C2D	-2.05	1.46	1.50
43	2	302	A86	C13-C11	-2.05	1.45	1.49
43	10	302	A86	C26-C27	-2.04	1.33	1.35
31	p	603	CLA	C3B-CAB	-2.04	1.43	1.47
31	4	312	CLA	C1A-CHA	-2.04	1.34	1.43
43	12	303	A86	O3-C36	2.04	1.46	1.43
31	8	312	CLA	C1A-CHA	-2.04	1.34	1.43
33	a	407	BCR	C38-C26	-2.04	1.47	1.50
31	p	601	CLA	C3B-CAB	-2.04	1.43	1.47
31	d	405	CLA	MG-ND	-2.04	2.01	2.05
39	h	102	DGD	O2G-C2G	-2.04	1.41	1.46
43	1	303	A86	O4-C34	-2.04	1.41	1.46
43	6	304	A86	C5-C6	-2.04	1.33	1.35
31	7	307	CLA	C4B-CHC	-2.04	1.35	1.41
31	18	309	CLA	MG-ND	-2.04	2.01	2.05
38	b	621	LMG	C4-C5	2.04	1.57	1.53
31	9	313	CLA	CAC-C3C	-2.04	1.45	1.51
31	15	312	CLA	CMD-C2D	-2.04	1.46	1.50
42	16	301	KC1	C4C-C3C	2.04	1.48	1.45
43	6	305	A86	C13-C11	-2.04	1.45	1.49
31	17	312	CLA	MG-ND	-2.04	2.01	2.05
43	10	303	A86	C32-C31	-2.04	1.51	1.54
31	5	314	CLA	C3B-C2B	-2.04	1.37	1.40
32	d	402	PHO	CMB-C2B	-2.04	1.46	1.51
39	H	102	DGD	O2G-C2G	-2.04	1.41	1.46
31	18	314	CLA	MG-ND	-2.04	2.01	2.05
38	F	102	LMG	O2-C2	-2.04	1.38	1.43
39	C	520	DGD	O4E-C4E	-2.04	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	c	520	DGD	O4E-C4E	-2.04	1.38	1.43
42	3	314	KC1	C1C-C2C	2.04	1.48	1.44
32	d	402	PHO	CHA-CBD	-2.03	1.49	1.52
31	b	605	CLA	C1C-NC	-2.03	1.34	1.37
32	d	402	PHO	C1C-NC	-2.03	1.32	1.38
31	16	311	CLA	CMD-C2D	-2.03	1.46	1.50
43	3	305	A86	C35-C34	2.03	1.55	1.51
43	17	301	A86	C37-C36	-2.03	1.49	1.52
36	L	101	LHG	P-O6	2.03	1.67	1.59
42	14	313	KC1	O2A-CGA	-2.03	1.25	1.30
31	b	606	CLA	MG-ND	-2.03	2.01	2.05
31	a	404	CLA	C3B-CAB	-2.03	1.43	1.47
42	2	313	KC1	C4A-C3A	2.03	1.48	1.44
45	14	308	KC2	C4A-C3A	2.03	1.48	1.44
31	d	405	CLA	C3B-CAB	-2.03	1.43	1.47
31	0	314	CLA	C3B-CAB	-2.03	1.43	1.47
38	Z	102	LMG	C1-C2	2.03	1.58	1.52
39	b	622	DGD	O2D-C2D	-2.03	1.38	1.43
43	16	307	A86	O3-C36	2.03	1.46	1.43
32	D	402	PHO	C1C-NC	-2.03	1.32	1.38
31	C	506	CLA	MG-ND	-2.03	2.01	2.05
42	1	314	KC1	C4C-C3C	2.03	1.48	1.45
31	D	401	CLA	C3B-CAB	-2.03	1.43	1.47
31	10	314	CLA	C3B-CAB	-2.03	1.43	1.47
31	8	307	CLA	CMA-C3A	-2.03	1.48	1.53
31	19	307	CLA	CMD-C2D	-2.03	1.46	1.50
32	D	402	PHO	CHA-CBD	-2.03	1.49	1.52
31	c	507	CLA	C4B-CHC	-2.03	1.35	1.41
31	6	309	CLA	CMC-C2C	-2.03	1.46	1.50
33	A	407	BCR	C38-C26	-2.03	1.47	1.50
31	3	307	CLA	C4B-CHC	-2.03	1.35	1.41
31	b	608	CLA	MG-ND	-2.03	2.01	2.05
43	11	304	A86	C2-C1	-2.03	1.33	1.35
42	5	313	KC1	C4C-C3C	2.03	1.48	1.45
31	P	601	CLA	C3B-CAB	-2.03	1.43	1.47
31	B	605	CLA	MG-ND	-2.03	2.01	2.05
31	18	306	CLA	CMC-C2C	-2.03	1.46	1.50
31	b	606	CLA	CAC-C3C	-2.03	1.45	1.51
42	6	315	KC1	C1A-CHA	2.03	1.45	1.40
45	1	311	KC2	C1D-CHD	2.03	1.46	1.41
31	2	315	CLA	CHD-C1D	-2.03	1.34	1.38
38	d	408	LMG	O1-C7	-2.03	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	12	306	A86	C5-C6	-2.02	1.33	1.35
31	19	311	CLA	CMD-C2D	-2.02	1.46	1.50
42	5	313	KC1	C4A-C3A	2.02	1.48	1.44
45	2	310	KC2	C4A-C3A	2.02	1.48	1.44
31	7	313	CLA	C1D-ND	2.02	1.40	1.37
31	17	312	CLA	C3B-C2B	-2.02	1.37	1.40
43	4	303	A86	C19-C18	2.02	1.55	1.52
45	16	310	KC2	C4A-C3A	2.02	1.48	1.44
31	1	316	CLA	CMD-C2D	-2.02	1.46	1.50
31	3	316	CLA	C3D-C4D	2.02	1.48	1.44
42	0	315	KC1	C4C-C3C	2.02	1.48	1.45
36	14	317	LHG	P-O6	2.02	1.67	1.59
31	9	307	CLA	CMD-C2D	-2.02	1.46	1.50
31	8	314	CLA	CMC-C2C	-2.02	1.46	1.50
31	B	610	CLA	MG-ND	-2.02	2.01	2.05
31	3	315	CLA	CMD-C2D	-2.02	1.46	1.50
31	12	313	CLA	C3B-CAB	-2.02	1.43	1.47
42	9	314	KC1	C1C-C2C	2.02	1.48	1.44
38	B	620	LMG	O8-C9	-2.02	1.40	1.45
38	4	316	LMG	O8-C9	-2.02	1.40	1.45
31	P	602	CLA	CMD-C2D	-2.02	1.46	1.50
43	17	305	A86	C13-C11	-2.02	1.45	1.49
43	1	303	A86	C2-C1	-2.02	1.33	1.35
43	3	305	A86	C14-C15	2.02	1.56	1.52
31	c	511	CLA	CAC-C3C	-2.02	1.45	1.51
45	3	309	KC2	O2A-CGA	-2.02	1.25	1.30
38	b	621	LMG	O8-C9	-2.02	1.40	1.45
31	C	509	CLA	C3B-C2B	-2.02	1.37	1.40
31	c	509	CLA	C3B-C2B	-2.02	1.37	1.40
38	f	102	LMG	O2-C2	-2.02	1.38	1.43
31	8	314	CLA	MG-ND	-2.02	2.01	2.05
31	C	511	CLA	C3B-CAB	-2.02	1.43	1.47
45	14	308	KC2	C4B-NB	-2.02	1.35	1.37
34	10	320	SQD	O47-C45	-2.02	1.41	1.46
43	5	304	A86	C40-C32	-2.02	1.49	1.53
39	W	203	DGD	C1D-C2D	2.02	1.58	1.52
34	a	408	SQD	O47-C45	-2.02	1.41	1.46
31	19	311	CLA	CMC-C2C	-2.02	1.46	1.50
39	W	203	DGD	C6D-C5D	2.02	1.57	1.51
31	B	605	CLA	CAC-C3C	-2.02	1.45	1.51
31	Z	101	CLA	C3B-CAB	-2.01	1.43	1.47
39	C	519	DGD	O4D-C4D	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	c	519	DGD	O4D-C4D	-2.01	1.38	1.43
43	3	304	A86	C5-C6	-2.01	1.33	1.35
43	6	303	A86	C13-C11	-2.01	1.45	1.49
43	6	304	A86	C26-C27	-2.01	1.33	1.35
36	8	315	LHG	O7-C5	-2.01	1.41	1.46
31	12	307	CLA	MG-ND	-2.01	2.01	2.05
36	l	102	LHG	O8-C6	-2.01	1.40	1.45
31	10	313	CLA	C3B-CAB	-2.01	1.43	1.47
43	11	302	A86	C13-C11	-2.01	1.45	1.49
43	8	305	A86	C17-C18	-2.01	1.49	1.52
31	4	315	CLA	CMD-C2D	-2.01	1.46	1.50
31	10	307	CLA	CMC-C2C	-2.01	1.46	1.50
31	A	403	CLA	C3B-CAB	-2.01	1.43	1.47
33	F	101	BCR	C33-C5	-2.01	1.47	1.50
33	f	101	BCR	C33-C5	-2.01	1.47	1.50
31	17	312	CLA	CMC-C2C	-2.01	1.46	1.50
31	12	313	CLA	C1D-ND	2.01	1.40	1.37
31	b	616	CLA	CAC-C3C	-2.01	1.46	1.51
42	18	313	KC1	O2A-CGA	-2.01	1.25	1.30
38	c	522	LMG	O1-C1	2.01	1.43	1.40
41	e	101	HEM	CMB-C2B	2.01	1.55	1.50
33	C	516	BCR	C33-C5	-2.01	1.47	1.50
33	c	516	BCR	C33-C5	-2.01	1.47	1.50
31	2	311	CLA	CMC-C2C	-2.01	1.46	1.50
31	17	308	CLA	CMC-C2C	-2.01	1.46	1.50
31	15	312	CLA	C1D-C2D	2.01	1.49	1.45
39	c	519	DGD	O2D-C2D	-2.01	1.38	1.43
42	6	315	KC1	C4B-NB	-2.01	1.35	1.37
34	A	408	SQD	O47-C45	-2.01	1.41	1.46
38	0	317	LMG	C7-C8	2.01	1.56	1.50
31	0	307	CLA	CMD-C2D	-2.01	1.46	1.50
45	7	309	KC2	C4B-NB	-2.01	1.35	1.37
31	B	607	CLA	MG-ND	-2.00	2.01	2.05
31	8	309	CLA	MG-ND	-2.00	2.01	2.05
31	C	507	CLA	C4B-CHC	-2.00	1.35	1.41
43	14	305	A86	C2-C1	-2.00	1.33	1.35
36	L	101	LHG	O8-C6	-2.00	1.40	1.45
45	6	310	KC2	C4A-C3A	2.00	1.48	1.44
42	9	314	KC1	C1B-NB	-2.00	1.35	1.37
42	p	609	KC1	O2A-CGA	-2.00	1.25	1.30
39	w	204	DGD	C1D-C2D	2.00	1.58	1.52
31	6	314	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	607	CLA	C4B-CHC	-2.00	1.35	1.41
31	b	608	CLA	C4B-CHC	-2.00	1.35	1.41
43	2	303	A86	C17-C18	-2.00	1.49	1.52
31	2	314	CLA	CMD-C2D	-2.00	1.46	1.50
42	16	301	KC1	C4B-NB	-2.00	1.35	1.37

All (8349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	304	A86	O1-C20-C19	-32.86	88.70	113.38
43	P	611	A86	O1-C20-C19	-27.13	93.00	113.38
43	p	611	A86	O1-C20-C19	-27.03	93.07	113.38
42	8	313	KC1	CMD-C2D-C1D	-25.69	88.98	128.46
42	6	315	KC1	OBD-CAD-CBD	23.59	159.59	125.89
43	2	302	A86	O1-C20-C19	22.66	130.41	113.38
43	12	301	A86	O1-C20-C19	22.61	130.37	113.38
42	6	315	KC1	CMD-C2D-C1D	-22.60	93.73	128.46
42	18	313	KC1	OBD-CAD-CBD	22.55	158.11	125.89
43	2	304	A86	C40-C32-C31	-22.54	90.30	110.47
43	6	305	A86	O1-C20-C19	-22.35	96.59	113.38
43	18	301	A86	O1-C20-C19	22.29	130.13	113.38
43	16	306	A86	O1-C20-C19	-22.19	96.71	113.38
42	8	313	KC1	CMD-C2D-C3D	22.11	166.05	124.68
43	3	305	A86	O1-C20-C19	-22.06	96.81	113.38
43	11	302	A86	O1-C20-C19	22.05	129.94	113.38
43	0	304	A86	O1-C20-C19	22.00	129.91	113.38
43	10	304	A86	O1-C20-C19	21.94	129.86	113.38
43	9	304	A86	O1-C20-C19	21.65	129.65	113.38
42	16	315	KC1	OBD-CAD-CBD	21.60	156.76	125.89
43	19	301	A86	O1-C20-C19	21.44	129.49	113.38
43	19	304	A86	O1-C20-C19	21.39	129.45	113.38
43	9	301	A86	O1-C20-C19	21.29	129.38	113.38
43	3	306	A86	C41-C32-C31	21.24	129.48	110.47
43	11	306	A86	O1-C20-C19	-20.94	97.65	113.38
43	13	304	A86	O1-C20-C19	-20.93	97.66	113.38
43	2	304	A86	O1-C20-C19	20.91	129.09	113.38
42	3	314	KC1	CMD-C2D-C1D	-20.89	96.35	128.46
43	19	305	A86	O1-C20-C19	-20.72	97.81	113.38
43	9	305	A86	O1-C20-C19	-20.67	97.85	113.38
42	17	314	KC1	CMD-C2D-C1D	-20.65	96.72	128.46
43	10	301	A86	O1-C20-C19	20.65	128.89	113.38
43	0	301	A86	O1-C20-C19	20.64	128.88	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	304	A86	O1-C20-C19	20.62	128.87	113.38
43	8	304	A86	O1-C20-C19	20.36	128.67	113.38
43	7	304	A86	O1-C20-C19	-20.17	98.23	113.38
43	18	304	A86	O1-C20-C19	20.01	128.41	113.38
43	19	302	A86	C28-C27-C29	-19.97	72.66	118.93
43	13	306	A86	O1-C20-C19	19.49	128.02	113.38
43	17	305	A86	O1-C20-C19	-19.43	98.79	113.38
43	1	306	A86	O1-C20-C19	18.86	127.55	113.38
42	16	315	KC1	CMD-C2D-C1D	-18.76	99.63	128.46
42	3	314	KC1	CMD-C2D-C3D	18.69	159.64	124.68
42	18	313	KC1	CMD-C2D-C1D	-18.67	99.77	128.46
42	17	314	KC1	CMD-C2D-C3D	18.61	159.49	124.68
45	14	308	KC2	CMD-C2D-C1D	-18.53	99.98	128.46
43	19	302	A86	C28-C27-C26	-18.44	97.10	122.92
42	3	314	KC1	OBD-CAD-CBD	18.37	152.14	125.89
42	6	315	KC1	CMD-C2D-C3D	17.95	158.25	124.68
45	4	308	KC2	CMD-C2D-C1D	-17.94	100.89	128.46
42	0	315	KC1	CMD-C2D-C1D	-17.92	100.93	128.46
43	15	304	A86	C40-C32-C31	-17.40	94.90	110.47
43	5	303	A86	O1-C20-C21	-17.26	94.37	115.06
43	15	303	A86	O1-C20-C21	-17.05	94.62	115.06
43	17	305	A86	O1-C20-C21	-17.04	94.64	115.06
43	6	303	A86	O1-C20-C19	-17.03	100.59	113.38
43	7	302	A86	O1-C20-C19	-17.03	100.59	113.38
43	15	302	A86	C41-C32-C31	16.90	125.60	110.47
43	P	611	A86	O1-C20-C21	-16.89	94.82	115.06
45	2	310	KC2	OBD-CAD-CBD	16.85	149.97	125.89
43	p	611	A86	O1-C20-C21	-16.85	94.86	115.06
45	8	310	KC2	CMD-C2D-C1D	-16.85	102.57	128.46
42	14	313	KC1	CMD-C2D-C1D	-16.82	102.61	128.46
45	10	310	KC2	OBD-CAD-CBD	16.82	149.92	125.89
42	2	313	KC1	OBD-CAD-CBD	16.76	149.84	125.89
45	18	310	KC2	CMD-C2D-C1D	-16.71	102.78	128.46
45	14	308	KC2	CMD-C2D-C3D	16.69	155.90	124.68
43	17	301	A86	C33-C32-C31	-16.67	93.01	109.21
43	7	304	A86	O1-C20-C21	-16.65	95.10	115.06
43	12	302	A86	C33-C32-C31	-16.65	93.03	109.21
45	14	310	KC2	OBD-CAD-CBD	16.63	149.66	125.89
45	16	312	KC2	CMD-C2D-C1D	-16.49	103.12	128.46
42	5	313	KC1	CMD-C2D-C1D	16.42	153.69	128.46
42	10	315	KC1	OBD-CAD-CBD	16.35	149.26	125.89
45	4	310	KC2	OBD-CAD-CBD	16.34	149.24	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	6	312	KC2	CMD-C2D-C1D	-16.30	103.40	128.46
42	12	314	KC1	OBD-CAD-CBD	16.21	149.06	125.89
45	7	311	KC2	OBD-CAD-CBD	16.19	149.03	125.89
45	4	308	KC2	CMD-C2D-C3D	16.18	154.95	124.68
45	17	311	KC2	OBD-CAD-CBD	16.12	148.93	125.89
43	8	301	A86	C33-C32-C31	-16.11	93.55	109.21
42	10	315	KC1	CMD-C2D-C1D	-16.03	103.82	128.46
42	8	313	KC1	OBD-CAD-CBD	16.01	148.77	125.89
45	3	311	KC2	OBD-CAD-CBD	16.01	148.77	125.89
45	3	311	KC2	CMD-C2D-C1D	-16.00	103.87	128.46
45	2	310	KC2	CMD-C2D-C1D	-16.00	103.88	128.46
42	0	315	KC1	CMD-C2D-C3D	15.97	154.56	124.68
42	18	313	KC1	CMD-C2D-C3D	15.90	154.43	124.68
43	9	305	A86	O1-C20-C21	-15.86	96.06	115.06
43	15	302	A86	C33-C32-C31	-15.80	93.86	109.21
43	19	305	A86	O1-C20-C21	-15.77	96.16	115.06
42	14	313	KC1	CMD-C2D-C3D	15.75	154.15	124.68
45	18	310	KC2	CMD-C2D-C3D	15.73	154.11	124.68
45	8	310	KC2	CMD-C2D-C3D	15.73	154.10	124.68
42	16	315	KC1	CMD-C2D-C3D	15.72	154.08	124.68
45	18	310	KC2	OBD-CAD-CBD	15.56	148.13	125.89
45	8	310	KC2	OBD-CAD-CBD	15.53	148.08	125.89
42	4	313	KC1	CMD-C2D-C1D	-15.45	104.72	128.46
43	6	301	A86	C33-C32-C31	-15.42	94.23	109.21
45	16	312	KC2	CMD-C2D-C3D	15.40	153.49	124.68
43	16	306	A86	O1-C20-C21	-15.31	96.72	115.06
42	10	315	KC1	CMD-C2D-C3D	15.30	153.31	124.68
45	12	309	KC2	OBD-CAD-CBD	15.30	147.76	125.89
43	15	305	A86	C40-C32-C31	15.29	124.16	110.47
45	6	312	KC2	CMD-C2D-C3D	15.21	153.14	124.68
42	11	314	KC1	OBD-CAD-CBD	15.21	147.62	125.89
45	3	311	KC2	CMD-C2D-C3D	15.20	153.11	124.68
45	7	311	KC2	CMD-C2D-C1D	-15.11	105.24	128.46
45	9	309	KC2	CMD-C2D-C1D	-15.06	105.32	128.46
45	6	312	KC2	OBD-CAD-CBD	15.06	147.41	125.89
43	17	301	A86	C41-C32-C31	15.06	123.95	110.47
43	6	305	A86	O1-C20-C21	-15.05	97.02	115.06
45	19	309	KC2	CMD-C2D-C1D	-14.99	105.42	128.46
45	16	312	KC2	OBD-CAD-CBD	14.94	147.24	125.89
43	14	305	A86	C33-C32-C31	-14.94	94.69	109.21
45	2	310	KC2	CMD-C2D-C3D	14.93	152.62	124.68
43	11	302	A86	C33-C32-C31	-14.86	94.77	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	4	313	KC1	CMD-C2D-C3D	14.86	152.49	124.68
43	1	319	A86	C33-C32-C31	-14.86	94.77	109.21
42	16	301	KC1	OBD-CAD-CBD	14.84	147.09	125.89
45	12	311	KC2	OBD-CAD-CBD	14.79	147.02	125.89
43	3	303	A86	C33-C32-C31	-14.78	94.85	109.21
43	4	305	A86	C40-C32-C31	-14.74	97.28	110.47
45	11	311	KC2	OBD-CAD-CBD	14.71	146.91	125.89
45	11	309	KC2	OBD-CAD-CBD	14.66	146.84	125.89
43	1	303	A86	C33-C32-C31	-14.63	94.99	109.21
43	10	303	A86	O1-C15-C14	-14.56	84.00	113.21
42	P	609	KC1	OBD-CAD-CBD	14.55	146.68	125.89
45	1	311	KC2	OBD-CAD-CBD	14.53	146.66	125.89
42	p	609	KC1	OBD-CAD-CBD	14.51	146.63	125.89
43	0	306	A86	O1-C15-C14	-14.49	84.13	113.21
43	17	316	A86	C41-C32-C31	14.47	123.42	110.47
43	8	303	A86	O1-C15-C14	-14.45	84.21	113.21
43	16	305	A86	O1-C15-C14	-14.43	84.25	113.21
45	7	311	KC2	CMD-C2D-C3D	14.42	151.66	124.68
42	19	314	KC1	OBD-CAD-CBD	14.41	146.48	125.89
43	10	306	A86	O1-C15-C14	-14.41	84.30	113.21
45	0	310	KC2	OBD-CAD-CBD	14.40	146.47	125.89
43	6	304	A86	O1-C15-C14	-14.39	84.34	113.21
43	13	304	A86	O1-C20-C21	-14.38	97.83	115.06
43	0	303	A86	O1-C15-C14	-14.31	84.48	113.21
31	c	503	CLA	C4A-NA-C1A	14.26	113.12	106.71
42	18	313	KC1	OBD-CAD-C3D	-14.24	104.34	127.98
31	C	503	CLA	C4A-NA-C1A	14.23	113.10	106.71
43	17	304	A86	O1-C15-C14	-14.22	84.66	113.21
43	7	303	A86	O1-C15-C14	-14.17	84.78	113.21
42	9	314	KC1	OBD-CAD-CBD	14.16	146.13	125.89
43	11	306	A86	O1-C20-C21	-14.13	98.13	115.06
43	19	306	A86	O1-C15-C14	-14.13	84.86	113.21
43	13	302	A86	C33-C32-C31	-14.11	95.50	109.21
43	9	306	A86	O1-C15-C14	-14.09	84.94	113.21
43	6	307	A86	C33-C32-C31	-14.06	95.55	109.21
45	15	308	KC2	OBD-CAD-CBD	14.01	145.91	125.89
45	9	309	KC2	CMD-C2D-C3D	13.97	150.81	124.68
43	6	307	A86	O1-C15-C14	-13.96	85.19	113.21
43	17	305	A86	C41-C32-C31	13.96	122.97	110.47
43	9	303	A86	O1-C15-C14	-13.95	85.22	113.21
45	5	308	KC2	OBD-CAD-CBD	13.91	145.78	125.89
43	1	302	A86	C33-C32-C31	-13.91	95.69	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	302	A86	O1-C15-C14	-13.91	85.30	113.21
43	19	303	A86	O1-C15-C14	-13.90	85.31	113.21
45	8	308	KC2	OBD-CAD-CBD	13.90	145.75	125.89
43	2	303	A86	O1-C15-C14	-13.87	85.38	113.21
43	12	303	A86	O1-C15-C14	-13.85	85.41	113.21
45	19	309	KC2	CMD-C2D-C3D	13.84	150.58	124.68
43	11	320	A86	O1-C15-C14	-13.84	85.43	113.21
45	1	309	KC2	OBD-CAD-CBD	13.83	145.65	125.89
42	7	314	KC1	OBD-CAD-CBD	13.73	145.51	125.89
43	19	302	A86	C33-C32-C31	-13.72	95.88	109.21
45	3	309	KC2	OBD-CAD-CBD	13.71	145.48	125.89
43	1	302	A86	C40-C32-C31	13.71	122.74	110.47
43	11	303	A86	C33-C32-C31	-13.69	95.90	109.21
45	2	310	KC2	OBD-CAD-C3D	-13.68	105.26	127.98
42	5	313	KC1	CMD-C2D-C3D	-13.67	99.09	124.68
45	13	309	KC2	OBD-CAD-CBD	13.63	145.37	125.89
42	6	315	KC1	OBD-CAD-C3D	-13.55	105.48	127.98
43	p	611	A86	C23-C16-C22	-13.54	87.39	107.37
43	P	611	A86	C23-C16-C22	-13.53	87.41	107.37
43	3	305	A86	O1-C20-C21	-13.50	98.88	115.06
43	17	301	A86	O1-C15-C14	-13.46	86.20	113.21
43	4	306	A86	C41-C32-C31	13.44	122.50	110.47
43	12	305	A86	O1-C15-C14	-13.43	86.26	113.21
45	18	308	KC2	OBD-CAD-CBD	13.41	145.05	125.89
42	16	315	KC1	OBD-CAD-C3D	-13.40	105.73	127.98
45	4	308	KC2	OBD-CAD-CBD	13.35	144.97	125.89
43	1	306	A86	O1-C15-C14	-13.31	86.50	113.21
45	14	310	KC2	OBD-CAD-C3D	-13.19	106.09	127.98
43	5	301	A86	C41-C32-C31	-13.18	98.68	110.47
45	10	310	KC2	OBD-CAD-C3D	-13.17	106.11	127.98
43	4	304	A86	O1-C15-C14	-13.15	86.81	113.21
43	14	303	A86	O1-C15-C14	-13.11	86.89	113.21
43	13	306	A86	C33-C32-C31	-13.08	96.50	109.21
43	1	320	A86	O1-C15-C14	-13.07	86.98	113.21
45	4	310	KC2	OBD-CAD-C3D	-13.05	106.31	127.98
31	P	606	CLA	C4A-NA-C1A	13.03	112.56	106.71
43	13	305	A86	O1-C15-C14	-13.03	87.07	113.21
31	p	606	CLA	C4A-NA-C1A	12.99	112.55	106.71
42	16	315	KC1	C1A-C2A-C3A	-12.98	96.81	107.11
45	14	308	KC2	OBD-CAD-CBD	12.97	144.42	125.89
43	5	318	A86	O1-C15-C14	-12.96	87.20	113.21
31	b	605	CLA	C4A-NA-C1A	12.95	112.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	303	A86	O1-C20-C19	-12.94	103.66	113.38
43	11	302	A86	C40-C32-C31	12.93	122.04	110.47
31	B	604	CLA	C4A-NA-C1A	12.91	112.51	106.71
43	6	301	A86	O1-C15-C14	-12.91	87.30	113.21
43	11	319	A86	O1-C20-C19	12.90	123.07	113.38
43	3	305	A86	C23-C16-C22	-12.89	88.36	107.37
43	4	301	A86	O1-C20-C19	-12.88	103.71	113.38
45	8	310	KC2	OBD-CAD-C3D	-12.86	106.63	127.98
43	16	302	A86	C33-C32-C31	-12.84	96.73	109.21
43	18	301	A86	O1-C15-C14	-12.81	87.51	113.21
45	7	311	KC2	OBD-CAD-C3D	-12.80	106.72	127.98
43	12	306	A86	O1-C15-C14	-12.76	87.60	113.21
43	5	302	A86	O1-C15-C14	-12.76	87.61	113.21
43	4	305	A86	O1-C15-C14	-12.75	87.62	113.21
45	3	311	KC2	OBD-CAD-C3D	-12.72	106.86	127.98
45	2	308	KC2	OBD-CAD-CBD	12.71	144.05	125.89
43	15	303	A86	O1-C15-C14	-12.69	87.74	113.21
43	6	303	A86	C23-C16-C22	-12.68	88.66	107.37
43	14	304	A86	O1-C15-C14	-12.65	87.82	113.21
42	0	315	KC1	OBD-CAD-CBD	12.65	143.97	125.89
42	2	313	KC1	OBD-CAD-C3D	-12.64	106.99	127.98
45	17	309	KC2	OBD-CAD-CBD	12.64	143.96	125.89
45	10	310	KC2	CHC-C4B-NB	12.60	136.03	124.45
42	5	313	KC1	C1A-NA-C4A	-12.59	101.05	106.71
45	18	310	KC2	OBD-CAD-C3D	-12.59	107.08	127.98
42	3	314	KC1	OBD-CAD-C3D	-12.59	107.08	127.98
43	13	302	A86	C40-C32-C31	12.58	121.73	110.47
43	5	303	A86	O1-C15-C14	-12.57	87.98	113.21
45	7	309	KC2	OBD-CAD-CBD	12.56	143.84	125.89
45	17	311	KC2	OBD-CAD-C3D	-12.53	107.18	127.98
43	15	301	A86	C41-C32-C31	-12.52	99.26	110.47
45	0	310	KC2	CHC-C4B-NB	12.51	135.95	124.45
45	9	309	KC2	OBD-CAD-CBD	12.50	143.75	125.89
43	17	316	A86	O1-C20-C21	-12.50	100.08	115.06
43	p	613	A86	O1-C15-C14	-12.49	88.14	113.21
43	P	613	A86	O1-C15-C14	-12.49	88.14	113.21
42	11	314	KC1	OBD-CAD-C3D	-12.46	107.28	127.98
45	1	309	KC2	C4C-C3C-C2C	-12.45	97.23	107.11
43	1	303	A86	O1-C20-C21	-12.45	100.14	115.06
45	15	310	KC2	OBD-CAD-CBD	12.44	143.67	125.89
42	5	313	KC1	C1A-C2A-C3A	-12.43	97.24	107.11
43	7	302	A86	C23-C16-C22	-12.41	89.06	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	8	313	KC1	OBD-CAD-C3D	-12.40	107.39	127.98
43	12	302	A86	C40-C32-C31	12.38	121.55	110.47
42	P	609	KC1	OBD-CAD-C3D	-12.35	107.47	127.98
45	11	309	KC2	OBD-CAD-C3D	-12.35	107.48	127.98
43	6	305	A86	C23-C16-C22	-12.34	89.16	107.37
43	11	306	A86	C23-C16-C22	-12.33	89.18	107.37
42	p	609	KC1	OBD-CAD-C3D	-12.32	107.52	127.98
43	1	303	A86	C40-C32-C31	12.25	121.44	110.47
45	6	312	KC2	OBD-CAD-C3D	-12.25	107.64	127.98
31	p	606	CLA	C1D-ND-C4D	-12.24	97.64	106.33
31	P	606	CLA	C1D-ND-C4D	-12.23	97.65	106.33
43	17	305	A86	C21-C20-C19	-12.22	100.53	114.28
43	3	302	A86	O1-C15-C14	-12.20	88.72	113.21
43	5	301	A86	O1-C15-C14	-12.20	88.72	113.21
45	12	309	KC2	OBD-CAD-C3D	-12.20	107.73	127.98
45	15	308	KC2	OBD-CAD-C3D	-12.18	107.75	127.98
43	16	306	A86	C23-C16-C22	-12.18	89.40	107.37
43	4	302	A86	O1-C15-C14	-12.18	88.78	113.21
45	15	308	KC2	C4C-C3C-C2C	-12.17	97.45	107.11
43	14	305	A86	C41-C32-C31	12.17	121.36	110.47
45	16	312	KC2	OBD-CAD-C3D	-12.14	107.83	127.98
31	p	606	CLA	CBA-CAA-C2A	12.13	139.62	114.02
31	P	606	CLA	CBA-CAA-C2A	12.13	139.61	114.02
43	7	306	A86	C33-C32-C31	-12.12	97.43	109.21
43	6	307	A86	C41-C32-C31	12.12	121.32	110.47
45	19	309	KC2	OBD-CAD-CBD	12.11	143.19	125.89
45	3	309	KC2	OBD-CAD-C3D	-12.09	107.90	127.98
43	13	301	A86	O1-C15-C14	-12.08	88.96	113.21
45	5	308	KC2	OBD-CAD-C3D	-12.07	107.94	127.98
43	11	303	A86	C40-C32-C31	12.05	121.26	110.47
45	11	311	KC2	OBD-CAD-C3D	-12.05	107.97	127.98
43	19	305	A86	C23-C16-C22	-12.04	89.62	107.37
45	1	311	KC2	OBD-CAD-C3D	-12.03	108.01	127.98
43	15	302	A86	O1-C15-C14	-12.02	89.09	113.21
45	0	310	KC2	OBD-CAD-C3D	-12.02	108.03	127.98
45	5	310	KC2	OBD-CAD-CBD	12.01	143.05	125.89
43	1	319	A86	O1-C20-C21	-12.00	100.68	115.06
43	0	302	A86	O1-C15-C14	-11.99	89.14	113.21
45	5	308	KC2	C4C-C3C-C2C	-11.99	97.60	107.11
43	10	302	A86	O1-C15-C14	-11.98	89.16	113.21
45	12	311	KC2	OBD-CAD-C3D	-11.98	108.09	127.98
45	4	310	KC2	CMD-C2D-C1D	-11.94	110.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	6	310	KC2	OBD-CAD-CBD	11.93	142.94	125.89
43	15	301	A86	O1-C15-C14	-11.92	89.29	113.21
43	18	301	A86	C33-C32-C31	-11.90	97.64	109.21
43	4	305	A86	C35-C34-C33	-11.90	89.11	109.88
45	7	311	KC2	CHC-C4B-NB	11.88	135.37	124.45
43	13	304	A86	C23-C16-C22	-11.86	89.88	107.37
43	17	303	A86	O1-C20-C19	-11.85	104.48	113.38
45	8	308	KC2	OBD-CAD-C3D	-11.84	108.32	127.98
45	4	310	KC2	CMD-C2D-C3D	11.84	146.83	124.68
42	16	315	KC1	C1A-NA-C4A	-11.83	101.39	106.71
43	8	301	A86	C40-C32-C31	11.82	121.05	110.47
43	9	305	A86	C23-C16-C22	-11.79	89.98	107.37
31	19	313	CLA	C4A-NA-C1A	11.78	112.00	106.71
42	0	315	KC1	C1A-C2A-C3A	-11.78	97.76	107.11
45	8	310	KC2	CHC-C4B-NB	11.75	135.25	124.45
42	4	313	KC1	OBD-CAD-C3D	-11.75	108.48	127.98
43	16	307	A86	C40-C32-C31	11.73	120.97	110.47
42	8	313	KC1	CHC-C4B-NB	11.72	135.23	124.45
43	7	304	A86	C21-C20-C19	-11.72	101.09	114.28
42	12	314	KC1	OBD-CAD-C3D	-11.72	108.52	127.98
42	6	315	KC1	CBD-CHA-C1A	11.72	150.72	128.88
43	4	302	A86	C33-C32-C31	-11.71	97.83	109.21
45	4	308	KC2	OBD-CAD-C3D	-11.70	108.56	127.98
43	6	306	A86	C40-C32-C31	11.70	120.94	110.47
43	7	306	A86	O1-C20-C19	-11.69	104.60	113.38
43	18	303	A86	O1-C20-C19	-11.69	104.60	113.38
43	7	305	A86	C40-C32-C31	11.68	120.93	110.47
45	13	309	KC2	OBD-CAD-C3D	-11.67	108.61	127.98
43	7	301	A86	O1-C15-C14	-11.66	89.81	113.21
45	11	309	KC2	C1A-NA-C4A	-11.66	101.46	106.71
42	19	314	KC1	OBD-CAD-C3D	-11.65	108.64	127.98
43	15	305	A86	O1-C15-C14	-11.64	89.85	113.21
43	17	303	A86	C23-C16-C22	-11.63	90.21	107.37
45	17	309	KC2	OBD-CAD-C3D	-11.62	108.69	127.98
42	16	301	KC1	OBD-CAD-C3D	-11.62	108.69	127.98
45	18	308	KC2	OBD-CAD-C3D	-11.60	108.71	127.98
45	14	310	KC2	CMD-C2D-C3D	11.60	146.39	124.68
45	1	309	KC2	OBD-CAD-C3D	-11.59	108.73	127.98
45	7	309	KC2	OBD-CAD-C3D	-11.59	108.73	127.98
42	9	314	KC1	OBD-CAD-C3D	-11.59	108.74	127.98
45	16	310	KC2	OBD-CAD-CBD	11.59	142.45	125.89
43	14	305	A86	O1-C15-C14	-11.57	89.99	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	305	A86	O1-C15-C14	-11.56	90.02	113.21
43	17	302	A86	O1-C15-C14	-11.54	90.04	113.21
45	18	310	KC2	CHC-C4B-NB	11.54	135.06	124.45
45	14	308	KC2	OBD-CAD-C3D	-11.54	108.82	127.98
43	11	303	A86	O1-C15-C14	-11.53	90.08	113.21
43	17	306	A86	C40-C32-C31	11.50	120.77	110.47
45	14	310	KC2	CMD-C2D-C1D	-11.50	110.79	128.46
43	19	302	A86	O1-C15-C14	-11.50	90.13	113.21
43	1	319	A86	O1-C15-C14	-11.50	90.13	113.21
43	9	302	A86	O1-C15-C14	-11.49	90.15	113.21
42	14	313	KC1	CHC-C4B-NB	11.49	135.01	124.45
45	13	311	KC2	OBD-CAD-CBD	11.47	142.28	125.89
43	11	304	A86	O1-C15-C14	-11.46	90.20	113.21
45	2	308	KC2	OBD-CAD-C3D	-11.45	108.96	127.98
42	4	313	KC1	CHC-C4B-NB	11.44	134.97	124.45
42	6	315	KC1	CHC-C4B-NB	11.41	134.94	124.45
43	6	302	A86	O1-C15-C14	-11.41	90.32	113.21
43	16	303	A86	O1-C15-C14	-11.40	90.34	113.21
31	9	313	CLA	C4A-NA-C1A	11.40	111.83	106.71
43	1	319	A86	C40-C32-C31	11.36	120.64	110.47
45	11	309	KC2	C1A-C2A-C3A	-11.35	98.10	107.11
43	1	303	A86	O1-C15-C14	-11.35	90.44	113.21
42	4	313	KC1	OBD-CAD-CBD	11.35	142.11	125.89
42	0	315	KC1	OBD-CAD-C3D	-11.34	109.16	127.98
45	3	309	KC2	C4C-C3C-C2C	-11.30	98.14	107.11
45	8	308	KC2	C4C-C3C-C2C	-11.30	98.14	107.11
45	19	309	KC2	OBD-CAD-C3D	-11.28	109.25	127.98
45	9	309	KC2	OBD-CAD-C3D	-11.28	109.25	127.98
43	7	304	A86	C23-C16-C22	-11.27	90.74	107.37
45	17	311	KC2	CHC-C4B-NB	11.27	134.81	124.45
43	0	305	A86	O1-C15-C14	-11.23	90.68	113.21
42	16	315	KC1	CHC-C4B-NB	11.23	134.77	124.45
42	10	315	KC1	C1A-NA-C4A	-11.23	101.66	106.71
43	3	304	A86	O1-C15-C14	-11.18	90.78	113.21
42	2	313	KC1	CMD-C2D-C3D	11.17	145.58	124.68
42	14	313	KC1	OBD-CAD-C3D	-11.16	109.45	127.98
42	11	314	KC1	CHC-C4B-NB	11.16	134.71	124.45
43	12	302	A86	O1-C15-C14	-11.16	90.82	113.21
43	3	303	A86	C40-C32-C31	11.14	120.44	110.47
43	11	303	A86	O1-C20-C21	-11.14	101.71	115.06
42	0	315	KC1	CHC-C4B-NB	11.13	134.68	124.45
43	13	303	A86	O1-C15-C14	-11.11	90.91	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	306	A86	O1-C15-C14	11.11	135.50	113.21
43	13	302	A86	O1-C20-C21	-11.08	101.78	115.06
43	12	306	A86	C33-C32-C31	-11.06	98.46	109.21
45	3	311	KC2	CHC-C4B-NB	11.06	134.61	124.45
43	17	316	A86	C33-C32-C31	-11.05	98.47	109.21
43	3	303	A86	O1-C15-C14	-11.03	91.07	113.21
45	15	310	KC2	OBD-CAD-C3D	-11.03	109.66	127.98
43	10	305	A86	O1-C15-C14	-11.03	91.07	113.21
42	3	314	KC1	CHC-C4B-NB	11.03	134.59	124.45
42	10	315	KC1	CHC-C4B-NB	11.03	134.59	124.45
43	3	305	A86	O1-C15-C14	11.02	135.32	113.21
42	19	314	KC1	CAB-C3B-C4B	11.00	151.47	124.90
42	17	314	KC1	OBD-CAD-CBD	10.99	141.59	125.89
43	13	302	A86	O1-C15-C14	-10.98	91.18	113.21
42	9	314	KC1	CAB-C3B-C4B	10.97	151.40	124.90
43	1	305	A86	O1-C20-C19	-10.96	105.15	113.38
43	1	304	A86	O1-C15-C14	-10.95	91.24	113.21
45	13	309	KC2	CHC-C4B-NB	10.93	134.50	124.45
45	6	310	KC2	OBD-CAD-C3D	-10.89	109.90	127.98
45	6	312	KC2	CHC-C4B-NB	10.88	134.45	124.45
45	5	308	KC2	CHC-C4B-NB	10.85	134.43	124.45
42	2	313	KC1	CMD-C2D-C1D	-10.85	111.78	128.46
43	5	304	A86	O1-C20-C19	-10.84	105.24	113.38
43	2	304	A86	C33-C32-C31	10.84	119.74	109.21
45	18	308	KC2	C4C-C3C-C2C	-10.82	98.52	107.11
43	15	304	A86	O1-C20-C19	-10.82	105.25	113.38
43	17	306	A86	O1-C15-C14	-10.80	91.53	113.21
43	16	307	A86	O1-C15-C14	-10.80	91.54	113.21
45	5	310	KC2	OBD-CAD-C3D	-10.80	110.05	127.98
42	1	314	KC1	CHC-C4B-NB	10.80	134.38	124.45
43	6	305	A86	O1-C15-C14	10.80	134.88	113.21
43	6	306	A86	O1-C15-C14	-10.79	91.56	113.21
45	5	310	KC2	CHC-C4B-NB	10.78	134.36	124.45
43	2	305	A86	O1-C15-C14	-10.77	91.60	113.21
43	3	301	A86	C41-C32-C31	10.77	120.11	110.47
43	10	318	A86	O1-C15-C14	-10.76	91.63	113.21
42	10	315	KC1	OBD-CAD-C3D	-10.75	110.13	127.98
43	7	305	A86	O1-C15-C14	-10.73	91.67	113.21
43	3	305	A86	C21-C20-C19	-10.72	102.22	114.28
45	16	312	KC2	CHC-C4B-NB	10.71	134.29	124.45
43	8	305	A86	O1-C15-C14	-10.71	91.72	113.21
42	13	314	KC1	C1A-C2A-C3A	-10.71	98.61	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	18	310	KC2	C1A-C2A-C3A	-10.67	98.65	107.11
42	17	314	KC1	CHC-C4B-NB	10.66	134.25	124.45
31	3	316	CLA	C4A-NA-C1A	10.63	111.48	106.71
45	16	310	KC2	CHC-C4B-NB	10.61	134.20	124.45
45	9	309	KC2	CHC-C4B-NB	10.60	134.19	124.45
42	16	301	KC1	C1A-C2A-C3A	-10.60	98.70	107.11
45	15	308	KC2	C1A-C2A-C3A	-10.59	98.70	107.11
45	16	310	KC2	OBD-CAD-C3D	-10.58	110.41	127.98
42	8	313	KC1	CHD-C4C-C3C	-10.57	105.49	125.33
42	12	314	KC1	CHD-C4C-C3C	-10.57	105.49	125.33
42	18	313	KC1	CHC-C4B-NB	10.53	134.13	124.45
43	5	304	A86	C40-C32-C31	10.53	119.89	110.47
42	7	314	KC1	CHC-C4B-NB	10.51	134.11	124.45
45	8	308	KC2	CHC-C4B-NB	10.51	134.11	124.45
45	18	308	KC2	CHC-C4B-NB	10.50	134.10	124.45
42	10	315	KC1	CHD-C4C-C3C	-10.49	105.63	125.33
42	13	314	KC1	CHD-C4C-C3C	-10.49	105.64	125.33
43	5	305	A86	C40-C32-C31	10.48	119.85	110.47
42	0	315	KC1	CAB-C3B-C4B	10.48	150.20	124.90
43	5	318	A86	O1-C20-C19	-10.48	105.51	113.38
45	19	309	KC2	CHC-C4B-NB	10.47	134.08	124.45
42	1	314	KC1	CMD-C2D-C1D	10.47	144.56	128.46
45	5	310	KC2	CAB-C3B-C4B	10.47	150.18	124.90
45	15	310	KC2	CHC-C4B-NB	10.46	134.06	124.45
42	17	314	KC1	CHD-C4C-C3C	-10.46	105.70	125.33
43	3	306	A86	O1-C15-C14	-10.45	92.23	113.21
45	15	310	KC2	CAB-C3B-C4B	10.44	150.11	124.90
42	5	313	KC1	CHC-C4B-NB	10.43	134.03	124.45
42	16	301	KC1	CHC-C4B-NB	10.41	134.02	124.45
42	8	313	KC1	CAB-C3B-C4B	10.39	149.99	124.90
43	8	302	A86	O1-C15-C14	-10.39	92.36	113.21
43	11	306	A86	O1-C15-C14	10.39	134.06	113.21
45	14	308	KC2	CHC-C4B-NB	10.37	133.99	124.45
43	4	306	A86	C33-C32-C31	-10.37	99.13	109.21
43	13	304	A86	O1-C15-C14	10.37	134.02	113.21
42	2	313	KC1	CHD-C4C-C3C	-10.36	105.89	125.33
45	8	310	KC2	C1A-C2A-C3A	-10.35	98.90	107.11
45	13	311	KC2	CAB-C3B-C4B	10.33	149.85	124.90
42	3	314	KC1	CHD-C4C-C3C	-10.33	105.94	125.33
43	3	305	A86	C41-C32-C31	10.32	119.71	110.47
43	P	611	A86	C40-C32-C31	-10.31	101.24	110.47
45	7	309	KC2	CHC-C4B-NB	10.31	133.93	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	14	302	A86	O1-C15-C14	-10.30	92.55	113.21
43	p	611	A86	C40-C32-C31	-10.29	101.27	110.47
45	17	309	KC2	CHC-C4B-NB	10.28	133.90	124.45
42	2	313	KC1	CAB-C3B-C4B	10.27	149.70	124.90
42	10	315	KC1	CAB-C3B-C4B	10.26	149.66	124.90
42	13	314	KC1	CHC-C4B-NB	10.25	133.88	124.45
42	18	313	KC1	CAB-C3B-C4B	10.25	149.64	124.90
43	15	305	A86	C35-C34-C33	-10.24	92.00	109.88
45	12	309	KC2	CHC-C4B-NB	10.24	133.86	124.45
42	10	315	KC1	C1A-C2A-C3A	-10.22	99.00	107.11
42	14	313	KC1	CHD-C4C-C3C	-10.21	106.16	125.33
31	0	313	CLA	C4A-NA-C1A	10.21	111.29	106.71
45	13	311	KC2	OBD-CAD-C3D	-10.19	111.06	127.98
43	2	305	A86	C41-C32-C31	10.19	119.59	110.47
43	6	305	A86	C21-C20-C19	-10.18	102.83	114.28
45	3	309	KC2	CHD-C4C-NC	-10.18	108.77	124.20
42	14	313	KC1	C1A-C2A-C3A	-10.18	99.04	107.11
45	12	311	KC2	CHC-C4B-NB	10.14	133.78	124.45
42	2	313	KC1	CHC-C4B-NB	10.13	133.76	124.45
43	17	305	A86	C17-C16-C15	10.11	119.48	109.16
42	3	314	KC1	CAB-C3B-C4B	10.11	149.31	124.90
42	19	314	KC1	CHD-C4C-C3C	-10.10	106.36	125.33
45	11	311	KC2	C1A-C2A-C3A	-10.09	99.10	107.11
43	17	316	A86	O1-C15-C14	-10.08	92.97	113.21
45	12	311	KC2	C1A-C2A-C3A	-10.08	99.11	107.11
42	11	314	KC1	CHD-C4C-C3C	-10.07	106.42	125.33
45	19	309	KC2	C1A-NA-C4A	-10.06	102.18	106.71
43	13	304	A86	C21-C20-C19	-10.06	102.97	114.28
42	4	313	KC1	CHD-C4C-C3C	-10.05	106.46	125.33
43	16	306	A86	C21-C20-C19	-10.05	102.97	114.28
43	4	306	A86	O1-C15-C14	-10.05	93.04	113.21
42	0	315	KC1	CHD-C4C-NC	10.05	139.45	124.20
45	12	309	KC2	CHB-C1B-NB	10.05	133.69	124.45
42	9	314	KC1	CHC-C4B-NB	10.04	133.68	124.45
42	P	609	KC1	CHC-C4B-NB	10.03	133.67	124.45
43	1	302	A86	O1-C20-C19	-10.03	105.85	113.38
43	2	301	A86	O1-C15-C14	10.03	133.33	113.21
43	19	305	A86	C21-C20-C19	-10.01	103.02	114.28
45	4	308	KC2	CHC-C4B-NB	10.00	133.64	124.45
45	15	308	KC2	CHB-C1B-NB	10.00	133.64	124.45
42	p	609	KC1	CHC-C4B-NB	9.99	133.64	124.45
45	15	308	KC2	CHC-C4B-NB	9.97	133.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	9	305	A86	C21-C20-C19	-9.96	103.07	114.28
42	6	315	KC1	C1A-C2A-C3A	-9.94	99.22	107.11
42	10	315	KC1	CHD-C4C-NC	9.94	139.28	124.20
42	17	314	KC1	OBD-CAD-C3D	-9.93	111.50	127.98
45	1	311	KC2	CHD-C4C-NC	9.92	139.26	124.20
42	9	314	KC1	CHD-C4C-C3C	-9.92	106.70	125.33
43	11	302	A86	O4-C38-C39	9.92	129.33	111.09
45	2	310	KC2	CHC-C4B-NB	9.92	133.57	124.45
43	1	302	A86	O1-C20-C21	-9.92	103.17	115.06
45	6	310	KC2	CHC-C4B-NB	9.91	133.56	124.45
45	12	311	KC2	CAB-C3B-C4B	9.89	148.79	124.90
42	19	314	KC1	CHC-C4B-NB	9.88	133.54	124.45
45	17	311	KC2	C1A-C2A-C3A	-9.87	99.28	107.11
42	13	314	KC1	CMD-C2D-C1D	9.87	143.63	128.46
43	15	305	A86	O1-C20-C19	9.86	120.79	113.38
45	12	309	KC2	CMD-C2D-C1D	-9.86	113.31	128.46
45	12	309	KC2	CMD-C2D-C3D	9.86	143.12	124.68
45	2	308	KC2	CHD-C4C-NC	-9.85	109.25	124.20
42	11	314	KC1	CHD-C4C-NC	9.84	139.14	124.20
45	11	309	KC2	CHC-C4B-NB	9.84	133.49	124.45
31	14	306	CLA	CMB-C2B-C1B	-9.81	113.39	128.46
45	1	311	KC2	CHC-C4B-NB	9.81	133.47	124.45
45	15	310	KC2	C1A-C2A-C3A	-9.80	99.33	107.11
43	3	303	A86	O1-C20-C21	-9.80	103.32	115.06
45	11	311	KC2	CHC-C4B-NB	9.79	133.45	124.45
45	5	308	KC2	CHB-C1B-NB	9.78	133.44	124.45
42	14	313	KC1	CAB-C3B-C4B	9.78	148.51	124.90
42	0	315	KC1	C1A-NA-C4A	-9.77	102.31	106.71
45	6	310	KC2	CHB-C1B-NB	9.75	133.42	124.45
43	11	305	A86	O1-C20-C19	-9.75	106.06	113.38
42	5	313	KC1	CAB-C3B-C4B	9.75	148.44	124.90
42	16	315	KC1	CAB-C3B-C4B	9.74	148.42	124.90
42	4	313	KC1	CAB-C3B-C4B	9.73	148.41	124.90
42	12	314	KC1	CHC-C4B-NB	9.65	133.32	124.45
43	17	316	A86	O1-C20-C19	9.64	120.62	113.38
43	9	305	A86	O1-C15-C14	9.64	132.55	113.21
42	6	315	KC1	CAB-C3B-C4B	9.64	148.18	124.90
43	19	305	A86	O1-C15-C14	9.63	132.54	113.21
42	6	315	KC1	C3D-CAD-CBD	-9.63	94.92	107.61
42	18	313	KC1	CHD-C4C-C3C	-9.63	107.26	125.33
42	0	315	KC1	CHD-C4C-C3C	-9.62	107.27	125.33
42	p	609	KC1	CHD-C4C-C3C	-9.62	107.27	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	0	303	A86	O1-C20-C21	-9.61	103.54	115.06
42	P	609	KC1	CHD-C4C-C3C	-9.61	107.29	125.33
43	4	306	A86	O4-C34-C35	-9.60	83.67	107.59
45	3	309	KC2	CHC-C4B-NB	9.60	133.28	124.45
43	4	301	A86	C23-C16-C22	-9.60	93.21	107.37
43	8	302	A86	O1-C20-C21	-9.59	103.57	115.06
45	16	310	KC2	CHB-C1B-NB	9.56	133.24	124.45
42	5	313	KC1	CHD-C4C-C3C	-9.56	107.39	125.33
43	4	302	A86	O4-C34-C33	9.56	131.40	107.59
31	B	606	CLA	C4A-NA-C1A	9.54	110.99	106.71
31	b	607	CLA	C4A-NA-C1A	9.53	110.99	106.71
45	1	311	KC2	C1A-C2A-C3A	-9.52	99.56	107.11
45	12	311	KC2	C1A-NA-C4A	-9.51	102.43	106.71
45	17	311	KC2	C1A-NA-C4A	-9.51	102.43	106.71
43	2	301	A86	C34-O4-C38	9.50	135.61	117.90
45	1	309	KC2	CHC-C4B-NB	9.48	133.16	124.45
45	18	308	KC2	CHB-C1B-NB	9.47	133.16	124.45
42	2	313	KC1	CHD-C4C-NC	9.47	138.57	124.20
45	19	309	KC2	C1A-C2A-C3A	-9.46	99.60	107.11
43	7	304	A86	O1-C15-C14	9.46	132.19	113.21
42	7	314	KC1	CHD-C4C-C3C	-9.44	107.61	125.33
31	1	321	CLA	CMB-C2B-C1B	-9.44	113.95	128.46
45	0	310	KC2	CHB-C1B-NB	9.42	133.11	124.45
45	2	308	KC2	CHC-C4B-NB	9.40	133.10	124.45
43	3	306	A86	C17-C16-C15	9.40	118.76	109.16
43	12	306	A86	C41-C32-C31	9.40	118.88	110.47
43	7	304	A86	C17-C16-C15	9.39	118.74	109.16
42	17	314	KC1	CHD-C4C-NC	9.38	138.44	124.20
45	5	310	KC2	CHB-C1B-NB	9.38	133.07	124.45
42	4	313	KC1	CHB-C1B-NB	9.37	133.07	124.45
45	16	310	KC2	C4C-C3C-C2C	-9.36	99.68	107.11
43	10	303	A86	O1-C20-C21	-9.36	103.84	115.06
45	18	310	KC2	C1A-NA-C4A	-9.35	102.50	106.71
42	16	301	KC1	CAB-C3B-C4B	9.35	147.47	124.90
45	10	310	KC2	CHB-C1B-NB	9.35	133.04	124.45
45	11	309	KC2	CHB-C1B-NB	9.32	133.02	124.45
42	17	314	KC1	CAB-C3B-C4B	9.32	147.40	124.90
45	1	309	KC2	CHB-C1B-NB	9.32	133.02	124.45
45	17	309	KC2	C4C-C3C-C2C	-9.32	99.72	107.11
43	12	302	A86	O1-C20-C21	-9.31	103.91	115.06
43	17	305	A86	C23-C16-C22	-9.30	93.66	107.37
45	7	309	KC2	C4C-C3C-C2C	-9.30	99.73	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	301	A86	O1-C20-C19	9.29	120.36	113.38
43	p	613	A86	O1-C20-C21	-9.28	103.94	115.06
43	1	302	A86	C21-C20-C19	-9.27	103.85	114.28
45	19	309	KC2	CHB-C1B-NB	9.27	132.98	124.45
42	6	315	KC1	C4D-C3D-CAD	9.27	122.80	107.81
42	11	314	KC1	CMD-C2D-C3D	9.27	142.02	124.68
43	P	613	A86	O1-C20-C21	-9.26	103.97	115.06
43	4	301	A86	C33-C32-C31	-9.25	100.22	109.21
45	0	310	KC2	CHD-C4C-NC	9.22	138.19	124.20
45	2	308	KC2	CHB-C1B-NB	9.22	132.93	124.45
43	2	301	A86	O4-C38-C39	9.22	128.05	111.09
43	11	306	A86	C21-C20-C19	-9.21	103.92	114.28
31	14	315	CLA	C4A-NA-C1A	9.20	110.84	106.71
42	18	313	KC1	CBD-CHA-C1A	9.20	146.03	128.88
42	14	313	KC1	OBD-CAD-CBD	9.20	139.03	125.89
44	P	612	DD6	O1-C20-C19	9.18	120.28	113.38
43	8	301	A86	O1-C15-C14	-9.17	94.81	113.21
43	6	304	A86	O1-C20-C21	-9.17	104.07	115.06
45	8	308	KC2	CHB-C1B-NB	9.16	132.87	124.45
42	1	314	KC1	CHD-C4C-C3C	-9.16	108.14	125.33
45	9	309	KC2	CHB-C1B-NB	9.15	132.87	124.45
42	11	314	KC1	CMD-C2D-C1D	-9.14	114.41	128.46
45	2	308	KC2	C4C-C3C-C2C	-9.14	99.86	107.11
42	16	315	KC1	CHD-C4C-C3C	-9.13	108.19	125.33
45	13	311	KC2	CHD-C4C-NC	-9.13	110.35	124.20
42	13	314	KC1	CAB-C3B-C4B	9.13	146.94	124.90
42	11	314	KC1	C1A-C2A-C3A	-9.12	99.87	107.11
42	16	301	KC1	CHD-C4C-C3C	-9.12	108.22	125.33
43	17	316	A86	O4-C38-C39	9.10	127.84	111.09
45	11	309	KC2	CHD-C4C-NC	9.10	138.01	124.20
31	C	509	CLA	C4A-NA-C1A	9.10	110.80	106.71
43	16	305	A86	O1-C20-C21	-9.09	104.16	115.06
31	c	509	CLA	C4A-NA-C1A	9.08	110.79	106.71
44	p	612	DD6	C4-C5-C6	-9.08	114.35	127.31
31	2	315	CLA	C4A-NA-C1A	9.06	110.78	106.71
43	p	613	A86	C33-C32-C31	-9.06	100.40	109.21
42	18	313	KC1	CHB-C1B-NB	9.06	132.78	124.45
43	P	613	A86	C33-C32-C31	-9.06	100.41	109.21
45	9	309	KC2	C1A-NA-C4A	-9.04	102.64	106.71
45	4	308	KC2	CHB-C1B-NB	9.04	132.76	124.45
45	5	308	KC2	C1A-C2A-C3A	-9.03	99.95	107.11
43	7	306	A86	O1-C20-C21	-9.03	104.24	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	7	314	KC1	CHD-C4C-NC	9.02	137.89	124.20
45	13	309	KC2	CMD-C2D-C3D	9.02	141.55	124.68
45	6	312	KC2	C1A-C2A-C3A	-9.01	99.96	107.11
43	0	302	A86	O1-C20-C19	8.99	120.14	113.38
45	8	310	KC2	C1A-NA-C4A	-8.99	102.67	106.71
31	9	311	CLA	C4A-NA-C1A	8.98	110.74	106.71
43	15	304	A86	O1-C20-C21	-8.98	104.30	115.06
42	7	314	KC1	CAB-C3B-C4B	8.97	146.57	124.90
42	19	314	KC1	CHD-C4C-NC	8.97	137.81	124.20
45	9	309	KC2	C1A-C2A-C3A	-8.97	99.99	107.11
43	11	320	A86	C41-C32-C31	8.96	118.49	110.47
43	9	302	A86	O1-C20-C21	-8.96	104.32	115.06
42	18	313	KC1	CHD-C4C-NC	8.95	137.78	124.20
31	b	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
43	8	305	A86	C41-C32-C31	8.94	118.47	110.47
45	2	310	KC2	C1A-C2A-C3A	-8.93	100.03	107.11
43	18	305	A86	O1-C15-C14	-8.93	95.29	113.21
45	7	311	KC2	CHB-C1B-NB	8.92	132.66	124.45
45	7	309	KC2	CHB-C1B-NB	8.92	132.65	124.45
31	B	611	CLA	C4A-NA-C1A	8.92	110.72	106.71
45	13	309	KC2	CMD-C2D-C1D	-8.91	114.77	128.46
45	3	309	KC2	CHB-C1B-NB	8.91	132.64	124.45
43	2	303	A86	O1-C20-C21	-8.90	104.40	115.06
43	13	302	A86	C34-O4-C38	-8.89	101.33	117.90
45	2	310	KC2	C1A-NA-C4A	-8.88	102.71	106.71
31	B	612	CLA	C4A-NA-C1A	8.88	110.70	106.71
42	3	314	KC1	CHD-C4C-NC	8.88	137.67	124.20
43	7	305	A86	C17-C16-C15	8.87	118.21	109.16
42	14	313	KC1	CHB-C1B-NB	8.85	132.59	124.45
45	14	308	KC2	CHB-C1B-NB	8.85	132.59	124.45
42	7	314	KC1	OBD-CAD-C3D	-8.85	113.30	127.98
45	15	310	KC2	CHB-C1B-NB	8.84	132.58	124.45
43	6	307	A86	C4-C5-C6	-8.84	114.70	127.31
45	17	309	KC2	CHD-C4C-NC	-8.82	110.82	124.20
31	b	613	CLA	C4A-NA-C1A	8.82	110.67	106.71
45	14	310	KC2	CHC-C4B-NB	8.81	132.55	124.45
45	15	308	KC2	C1A-NA-C4A	-8.80	102.75	106.71
43	11	305	A86	C23-C16-C22	-8.80	94.38	107.37
42	3	314	KC1	CBD-CHA-C1A	8.80	145.29	128.88
45	4	310	KC2	CHC-C4B-NB	8.79	132.53	124.45
43	6	306	A86	O4-C38-C39	8.78	127.25	111.09
43	17	303	A86	O1-C20-C21	-8.78	104.54	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	16	312	KC2	C1A-C2A-C3A	-8.77	100.15	107.11
43	2	302	A86	C21-C20-C19	-8.76	104.43	114.28
43	11	320	A86	C33-C32-C31	-8.76	100.70	109.21
42	0	315	KC1	CHB-C1B-NB	8.73	132.47	124.45
42	9	314	KC1	CHD-C4C-NC	8.73	137.44	124.20
42	1	314	KC1	CHD-C4C-NC	8.73	137.44	124.20
43	15	301	A86	C34-O4-C38	8.72	134.15	117.90
43	10	318	A86	C40-C32-C31	8.72	118.28	110.47
43	16	306	A86	C17-C16-C15	8.72	118.06	109.16
42	8	313	KC1	CHB-C1B-NB	8.72	132.47	124.45
42	9	314	KC1	CHB-C1B-NB	8.72	132.46	124.45
45	6	310	KC2	CHD-C4C-NC	-8.70	111.00	124.20
31	10	313	CLA	C4A-NA-C1A	8.70	110.62	106.71
43	11	302	A86	C21-C20-C19	-8.69	104.50	114.28
43	17	306	A86	C17-C16-C15	8.69	118.02	109.16
45	17	309	KC2	CHB-C1B-NB	8.68	132.43	124.45
31	11	307	CLA	CMB-C2B-C1B	-8.67	115.14	128.46
43	6	305	A86	C17-C16-C15	8.66	118.00	109.16
31	c	505	CLA	C4A-NA-C1A	8.66	110.60	106.71
45	15	308	KC2	CMD-C2D-C3D	8.66	140.88	124.68
43	11	306	A86	C17-C16-C15	8.66	118.00	109.16
43	16	307	A86	O4-C38-C39	8.65	127.01	111.09
31	b	606	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	4	315	CLA	C4A-NA-C1A	8.65	110.59	106.71
45	12	309	KC2	CHD-C4C-NC	8.64	137.31	124.20
43	2	304	A86	C41-C32-C31	8.64	118.20	110.47
45	7	309	KC2	CHD-C4C-NC	-8.64	111.09	124.20
45	15	308	KC2	CMD-C2D-C1D	-8.63	115.20	128.46
31	B	605	CLA	C4A-NA-C1A	8.62	110.58	106.71
43	19	302	A86	O1-C20-C21	-8.61	104.73	115.06
43	3	306	A86	O4-C34-C35	8.61	129.04	107.59
42	13	314	KC1	C1A-NA-C4A	-8.60	102.84	106.71
42	13	314	KC1	CMD-C2D-C3D	-8.60	108.58	124.68
43	9	304	A86	O1-C15-C14	-8.59	95.97	113.21
43	10	304	A86	O1-C15-C14	-8.59	95.97	113.21
43	2	301	A86	O1-C20-C19	8.59	119.83	113.38
43	0	304	A86	O1-C15-C14	-8.59	95.97	113.21
43	12	301	A86	O1-C15-C14	-8.58	95.99	113.21
43	15	301	A86	O4-C38-C39	8.58	126.87	111.09
31	b	616	CLA	C4A-NA-C1A	8.57	110.56	106.71
43	7	304	A86	C36-C31-C32	-8.56	111.20	119.70
42	19	314	KC1	CHB-C1B-NB	8.56	132.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	304	A86	C23-C16-C22	-8.56	94.74	107.37
45	1	311	KC2	CHB-C1B-NB	8.56	132.32	124.45
42	14	313	KC1	C1A-NA-C4A	-8.55	102.86	106.71
43	11	319	A86	O4-C38-C39	8.54	126.81	111.09
45	11	311	KC2	CHD-C4C-NC	8.54	137.16	124.20
43	5	301	A86	O4-C38-C39	8.54	126.81	111.09
43	19	304	A86	O1-C15-C14	-8.54	96.07	113.21
42	6	315	KC1	CHD-C4C-C3C	-8.54	109.30	125.33
42	10	315	KC1	CHB-C4A-C3A	-8.54	111.64	124.98
31	C	505	CLA	C4A-NA-C1A	8.53	110.54	106.71
43	5	304	A86	C23-C16-C22	-8.53	94.79	107.37
43	3	303	A86	C17-C16-C15	8.52	117.85	109.16
44	p	612	DD6	C8-C6-C5	8.52	132.01	118.94
31	19	311	CLA	C4A-NA-C1A	8.50	110.53	106.71
45	18	310	KC2	CHD-C4C-NC	8.49	137.09	124.20
43	16	302	A86	C41-C32-C31	8.49	118.07	110.47
31	c	508	CLA	C4A-NA-C1A	8.47	110.51	106.71
43	2	302	A86	O1-C15-C14	-8.45	96.24	113.21
43	5	301	A86	C34-O4-C38	8.45	133.64	117.90
42	7	314	KC1	CBD-CHA-C1A	8.44	144.62	128.88
43	6	303	A86	O4-C38-C39	8.44	126.61	111.09
43	6	306	A86	C17-C16-C15	8.43	117.76	109.16
43	3	305	A86	C17-C16-C15	8.42	117.76	109.16
45	12	311	KC2	CMD-C2D-C3D	8.42	140.43	124.68
43	12	302	A86	C17-C16-C15	8.41	117.75	109.16
43	8	304	A86	C40-C32-C31	8.40	117.99	110.47
45	12	311	KC2	CMD-C2D-C1D	-8.39	115.57	128.46
42	p	609	KC1	CHB-C1B-NB	8.38	132.15	124.45
45	8	310	KC2	CHB-C1B-NB	8.37	132.15	124.45
43	16	307	A86	C17-C16-C15	8.36	117.69	109.16
43	8	302	A86	O4-C38-C39	8.36	126.47	111.09
31	B	615	CLA	C4A-NA-C1A	8.35	110.46	106.71
45	15	310	KC2	C1A-NA-C4A	-8.35	102.95	106.71
42	1	314	KC1	CMD-C2D-C3D	-8.35	109.05	124.68
42	P	609	KC1	CHB-C1B-NB	8.35	132.13	124.45
43	7	305	A86	O4-C34-C35	8.34	128.37	107.59
42	12	314	KC1	CAB-C3B-C4B	8.34	145.03	124.90
43	7	306	A86	C41-C32-C31	8.34	117.93	110.47
43	17	305	A86	O1-C15-C14	8.33	129.93	113.21
43	8	304	A86	C41-C32-C31	8.33	117.93	110.47
43	8	305	A86	C17-C16-C15	8.33	117.66	109.16
45	6	310	KC2	C4C-C3C-C2C	-8.32	100.51	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	13	302	A86	C17-C16-C15	8.31	117.64	109.16
42	4	313	KC1	CHD-C4C-NC	8.30	136.79	124.20
43	1	305	A86	O1-C20-C21	-8.29	105.13	115.06
43	7	302	A86	O1-C20-C21	-8.29	105.13	115.06
42	17	314	KC1	C1A-C2A-C3A	-8.28	100.54	107.11
31	C	508	CLA	C4A-NA-C1A	8.28	110.43	106.71
43	10	301	A86	O1-C15-C14	-8.27	96.61	113.21
43	1	320	A86	O4-C38-C39	8.27	126.30	111.09
43	0	301	A86	O1-C15-C14	-8.26	96.64	113.21
45	11	311	KC2	CHB-C1B-NB	8.26	132.04	124.45
43	17	306	A86	O4-C34-C35	8.26	128.16	107.59
45	4	310	KC2	CHD-C4C-NC	8.25	136.72	124.20
45	13	311	KC2	CHB-C1B-NB	8.24	132.02	124.45
43	13	306	A86	C17-C16-C15	-8.23	100.77	109.16
42	16	301	KC1	CMD-C2D-C3D	8.23	140.08	124.68
43	8	303	A86	C41-C32-C31	8.22	117.83	110.47
45	12	311	KC2	CHB-C1B-NB	8.21	132.00	124.45
43	19	305	A86	C17-C16-C15	8.21	117.54	109.16
31	2	315	CLA	CAC-C3C-C2C	8.21	141.57	127.53
43	9	305	A86	C17-C16-C15	8.20	117.53	109.16
43	17	302	A86	C35-C34-C33	-8.20	95.57	109.88
43	11	305	A86	O1-C15-C14	-8.19	96.77	113.21
42	6	315	KC1	CHB-C1B-NB	8.19	131.98	124.45
45	1	309	KC2	CBD-CHA-C1A	8.18	144.12	128.88
43	1	319	A86	C17-C16-C15	8.17	117.49	109.16
42	13	314	KC1	CHD-C4C-NC	8.16	136.58	124.20
43	1	305	A86	C23-C16-C22	-8.15	95.34	107.37
43	2	305	A86	O4-C34-C35	8.15	127.89	107.59
45	13	309	KC2	CHB-C1B-NB	8.14	131.94	124.45
43	P	611	A86	C21-C20-C19	-8.12	105.14	114.28
45	18	310	KC2	CHB-C1B-NB	8.12	131.91	124.45
43	p	611	A86	C21-C20-C19	-8.11	105.16	114.28
43	9	301	A86	O1-C15-C14	-8.11	96.94	113.21
43	10	302	A86	C17-C16-C15	8.10	117.43	109.16
42	8	313	KC1	CHD-C4C-NC	8.10	136.50	124.20
43	10	318	A86	O4-C38-C39	8.10	125.99	111.09
42	P	609	KC1	C1A-C2A-C3A	-8.10	100.69	107.11
43	8	305	A86	O4-C38-C39	8.09	125.98	111.09
43	5	304	A86	O1-C15-C14	-8.07	97.01	113.21
45	11	311	KC2	C4C-C3C-C2C	-8.07	100.71	107.11
31	14	309	CLA	C4A-NA-C1A	8.07	110.33	106.71
43	11	319	A86	O1-C15-C14	8.06	129.39	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	p	612	DD6	C10-C9-C8	-8.05	98.09	123.22
43	19	301	A86	O1-C15-C14	-8.05	97.06	113.21
31	C	510	CLA	C4A-NA-C1A	8.05	110.32	106.71
43	3	303	A86	O4-C38-C39	8.04	125.89	111.09
43	3	301	A86	O1-C15-C14	8.03	129.32	113.21
43	18	304	A86	C41-C32-C31	8.03	117.66	110.47
42	p	609	KC1	C1A-C2A-C3A	-8.03	100.74	107.11
43	2	302	A86	C35-C34-C33	-8.02	95.88	109.88
43	15	304	A86	C41-C32-C31	8.02	117.65	110.47
43	3	303	A86	C34-O4-C38	-8.01	102.97	117.90
31	c	506	CLA	C4A-NA-C1A	7.99	110.30	106.71
43	10	318	A86	C17-C16-C15	7.99	117.32	109.16
43	3	301	A86	C33-C32-C31	-7.99	101.44	109.21
45	8	310	KC2	CHD-C4C-NC	7.99	136.33	124.20
42	5	313	KC1	CHB-C1B-NB	7.98	131.79	124.45
31	p	608	CLA	C4A-NA-C1A	7.98	110.29	106.71
43	2	305	A86	C17-C16-C15	7.97	117.30	109.16
31	4	309	CLA	C4A-NA-C1A	7.97	110.29	106.71
31	C	506	CLA	C4A-NA-C1A	7.97	110.29	106.71
31	4	312	CLA	CMB-C2B-C1B	-7.97	116.22	128.46
45	13	311	KC2	CHC-C4B-NB	7.97	131.78	124.45
42	16	315	KC1	CHD-C4C-NC	7.96	136.29	124.20
43	5	303	A86	C21-C20-C19	-7.96	105.32	114.28
45	2	310	KC2	C2C-C1C-NC	7.96	119.26	110.57
45	15	310	KC2	C4C-C3C-C2C	-7.94	100.81	107.11
31	10	312	CLA	C4A-NA-C1A	7.92	110.27	106.71
43	17	304	A86	O1-C20-C21	-7.91	105.58	115.06
45	17	311	KC2	CHD-C4C-NC	7.91	136.21	124.20
45	5	310	KC2	C1A-C2A-C3A	-7.91	100.84	107.11
31	c	510	CLA	C4A-NA-C1A	7.89	110.25	106.71
31	1	310	CLA	C4A-NA-C1A	7.89	110.25	106.71
44	p	612	DD6	C21-C20-C19	7.88	123.15	114.28
43	7	304	A86	C34-O4-C38	-7.86	103.25	117.90
43	13	306	A86	C41-C32-C31	7.85	117.50	110.47
42	8	313	KC1	C3C-C4C-NC	7.84	117.26	109.88
44	p	612	DD6	C13-C11-C10	7.83	130.95	118.94
42	18	313	KC1	C1A-C2A-C3A	-7.83	100.90	107.11
45	14	310	KC2	CHD-C4C-NC	7.82	136.06	124.20
45	10	310	KC2	CHD-C4C-NC	7.81	136.06	124.20
43	19	304	A86	O4-C38-C39	7.81	125.45	111.09
43	12	301	A86	O4-C38-C39	7.81	125.45	111.09
43	7	303	A86	O1-C20-C21	-7.80	105.71	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	3	311	KC2	C1A-C2A-C3A	-7.79	100.93	107.11
43	8	305	A86	C40-C32-C31	7.79	117.44	110.47
43	13	304	A86	C17-C16-C15	7.79	117.11	109.16
31	P	608	CLA	C4A-NA-C1A	7.79	110.21	106.71
43	12	301	A86	C35-C34-C33	-7.78	96.29	109.88
31	0	312	CLA	C4A-NA-C1A	7.78	110.20	106.71
43	p	611	A86	C17-C16-C15	7.77	117.09	109.16
45	5	308	KC2	CMD-C2D-C3D	7.77	139.21	124.68
43	P	611	A86	C17-C16-C15	7.76	117.08	109.16
43	1	305	A86	O1-C15-C14	-7.76	97.65	113.21
43	12	301	A86	C21-C20-C19	-7.75	105.56	114.28
43	5	302	A86	C21-C20-C19	7.75	122.99	114.28
43	10	305	A86	C17-C16-C15	7.73	117.05	109.16
31	14	306	CLA	CMB-C2B-C3B	7.72	139.12	124.68
31	14	312	CLA	CMB-C2B-C1B	-7.72	116.60	128.46
43	19	301	A86	O4-C38-C39	7.71	125.27	111.09
31	C	514	CLA	C4A-NA-C1A	7.71	110.17	106.71
31	D	401	CLA	C4A-NA-C1A	7.70	110.17	106.71
42	16	301	KC1	CHB-C1B-NB	7.70	131.53	124.45
43	2	302	A86	O4-C38-C39	7.70	125.25	111.09
42	11	314	KC1	CAB-C3B-C4B	7.70	143.48	124.90
31	2	315	CLA	CAC-C3C-C4C	-7.68	114.84	124.81
43	8	301	A86	C23-C16-C22	-7.68	96.04	107.37
43	11	303	A86	C17-C16-C15	7.68	117.00	109.16
45	8	310	KC2	C2C-C1C-NC	7.68	118.95	110.57
43	3	301	A86	C3-C2-C1	-7.67	116.36	127.31
42	16	315	KC1	C3D-CAD-CBD	-7.67	97.50	107.61
43	17	302	A86	O4-C38-C39	7.67	125.20	111.09
42	17	314	KC1	C1A-NA-C4A	-7.66	103.26	106.71
31	P	606	CLA	C1B-CHB-C4A	-7.66	114.94	130.12
31	p	606	CLA	C1B-CHB-C4A	-7.66	114.94	130.12
42	16	301	KC1	C1A-NA-C4A	-7.66	103.26	106.71
45	16	310	KC2	CHD-C4C-NC	-7.66	112.58	124.20
31	16	314	CLA	C2D-C1D-ND	-7.66	104.46	110.10
45	12	311	KC2	CHD-C4C-NC	7.66	135.82	124.20
43	1	303	A86	C17-C16-C15	7.66	116.97	109.16
43	0	301	A86	C35-C34-C33	-7.65	96.52	109.88
42	18	313	KC1	C3D-CAD-CBD	-7.65	97.53	107.61
31	6	311	CLA	C4A-NA-C1A	7.65	110.14	106.71
43	11	320	A86	O4-C38-C39	7.64	125.14	111.09
43	8	304	A86	O1-C15-C14	-7.64	97.88	113.21
31	13	316	CLA	C4A-NA-C1A	7.64	110.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	401	CLA	C4A-NA-C1A	7.63	110.14	106.71
42	7	314	KC1	C1A-C2A-C3A	-7.63	101.06	107.11
31	c	514	CLA	C4A-NA-C1A	7.63	110.14	106.71
42	8	313	KC1	C2C-C1C-NC	7.62	118.89	110.57
43	3	306	A86	C41-C32-C40	-7.62	85.15	108.53
42	6	315	KC1	CAC-C3C-C4C	7.62	134.69	124.81
31	2	307	CLA	C4A-NA-C1A	7.61	110.13	106.71
45	9	309	KC2	CHD-C4C-NC	7.61	135.75	124.20
42	6	315	KC1	C2C-C1C-NC	7.61	118.88	110.57
43	16	303	A86	C17-C16-C15	7.60	116.92	109.16
31	8	309	CLA	C4A-NA-C1A	7.60	110.12	106.71
31	16	311	CLA	C4A-NA-C1A	7.59	110.12	106.71
42	8	313	KC1	CBD-CHA-C1A	7.59	143.03	128.88
45	5	308	KC2	CMD-C2D-C1D	-7.59	116.80	128.46
43	6	302	A86	C17-C16-C15	7.58	116.90	109.16
31	18	309	CLA	C4A-NA-C1A	7.58	110.12	106.71
31	B	603	CLA	C4A-NA-C1A	7.57	110.11	106.71
45	3	311	KC2	CHB-C1B-NB	7.57	131.41	124.45
43	P	613	A86	C41-C32-C31	7.57	117.25	110.47
43	8	303	A86	O1-C20-C21	-7.57	105.98	115.06
43	11	302	A86	O1-C15-C14	-7.56	98.04	113.21
43	p	613	A86	C41-C32-C31	7.56	117.24	110.47
43	1	303	A86	O4-C34-C35	7.56	126.41	107.59
45	7	311	KC2	C1A-C2A-C3A	-7.55	101.12	107.11
31	9	310	CLA	C4A-NA-C1A	7.54	110.10	106.71
43	3	301	A86	C25-C26-C27	-7.54	116.55	127.31
42	14	313	KC1	CHD-C4C-NC	7.54	135.64	124.20
31	1	321	CLA	CMB-C2B-C3B	7.54	138.78	124.68
42	13	314	KC1	CHB-C1B-NB	7.54	131.38	124.45
43	0	305	A86	C17-C16-C15	7.53	116.85	109.16
43	1	302	A86	O1-C15-C14	-7.53	98.09	113.21
43	2	305	A86	C40-C32-C31	7.53	117.21	110.47
31	19	310	CLA	C4A-NA-C1A	7.53	110.09	106.71
45	8	308	KC2	CBD-CHA-C1A	7.52	142.90	128.88
43	12	304	A86	O1-C15-C14	-7.51	98.13	113.21
43	12	302	A86	O4-C38-C39	7.51	124.91	111.09
42	1	314	KC1	C1A-C2A-C3A	-7.51	101.15	107.11
42	3	314	KC1	C1A-C2A-C3A	-7.51	101.15	107.11
43	16	303	A86	O4-C38-C39	7.51	124.91	111.09
31	4	311	CLA	C4A-NA-C1A	7.51	110.08	106.71
43	7	304	A86	C41-C32-C31	7.51	117.19	110.47
43	1	306	A86	C20-C19-C18	7.50	127.59	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	17	311	KC2	C2C-C1C-NC	7.50	118.76	110.57
43	11	303	A86	O4-C34-C35	7.50	126.28	107.59
43	9	301	A86	O4-C38-C39	7.49	124.87	111.09
43	12	306	A86	C25-C26-C27	-7.49	116.62	127.31
31	b	604	CLA	C4A-NA-C1A	7.48	110.07	106.71
43	3	302	A86	O4-C38-C39	7.48	124.86	111.09
43	6	302	A86	C35-C34-C33	-7.47	96.85	109.88
43	9	301	A86	C35-C34-C33	-7.46	96.86	109.88
43	7	305	A86	O4-C38-C39	7.46	124.81	111.09
43	10	301	A86	C35-C34-C33	-7.45	96.87	109.88
45	3	309	KC2	CBD-CHA-C1A	7.45	142.76	128.88
31	c	507	CLA	C4A-NA-C1A	7.45	110.05	106.71
31	2	309	CLA	C4A-NA-C1A	7.44	110.05	106.71
31	11	310	CLA	C4A-NA-C1A	7.44	110.05	106.71
45	18	308	KC2	CBD-CHA-C1A	7.44	142.74	128.88
31	1	307	CLA	CMB-C2B-C1B	-7.43	117.05	128.46
43	11	305	A86	O1-C20-C21	-7.43	106.16	115.06
45	17	311	KC2	CHB-C1B-NB	7.43	131.28	124.45
43	13	301	A86	C4-C5-C6	-7.42	116.72	127.31
43	4	306	A86	O4-C34-C33	7.42	126.08	107.59
43	0	301	A86	O4-C38-C39	7.42	124.73	111.09
43	17	306	A86	O4-C38-C39	7.41	124.72	111.09
43	7	301	A86	C35-C34-C33	-7.41	96.95	109.88
42	16	315	KC1	C2C-C1C-NC	7.41	118.66	110.57
31	15	309	CLA	C4A-NA-C1A	7.40	110.03	106.71
45	10	310	KC2	C1A-NA-C4A	-7.40	103.38	106.71
43	19	301	A86	C35-C34-C33	-7.39	96.98	109.88
31	C	507	CLA	C4A-NA-C1A	7.39	110.03	106.71
42	8	313	KC1	CHB-C4A-C3A	-7.39	113.44	124.98
43	2	305	A86	O4-C38-C39	7.38	124.67	111.09
43	13	303	A86	C25-C26-C27	-7.38	116.77	127.31
31	14	311	CLA	C4A-NA-C1A	7.38	110.02	106.71
31	p	606	CLA	CAA-C2A-C1A	-7.38	87.80	111.97
45	11	309	KC2	CHB-C4A-C3A	-7.38	113.45	124.98
42	18	313	KC1	C4D-C3D-CAD	7.38	119.73	107.81
43	7	301	A86	O4-C38-C39	7.37	124.65	111.09
31	P	606	CLA	CAA-C2A-C1A	-7.36	87.84	111.97
45	18	310	KC2	C2C-C1C-NC	7.36	118.61	110.57
45	17	311	KC2	CMD-C2D-C3D	7.36	138.45	124.68
43	10	318	A86	C41-C32-C31	7.36	117.06	110.47
43	0	304	A86	C41-C32-C31	7.36	117.06	110.47
42	19	314	KC1	C1A-C2A-C3A	-7.35	101.28	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	303	A86	O1-C15-C14	-7.35	98.47	113.21
43	6	307	A86	C4-C3-C2	-7.34	108.43	123.47
43	15	301	A86	C4-C5-C6	-7.34	116.84	127.31
45	3	311	KC2	C2C-C1C-NC	7.34	118.58	110.57
43	11	302	A86	C34-O4-C38	7.34	131.57	117.90
45	10	310	KC2	C2C-C1C-NC	7.34	118.58	110.57
31	c	512	CLA	C4A-NA-C1A	7.33	110.00	106.71
45	7	311	KC2	C2C-C1C-NC	7.33	118.58	110.57
43	6	302	A86	O4-C38-C39	7.33	124.58	111.09
43	18	304	A86	O1-C15-C14	-7.33	98.51	113.21
43	13	301	A86	C35-C34-C33	-7.33	97.09	109.88
31	b	602	CLA	C4A-NA-C1A	7.32	110.00	106.71
31	18	314	CLA	C4A-NA-C1A	7.32	110.00	106.71
43	16	303	A86	C35-C34-C33	-7.32	97.11	109.88
42	9	314	KC1	C1A-C2A-C3A	-7.32	101.31	107.11
43	18	301	A86	C20-C19-C18	7.31	127.21	112.75
43	19	306	A86	O1-C20-C21	-7.31	106.30	115.06
43	1	319	A86	O4-C38-C39	7.30	124.52	111.09
31	C	512	CLA	C4A-NA-C1A	7.30	109.99	106.71
45	0	310	KC2	O2D-CGD-CBD	7.30	124.23	111.27
42	16	315	KC1	C4D-C3D-CAD	7.29	119.59	107.81
43	6	305	A86	C35-C34-C33	-7.29	97.16	109.88
43	17	305	A86	O4-C34-C35	7.28	125.72	107.59
45	2	310	KC2	CHB-C1B-NB	7.28	131.14	124.45
31	12	312	CLA	C4A-NA-C1A	7.28	109.98	106.71
43	15	303	A86	C21-C20-C19	-7.27	106.10	114.28
45	5	310	KC2	C4C-C3C-C2C	-7.27	101.34	107.11
45	6	312	KC2	C2C-C1C-NC	7.26	118.50	110.57
43	13	301	A86	O4-C38-C39	7.26	124.45	111.09
45	19	309	KC2	CHD-C4C-NC	7.26	135.22	124.20
31	B	601	CLA	C4A-NA-C1A	7.26	109.97	106.71
45	16	312	KC2	C2C-C1C-NC	7.26	118.49	110.57
31	16	314	CLA	CMB-C2B-C1B	-7.25	117.32	128.46
43	16	307	A86	O4-C34-C35	7.24	125.63	107.59
43	8	305	A86	O4-C34-C35	7.24	125.63	107.59
43	15	304	A86	O1-C15-C14	-7.24	98.68	113.21
42	p	609	KC1	C2C-C1C-NC	7.24	118.47	110.57
43	2	304	A86	O1-C15-C14	-7.24	98.69	113.21
31	16	309	CLA	C4A-NA-C1A	7.23	109.96	106.71
43	8	301	A86	O1-C20-C21	-7.23	106.40	115.06
43	10	301	A86	O4-C38-C39	7.23	124.38	111.09
31	16	308	CLA	C4A-NA-C1A	7.22	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	0	310	KC2	C2C-C1C-NC	7.22	118.46	110.57
31	8	307	CLA	C4A-NA-C1A	7.22	109.95	106.71
31	8	314	CLA	C4A-NA-C1A	7.22	109.95	106.71
45	12	309	KC2	C1A-C2A-C3A	-7.21	101.39	107.11
31	2	312	CLA	CMB-C2B-C1B	-7.21	117.38	128.46
31	B	607	CLA	C4A-NA-C1A	7.21	109.95	106.71
42	19	314	KC1	CAB-C3B-C2B	-7.21	104.85	128.60
31	p	605	CLA	C4A-NA-C1A	7.20	109.94	106.71
31	10	311	CLA	C4A-NA-C1A	7.20	109.94	106.71
43	12	303	A86	O1-C20-C21	-7.19	106.44	115.06
43	0	303	A86	O4-C38-C39	7.19	124.32	111.09
31	b	610	CLA	C4A-NA-C1A	7.19	109.94	106.71
42	P	609	KC1	C2C-C1C-NC	7.19	118.42	110.57
43	10	304	A86	O4-C38-C39	7.19	124.31	111.09
45	0	310	KC2	C1A-NA-C4A	-7.18	103.48	106.71
31	B	609	CLA	C4A-NA-C1A	7.18	109.94	106.71
43	10	303	A86	O4-C38-C39	7.18	124.30	111.09
45	13	309	KC2	C1A-C2A-C3A	-7.17	101.42	107.11
43	0	304	A86	O4-C38-C39	7.17	124.28	111.09
31	12	310	CLA	C4A-NA-C1A	7.16	109.93	106.71
43	14	304	A86	C17-C16-C15	7.16	116.47	109.16
45	19	309	KC2	C2C-C1C-NC	7.16	118.39	110.57
43	16	306	A86	C35-C34-C33	-7.16	97.39	109.88
43	5	302	A86	C17-C16-C15	7.15	116.46	109.16
42	9	314	KC1	CAB-C3B-C2B	-7.15	105.05	128.60
42	16	301	KC1	CMD-C2D-C1D	-7.15	117.48	128.46
31	5	309	CLA	C4A-NA-C1A	7.14	109.92	106.71
31	16	316	CLA	C4A-NA-C1A	7.14	109.92	106.71
45	17	311	KC2	CHB-C4A-C3A	-7.14	113.82	124.98
43	3	302	A86	C35-C34-C33	-7.14	97.42	109.88
31	b	608	CLA	C4A-NA-C1A	7.14	109.91	106.71
31	13	307	CLA	C4A-NA-C1A	7.14	109.91	106.71
43	p	611	A86	O1-C15-C20	-7.13	52.43	59.40
31	r	101	CLA	C4A-NA-C1A	7.13	109.91	106.71
43	7	306	A86	C40-C32-C31	7.13	116.85	110.47
42	2	313	KC1	CHB-C1B-NB	7.13	131.00	124.45
31	z	101	CLA	C4A-NA-C1A	7.12	109.91	106.71
31	6	314	CLA	CMB-C2B-C1B	-7.12	117.52	128.46
43	9	304	A86	O4-C38-C39	7.12	124.19	111.09
43	10	318	A86	O4-C34-C35	7.12	125.32	107.59
42	2	313	KC1	CHB-C4A-C3A	-7.11	113.86	124.98
42	3	314	KC1	C2C-C1C-NC	7.11	118.34	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	309	CLA	C4A-NA-C1A	7.11	109.90	106.71
42	16	315	KC1	CBD-CHA-C1A	7.11	142.14	128.88
31	12	316	CLA	C4A-NA-C1A	7.11	109.90	106.71
31	0	311	CLA	C4A-NA-C1A	7.11	109.90	106.71
31	P	605	CLA	C4A-NA-C1A	7.10	109.90	106.71
43	1	302	A86	C23-C16-C22	-7.08	96.92	107.37
43	1	320	A86	C36-C31-C32	-7.08	112.67	119.70
31	R	101	CLA	C4A-NA-C1A	7.08	109.89	106.71
45	18	310	KC2	CHB-C4A-C3A	-7.08	113.92	124.98
43	P	611	A86	O1-C15-C20	-7.08	52.48	59.40
43	5	301	A86	C4-C5-C6	-7.07	117.22	127.31
31	10	307	CLA	CMB-C2B-C1B	-7.07	117.60	128.46
43	5	301	A86	O4-C34-C33	7.07	125.19	107.59
43	18	303	A86	O1-C15-C14	-7.06	99.04	113.21
42	5	313	KC1	C2C-C1C-NC	7.06	118.28	110.57
45	12	311	KC2	CHB-C4A-C3A	-7.06	113.95	124.98
43	4	301	A86	O1-C20-C21	-7.06	106.60	115.06
42	1	314	KC1	CAB-C3B-C4B	7.05	141.93	124.90
31	Z	101	CLA	C4A-NA-C1A	7.04	109.87	106.71
31	3	312	CLA	C4A-NA-C1A	7.04	109.87	106.71
31	11	307	CLA	CMB-C2B-C3B	7.04	137.85	124.68
45	6	312	KC2	CHB-C1B-NB	7.04	130.92	124.45
45	9	309	KC2	C2C-C1C-NC	7.04	118.25	110.57
43	15	305	A86	C41-C32-C31	-7.03	104.18	110.47
31	c	502	CLA	C4A-NA-C1A	7.02	109.86	106.71
43	3	306	A86	O4-C38-C39	7.00	123.97	111.09
31	6	316	CLA	C4A-NA-C1A	7.00	109.85	106.71
42	18	313	KC1	C2C-C1C-NC	7.00	118.21	110.57
45	12	311	KC2	C2C-C1C-NC	6.99	118.21	110.57
42	16	315	KC1	CAC-C3C-C4C	6.99	133.88	124.81
45	12	311	KC2	C4C-C3C-C2C	-6.98	101.57	107.11
31	b	611	CLA	C4A-NA-C1A	6.98	109.84	106.71
31	8	311	CLA	C4A-NA-C1A	6.98	109.84	106.71
45	18	310	KC2	C4C-C3C-C2C	-6.98	101.58	107.11
43	15	302	A86	C17-C16-C15	6.97	116.28	109.16
43	15	301	A86	O4-C34-C33	6.97	124.95	107.59
42	6	315	KC1	C1A-NA-C4A	-6.97	103.57	106.71
42	10	315	KC1	C2C-C1C-NC	6.97	118.18	110.57
31	19	307	CLA	C4A-NA-C1A	6.96	109.84	106.71
45	16	312	KC2	CHB-C1B-NB	6.96	130.85	124.45
31	B	610	CLA	C4A-NA-C1A	6.96	109.83	106.71
31	0	307	CLA	CMB-C2B-C1B	-6.96	117.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	6	315	KC1	C3C-C4C-NC	6.95	116.42	109.88
42	p	609	KC1	CMD-C2D-C3D	6.95	137.68	124.68
42	P	609	KC1	CMD-C2D-C3D	6.95	137.67	124.68
43	13	305	A86	C17-C16-C15	6.94	116.24	109.16
31	C	502	CLA	C4A-NA-C1A	6.94	109.83	106.71
43	12	306	A86	C3-C2-C1	-6.93	117.42	127.31
42	10	315	KC1	CHB-C1B-NB	6.93	130.82	124.45
43	4	302	A86	C17-C16-C15	6.93	116.23	109.16
31	1	316	CLA	C4A-NA-C1A	6.93	109.82	106.71
45	8	310	KC2	C4C-C3C-C2C	-6.92	101.62	107.11
31	15	311	CLA	CMA-C3A-C2A	-6.92	85.90	113.83
31	2	306	CLA	CED-O2D-CGD	6.92	131.59	115.94
31	7	310	CLA	C4A-NA-C1A	6.92	109.82	106.71
43	17	303	A86	C17-C16-C15	6.92	116.22	109.16
31	C	504	CLA	C4A-NA-C1A	6.92	109.82	106.71
43	19	303	A86	C33-C32-C31	-6.92	102.49	109.21
43	5	318	A86	C23-C16-C22	6.92	117.57	107.37
45	8	310	KC2	CHC-C4B-C3B	-6.92	113.43	125.26
42	3	314	KC1	CHB-C1B-NB	6.91	130.81	124.45
31	3	316	CLA	CAC-C3C-C4C	-6.91	115.84	124.81
31	1	312	CLA	C4A-NA-C1A	6.91	109.81	106.71
42	8	313	KC1	CAB-C3B-C2B	-6.91	105.85	128.60
42	5	313	KC1	CHB-C4A-C3A	-6.91	114.19	124.98
43	13	302	A86	O4-C38-C39	6.90	123.79	111.09
45	10	310	KC2	CHC-C4B-C3B	-6.90	113.45	125.26
42	0	315	KC1	CAB-C3B-C2B	-6.90	105.88	128.60
43	17	305	A86	C25-C26-C27	-6.90	117.47	127.31
42	0	315	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
31	3	313	CLA	CMB-C2B-C1B	-6.90	117.86	128.46
45	7	309	KC2	CBD-CHA-C1A	6.89	141.72	128.88
31	17	310	CLA	C4A-NA-C1A	6.88	109.80	106.71
42	16	315	KC1	CHB-C1B-NB	6.88	130.78	124.45
43	4	305	A86	C17-C16-C15	6.88	116.18	109.16
45	17	309	KC2	CBD-CHA-C1A	6.88	141.70	128.88
45	0	310	KC2	CHC-C4B-C3B	-6.88	113.50	125.26
43	5	305	A86	O4-C34-C35	6.87	124.71	107.59
43	18	302	A86	O1-C15-C14	-6.87	99.42	113.21
31	B	602	CLA	C4A-NA-C1A	6.87	109.79	106.71
45	17	309	KC2	C1A-C2A-C3A	-6.86	101.67	107.11
45	6	310	KC2	CBD-CHA-C1A	6.86	141.67	128.88
43	16	304	A86	O1-C15-C14	6.86	126.98	113.21
43	P	611	A86	O1-C15-C14	6.86	126.98	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	p	612	DD6	C9-C10-C11	6.85	137.09	127.31
31	c	504	CLA	C4A-NA-C1A	6.85	109.79	106.71
31	6	308	CLA	C4A-NA-C1A	6.85	109.79	106.71
45	18	310	KC2	CHC-C4B-C3B	-6.85	113.54	125.26
43	15	303	A86	O4-C38-C39	6.85	123.69	111.09
31	d	405	CLA	C4A-NA-C1A	6.85	109.78	106.71
31	12	307	CLA	CMB-C2B-C1B	-6.85	117.94	128.46
42	8	313	KC1	CHC-C1C-NC	-6.85	113.42	124.20
31	9	307	CLA	C4A-NA-C1A	6.84	109.78	106.71
43	8	301	A86	C25-C26-C27	-6.84	117.55	127.31
43	10	305	A86	C41-C32-C31	6.83	116.59	110.47
45	4	310	KC2	C1A-C2A-C3A	-6.83	101.69	107.11
31	5	311	CLA	CMA-C3A-C2A	-6.83	86.28	113.83
43	13	304	A86	C35-C34-C33	-6.83	97.96	109.88
43	17	301	A86	C25-C26-C27	-6.83	117.57	127.31
43	p	611	A86	O1-C15-C14	6.83	126.91	113.21
42	1	314	KC1	C2C-C1C-NC	6.83	118.02	110.57
31	18	307	CLA	C4A-NA-C1A	6.82	109.77	106.71
43	6	306	A86	O4-C34-C35	6.82	124.58	107.59
43	17	316	A86	C21-C20-C19	-6.82	106.61	114.28
31	3	307	CLA	C4A-NA-C1A	6.81	109.77	106.71
42	2	313	KC1	C2C-C1C-NC	6.81	118.01	110.57
43	0	302	A86	C22-C16-C17	6.81	120.81	108.98
42	18	313	KC1	C1A-NA-C4A	-6.81	103.64	106.71
43	13	301	A86	C25-C26-C27	-6.80	117.60	127.31
43	2	305	A86	C41-C32-C40	-6.80	87.66	108.53
43	13	306	A86	C40-C32-C31	6.80	116.56	110.47
31	3	308	CLA	C4A-NA-C1A	6.80	109.76	106.71
43	9	306	A86	O1-C20-C21	-6.78	106.93	115.06
31	B	608	CLA	C4A-NA-C1A	6.77	109.75	106.71
31	C	513	CLA	C4A-NA-C1A	6.77	109.75	106.71
43	1	320	A86	O1-C20-C19	6.77	118.47	113.38
43	8	302	A86	C41-C32-C31	6.77	116.53	110.47
31	D	405	CLA	C4A-NA-C1A	6.77	109.75	106.71
45	14	310	KC2	C1A-C2A-C3A	-6.77	101.74	107.11
42	17	314	KC1	CHB-C4A-C3A	-6.76	114.42	124.98
31	12	308	CLA	C4A-NA-C1A	6.76	109.74	106.71
45	7	309	KC2	C1A-C2A-C3A	-6.76	101.75	107.11
42	10	315	KC1	CAB-C3B-C2B	-6.75	106.36	128.60
31	9	308	CLA	C4A-NA-C1A	6.75	109.74	106.71
42	12	314	KC1	CMD-C2D-C3D	6.75	137.31	124.68
45	15	310	KC2	CAB-C3B-C2B	-6.75	106.36	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	13	304	A86	C41-C32-C31	6.75	116.51	110.47
31	p	601	CLA	C4A-NA-C1A	6.75	109.74	106.71
45	14	308	KC2	C1A-C2A-C3A	-6.74	101.76	107.11
31	c	513	CLA	C4A-NA-C1A	6.74	109.73	106.71
31	2	311	CLA	C4A-NA-C1A	6.74	109.73	106.71
43	0	305	A86	C41-C32-C31	6.74	116.50	110.47
43	5	304	A86	C41-C32-C31	6.73	116.50	110.47
43	3	301	A86	C4-C5-C6	-6.73	117.70	127.31
45	5	310	KC2	CAB-C3B-C2B	-6.73	106.44	128.60
45	4	308	KC2	C1A-C2A-C3A	-6.72	101.78	107.11
31	9	312	CLA	C4A-NA-C1A	6.72	109.73	106.71
43	18	305	A86	C4-C5-C6	-6.72	117.72	127.31
43	11	305	A86	C35-C34-C33	-6.72	98.15	109.88
42	11	314	KC1	C2C-C1C-NC	6.72	117.91	110.57
31	15	306	CLA	C4A-NA-C1A	6.72	109.73	106.71
42	8	313	KC1	CHC-C4B-C3B	-6.72	113.77	125.26
45	5	308	KC2	CBD-CHA-C1A	6.72	141.40	128.88
31	b	609	CLA	C4A-NA-C1A	6.72	109.73	106.71
42	0	315	KC1	CHC-C4B-C3B	-6.72	113.77	125.26
31	b	603	CLA	C4A-NA-C1A	6.71	109.72	106.71
31	p	604	CLA	C4A-NA-C1A	6.71	109.72	106.71
31	6	308	CLA	CED-O2D-CGD	6.71	131.10	115.94
43	2	304	A86	C36-C31-C32	-6.70	113.04	119.70
42	2	313	KC1	CAB-C3B-C2B	-6.70	106.52	128.60
45	10	310	KC2	CMD-C2D-C3D	6.70	137.22	124.68
43	5	301	A86	C35-C34-C33	-6.70	98.18	109.88
42	18	313	KC1	CAB-C3B-C2B	-6.70	106.54	128.60
31	P	610	CLA	C4A-NA-C1A	6.69	109.71	106.71
45	2	310	KC2	CHB-C4A-C3A	-6.69	114.53	124.98
43	8	301	A86	C17-C16-C15	6.68	115.98	109.16
43	15	304	A86	C33-C32-C31	6.67	115.70	109.21
43	17	316	A86	C34-O4-C38	6.67	130.33	117.90
43	12	306	A86	C4-C5-C6	-6.67	117.79	127.31
43	3	306	A86	C40-C32-C31	6.67	116.44	110.47
45	2	308	KC2	CBD-CHA-C1A	6.67	141.31	128.88
42	10	315	KC1	CHC-C4B-C3B	-6.67	113.85	125.26
45	16	310	KC2	CBD-CHA-C1A	6.67	141.31	128.88
31	c	511	CLA	C4A-NA-C1A	6.67	109.70	106.71
42	P	609	KC1	CHD-C4C-NC	6.67	134.32	124.20
43	13	301	A86	C17-C16-C15	6.67	115.96	109.16
43	6	303	A86	C34-O4-C38	-6.66	105.48	117.90
42	14	313	KC1	O2D-CGD-CBD	6.66	123.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	303	A86	C17-C16-C15	6.66	115.95	109.16
31	P	601	CLA	C4A-NA-C1A	6.65	109.69	106.71
45	3	311	KC2	CHC-C4B-C3B	-6.64	113.89	125.26
31	P	607	CLA	C4A-NA-C1A	6.64	109.69	106.71
43	3	304	A86	C25-C26-C27	-6.64	117.83	127.31
31	1	308	CLA	CMB-C2B-C1B	-6.64	118.26	128.46
31	10	308	CLA	C4A-NA-C1A	6.64	109.69	106.71
45	13	311	KC2	CAB-C3B-C2B	-6.63	106.77	128.60
31	6	313	CLA	C4A-NA-C1A	6.63	109.69	106.71
42	p	609	KC1	CHD-C4C-NC	6.63	134.26	124.20
43	6	302	A86	C25-C26-C27	-6.63	117.85	127.31
31	19	312	CLA	C4A-NA-C1A	6.63	109.69	106.71
31	3	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
45	17	311	KC2	C4C-C3C-C2C	-6.62	101.86	107.11
42	14	313	KC1	CAB-C3B-C2B	-6.62	106.80	128.60
42	17	314	KC1	CHC-C4B-C3B	-6.61	113.95	125.26
31	0	308	CLA	C4A-NA-C1A	6.61	109.68	106.71
42	11	314	KC1	CHB-C1B-NB	6.60	130.52	124.45
31	2	306	CLA	C4A-NA-C1A	6.60	109.67	106.71
31	13	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
31	14	314	CLA	C4A-NA-C1A	6.60	109.67	106.71
43	9	303	A86	O4-C38-C39	6.60	123.23	111.09
42	4	313	KC1	CAB-C3B-C2B	-6.60	106.87	128.60
42	3	314	KC1	CAB-C3B-C2B	-6.59	106.88	128.60
31	p	610	CLA	C4A-NA-C1A	6.59	109.67	106.71
45	1	311	KC2	CHB-C4A-C3A	-6.59	114.68	124.98
43	6	301	A86	C41-C32-C31	6.59	116.37	110.47
45	12	311	KC2	CHC-C4B-C3B	-6.59	113.98	125.26
43	16	303	A86	C23-C16-C17	-6.59	97.54	108.98
31	C	511	CLA	C4A-NA-C1A	6.59	109.67	106.71
31	10	317	CLA	C4A-NA-C1A	6.58	109.67	106.71
43	1	305	A86	C35-C34-C33	-6.58	98.39	109.88
31	12	315	CLA	C4A-NA-C1A	6.58	109.67	106.71
43	5	303	A86	C17-C16-C15	6.58	115.87	109.16
43	10	302	A86	C23-C16-C17	-6.58	97.55	108.98
45	5	310	KC2	CHC-C4B-C3B	-6.57	114.01	125.26
42	17	314	KC1	C2C-C1C-NC	6.57	117.75	110.57
45	7	311	KC2	CHC-C4B-C3B	-6.56	114.04	125.26
31	11	312	CLA	C4A-NA-C1A	6.56	109.66	106.71
31	A	406	CLA	C4A-NA-C1A	6.56	109.65	106.71
45	17	311	KC2	CMD-C2D-C1D	-6.56	118.39	128.46
43	0	302	A86	O1-C20-C21	-6.56	107.20	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	10	310	KC2	CHB-C4A-C3A	-6.55	114.74	124.98
43	7	304	A86	C35-C34-C33	-6.55	98.44	109.88
42	5	313	KC1	CHC-C4B-C3B	-6.55	114.05	125.26
43	17	305	A86	C41-C32-C40	-6.55	88.43	108.53
31	a	406	CLA	C4A-NA-C1A	6.54	109.65	106.71
31	P	604	CLA	C4A-NA-C1A	6.54	109.65	106.71
31	p	607	CLA	C4A-NA-C1A	6.54	109.65	106.71
43	1	305	A86	C41-C32-C31	6.54	116.32	110.47
43	13	302	A86	C36-C31-C32	6.53	126.17	119.70
42	1	314	KC1	CHB-C1B-NB	6.52	130.45	124.45
45	6	312	KC2	CHC-C4B-C3B	-6.52	114.10	125.26
45	11	309	KC2	C4C-C3C-C2C	-6.52	101.94	107.11
45	16	312	KC2	CHC-C4B-C3B	-6.52	114.11	125.26
43	3	301	A86	C23-C16-C17	-6.51	97.67	108.98
43	8	301	A86	O4-C34-C33	6.51	123.81	107.59
42	4	313	KC1	O2D-CGD-CBD	6.51	122.83	111.27
31	D	404	CLA	C4A-NA-C1A	6.51	109.63	106.71
31	19	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
43	2	303	A86	C3-C2-C1	-6.50	118.03	127.31
43	11	305	A86	C41-C32-C31	6.49	116.28	110.47
31	19	315	CLA	C4A-NA-C1A	6.49	109.62	106.71
31	d	404	CLA	C4A-NA-C1A	6.49	109.62	106.71
43	6	307	A86	C25-C26-C27	-6.49	118.05	127.31
42	0	315	KC1	C2C-C1C-NC	6.48	117.65	110.57
42	1	314	KC1	CHC-C4B-C3B	-6.47	114.19	125.26
42	4	313	KC1	CHC-C4B-C3B	-6.47	114.19	125.26
43	17	302	A86	C17-C16-C15	6.47	115.76	109.16
42	14	313	KC1	CHC-C4B-C3B	-6.47	114.19	125.26
43	19	303	A86	O4-C38-C39	6.46	122.98	111.09
42	12	314	KC1	C2C-C1C-NC	6.46	117.63	110.57
31	a	404	CLA	C4A-NA-C1A	6.46	109.61	106.71
31	7	312	CLA	C4A-NA-C1A	6.46	109.61	106.71
43	P	611	A86	C36-C31-C32	-6.46	113.29	119.70
42	16	301	KC1	C2C-C1C-NC	6.46	117.62	110.57
31	z	103	CLA	C4A-NA-C1A	6.45	109.61	106.71
45	15	310	KC2	CHC-C4B-C3B	-6.45	114.22	125.26
43	17	302	A86	C23-C16-C17	-6.45	97.78	108.98
43	6	302	A86	C23-C16-C17	-6.44	97.79	108.98
31	0	316	CLA	C4A-NA-C1A	6.44	109.60	106.71
43	3	303	A86	C36-C31-C32	6.44	126.09	119.70
31	16	313	CLA	C4A-NA-C1A	6.44	109.60	106.71
42	3	314	KC1	CHC-C1C-NC	-6.44	114.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	314	KC1	CHC-C4B-C3B	-6.44	114.24	125.26
45	1	311	KC2	C2C-C1C-NC	6.43	117.59	110.57
43	p	611	A86	C36-C31-C32	-6.43	113.32	119.70
43	1	320	A86	C40-C32-C31	6.42	116.22	110.47
31	1	315	CLA	C4A-NA-C1A	6.42	109.59	106.71
42	2	313	KC1	CHC-C4B-C3B	-6.42	114.27	125.26
43	13	306	A86	C25-C26-C27	-6.42	118.15	127.31
43	4	306	A86	C17-C16-C15	6.42	115.71	109.16
42	14	313	KC1	C2C-C1C-NC	6.41	117.57	110.57
43	4	302	A86	C4-C5-C6	-6.40	118.17	127.31
42	13	314	KC1	CHB-C4A-C3A	-6.40	114.98	124.98
43	0	302	A86	C21-C20-C19	-6.40	107.08	114.28
43	5	318	A86	C4-C5-C6	-6.40	118.18	127.31
43	8	304	A86	C23-C16-C22	-6.40	97.94	107.37
45	11	311	KC2	CHC-C4B-C3B	-6.39	114.33	125.26
43	17	316	A86	C17-C16-C15	6.39	115.68	109.16
31	7	315	CLA	C4A-NA-C1A	6.39	109.58	106.71
31	2	314	CLA	C4A-NA-C1A	6.38	109.58	106.71
43	4	304	A86	O1-C20-C21	-6.38	107.41	115.06
42	13	314	KC1	C2C-C1C-NC	6.38	117.54	110.57
45	0	310	KC2	CHB-C4A-C3A	-6.38	115.02	124.98
45	17	311	KC2	CHC-C4B-C3B	-6.37	114.36	125.26
31	11	308	CLA	CMB-C2B-C1B	-6.37	118.67	128.46
43	11	302	A86	C4-C5-C6	-6.37	118.22	127.31
42	16	315	KC1	CHC-C4B-C3B	-6.37	114.36	125.26
42	11	314	KC1	CHC-C4B-C3B	-6.37	114.37	125.26
45	13	311	KC2	C1A-C2A-C3A	-6.36	102.06	107.11
44	p	612	DD6	C15-C14-C13	6.36	139.43	125.99
43	16	302	A86	O1-C20-C19	-6.36	108.61	113.38
42	12	314	KC1	CHB-C4A-C3A	-6.36	115.05	124.98
42	16	315	KC1	CAB-C3B-C2B	-6.35	107.67	128.60
43	P	611	A86	O4-C34-C33	6.35	123.41	107.59
43	p	611	A86	O4-C34-C33	6.35	123.41	107.59
45	18	308	KC2	C2C-C1C-NC	6.35	117.50	110.57
42	12	314	KC1	CBD-CHA-C1A	6.35	140.71	128.88
31	13	312	CLA	C4A-NA-C1A	6.34	109.56	106.71
43	12	304	A86	C35-C34-C33	-6.34	98.81	109.88
43	11	306	A86	O1-C15-C20	-6.34	53.20	59.40
31	13	310	CLA	C4A-NA-C1A	6.34	109.56	106.71
31	C	509	CLA	CMB-C2B-C1B	-6.34	118.72	128.46
43	1	305	A86	C21-C20-C19	-6.33	107.15	114.28
31	9	315	CLA	C4A-NA-C1A	6.33	109.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	314	KC1	C3C-C4C-NC	6.33	115.84	109.88
45	2	310	KC2	C4C-C3C-C2C	-6.33	102.09	107.11
31	4	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
43	15	301	A86	C17-C16-C15	6.33	115.62	109.16
31	17	312	CLA	C4A-NA-C1A	6.33	109.55	106.71
42	6	315	KC1	CAB-C3B-C2B	-6.32	107.77	128.60
43	4	305	A86	C25-C26-C27	-6.32	118.29	127.31
31	c	509	CLA	CMB-C2B-C1B	-6.32	118.75	128.46
42	6	315	KC1	CHC-C1C-NC	-6.31	114.27	124.20
45	11	311	KC2	C2C-C1C-NC	6.31	117.46	110.57
43	13	301	A86	C3-C2-C1	-6.30	118.32	127.31
31	A	404	CLA	C4A-NA-C1A	6.30	109.54	106.71
45	14	310	KC2	C4B-CHC-C1C	-6.30	112.47	126.06
45	9	309	KC2	CHC-C4B-C3B	-6.30	114.48	125.26
43	1	320	A86	C25-C26-C27	-6.30	118.32	127.31
31	7	313	CLA	CMB-C2B-C1B	-6.30	118.78	128.46
31	p	603	CLA	C4A-NA-C1A	6.30	109.54	106.71
43	8	302	A86	O1-C20-C19	6.30	118.11	113.38
45	4	310	KC2	C4B-CHC-C1C	-6.30	112.48	126.06
43	18	302	A86	C4-C5-C6	-6.29	118.33	127.31
31	P	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
43	13	305	A86	C23-C16-C17	-6.29	98.05	108.98
43	7	306	A86	C17-C16-C15	6.29	115.58	109.16
43	p	611	A86	C41-C32-C31	6.29	116.10	110.47
45	5	310	KC2	C2C-C1C-NC	6.29	117.44	110.57
42	P	609	KC1	CHC-C4B-C3B	-6.28	114.51	125.26
45	8	310	KC2	CHB-C4A-C3A	-6.28	115.16	124.98
31	17	307	CLA	C4A-NA-C1A	6.28	109.53	106.71
43	P	611	A86	C41-C32-C31	6.28	116.09	110.47
42	p	609	KC1	CHC-C4B-C3B	-6.28	114.52	125.26
45	13	309	KC2	CHC-C4B-C3B	-6.27	114.53	125.26
43	4	302	A86	C34-O4-C38	6.27	129.59	117.90
42	5	313	KC1	CAB-C3B-C2B	-6.27	107.94	128.60
45	12	311	KC2	CAB-C3B-C2B	-6.27	107.94	128.60
45	1	311	KC2	CHC-C4B-C3B	-6.27	114.54	125.26
43	7	301	A86	C17-C16-C15	6.27	115.56	109.16
43	6	301	A86	C40-C32-C31	6.27	116.08	110.47
31	1	307	CLA	CMB-C2B-C3B	6.27	136.40	124.68
43	18	304	A86	C40-C32-C31	6.27	116.08	110.47
43	17	301	A86	C3-C2-C1	-6.26	118.37	127.31
31	10	316	CLA	C4A-NA-C1A	6.26	109.52	106.71
45	19	309	KC2	CHC-C4B-C3B	-6.26	114.55	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	4	313	KC1	C2C-C1C-NC	6.26	117.41	110.57
31	5	307	CLA	C4A-NA-C1A	6.26	109.52	106.71
42	14	313	KC1	CAC-C3C-C4C	6.26	132.93	124.81
31	10	314	CLA	C4A-NA-C1A	6.25	109.52	106.71
45	11	311	KC2	CMD-C2D-C3D	6.25	136.38	124.68
31	17	315	CLA	C4A-NA-C1A	6.25	109.51	106.71
43	3	303	A86	C21-C20-C19	-6.25	107.25	114.28
31	7	307	CLA	C4A-NA-C1A	6.23	109.51	106.71
31	b	614	CLA	C4A-NA-C1A	6.23	109.51	106.71
42	9	314	KC1	CHC-C4B-C3B	-6.23	114.61	125.26
42	6	315	KC1	CHC-C4B-C3B	-6.22	114.61	125.26
45	7	311	KC2	C1A-NA-C4A	-6.22	103.91	106.71
43	6	305	A86	O4-C38-C39	6.22	122.53	111.09
45	15	308	KC2	C2C-C1C-NC	6.22	117.36	110.57
45	5	308	KC2	CHC-C4B-C3B	-6.22	114.63	125.26
45	6	312	KC2	C1A-NA-C4A	-6.21	103.91	106.71
43	0	305	A86	C3-C2-C1	-6.21	118.45	127.31
45	15	310	KC2	C2C-C1C-NC	6.21	117.35	110.57
43	11	305	A86	C21-C20-C19	-6.21	107.30	114.28
43	12	306	A86	C17-C16-C15	6.20	115.49	109.16
43	17	316	A86	C25-C26-C27	-6.20	118.46	127.31
42	12	314	KC1	CHC-C4B-C3B	-6.19	114.67	125.26
45	13	309	KC2	C4C-C3C-C2C	-6.18	102.21	107.11
45	7	311	KC2	CHD-C4C-NC	6.18	133.57	124.20
45	3	311	KC2	CHD-C4C-NC	6.18	133.57	124.20
43	7	301	A86	C23-C16-C17	-6.18	98.25	108.98
43	15	305	A86	C23-C16-C22	-6.17	98.26	107.37
42	16	301	KC1	CHB-C4A-C3A	-6.17	115.33	124.98
43	0	305	A86	C25-C26-C27	-6.17	118.50	127.31
31	15	307	CLA	C4A-NA-C1A	6.17	109.48	106.71
43	10	301	A86	C19-C18-C17	-6.17	98.86	110.77
42	7	314	KC1	CHC-C4B-C3B	-6.17	114.71	125.26
42	2	313	KC1	CBD-CHA-C1A	6.16	140.37	128.88
42	13	314	KC1	CAC-C3C-C4C	6.16	132.80	124.81
42	1	314	KC1	CHC-C1C-NC	-6.15	114.51	124.20
43	6	304	A86	C3-C2-C1	-6.14	118.55	127.31
43	15	301	A86	C35-C34-C33	-6.14	99.16	109.88
43	16	304	A86	C23-C16-C17	6.14	119.65	108.98
45	5	308	KC2	C2C-C1C-NC	6.14	117.27	110.57
43	14	301	A86	C3-C4-C5	-6.14	110.90	123.47
43	3	302	A86	C17-C16-C15	6.14	115.42	109.16
42	9	314	KC1	C2C-C1C-NC	6.14	117.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	316	CLA	C4A-NA-C1A	6.13	109.46	106.71
43	8	304	A86	O4-C34-C35	6.13	122.87	107.59
31	B	613	CLA	C4A-NA-C1A	6.13	109.46	106.71
42	13	314	KC1	CAB-C3B-C2B	-6.13	108.41	128.60
45	11	309	KC2	C2C-C1C-NC	6.13	117.26	110.57
31	b	612	CLA	CMB-C2B-C1B	-6.13	119.04	128.46
31	4	312	CLA	CMB-C2B-C3B	6.12	136.13	124.68
42	18	313	KC1	CHB-C4A-C3A	-6.12	115.42	124.98
43	12	302	A86	C36-C31-C32	6.11	125.76	119.70
43	13	306	A86	O1-C15-C14	-6.11	100.96	113.21
42	12	314	KC1	CHB-C4A-NA	6.11	133.82	124.20
43	10	305	A86	C3-C2-C1	-6.11	118.60	127.31
43	16	305	A86	C3-C2-C1	-6.11	118.60	127.31
43	10	304	A86	C34-O4-C38	-6.10	106.52	117.90
31	3	315	CLA	C4A-NA-C1A	6.10	109.45	106.71
31	B	611	CLA	CMB-C2B-C1B	-6.09	119.10	128.46
43	19	302	A86	C40-C32-C31	6.09	115.93	110.47
43	2	302	A86	C19-C18-C17	-6.09	99.01	110.77
43	3	302	A86	C4-C5-C6	-6.09	118.62	127.31
42	12	314	KC1	CHD-C4C-NC	6.08	133.43	124.20
43	15	301	A86	C25-C26-C27	-6.08	118.63	127.31
43	0	304	A86	C34-O4-C38	-6.08	106.56	117.90
43	7	306	A86	C23-C16-C22	-6.08	98.40	107.37
42	16	301	KC1	CAB-C3B-C2B	-6.07	108.59	128.60
45	13	309	KC2	C2C-C1C-NC	6.07	117.20	110.57
31	11	308	CLA	C4A-NA-C1A	6.07	109.44	106.71
42	P	609	KC1	CBD-CHA-C1A	6.07	140.19	128.88
45	11	311	KC2	CHB-C4A-C3A	-6.07	115.50	124.98
31	6	314	CLA	C2D-C1D-ND	-6.07	105.63	110.10
42	16	301	KC1	CHC-C4B-C3B	-6.06	114.89	125.26
43	1	302	A86	C4-C5-C6	-6.06	118.66	127.31
42	19	314	KC1	CHC-C4B-C3B	-6.06	114.89	125.26
42	12	314	KC1	CHB-C1B-NB	6.06	130.02	124.45
45	5	308	KC2	C1A-NA-C4A	-6.06	103.98	106.71
45	4	308	KC2	O2D-CGD-CBD	6.06	122.03	111.27
42	p	609	KC1	CBD-CHA-C1A	6.06	140.17	128.88
42	13	314	KC1	CHC-C1C-NC	-6.05	114.67	124.20
42	17	314	KC1	CAB-C3B-C2B	-6.05	108.67	128.60
43	14	301	A86	O-C13-C11	-6.05	107.78	121.15
31	a	403	CLA	CMB-C2B-C1B	-6.05	119.16	128.46
31	b	615	CLA	C4A-NA-C1A	6.05	109.43	106.71
31	p	602	CLA	C4A-NA-C1A	6.05	109.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	308	CLA	CED-O2D-CGD	6.05	129.61	115.94
31	A	403	CLA	CMB-C2B-C1B	-6.04	119.18	128.46
45	7	311	KC2	CHB-C4A-C3A	-6.04	115.54	124.98
43	1	306	A86	C23-C16-C22	-6.04	98.46	107.37
43	0	302	A86	C23-C16-C22	-6.04	98.46	107.37
42	13	314	KC1	C3C-C4C-NC	6.04	115.56	109.88
31	8	306	CLA	C4A-NA-C1A	6.04	109.42	106.71
31	10	309	CLA	C4A-NA-C1A	6.04	109.42	106.71
43	1	302	A86	O2-C18-C19	-6.04	97.81	109.80
45	6	312	KC2	CHD-C4C-NC	6.03	133.36	124.20
45	11	309	KC2	CMD-C2D-C3D	6.03	135.96	124.68
43	7	302	A86	C25-C26-C27	-6.03	118.71	127.31
31	17	313	CLA	CMB-C2B-C1B	-6.02	119.21	128.46
42	P	609	KC1	CMD-C2D-C1D	-6.02	119.21	128.46
43	5	304	A86	O1-C20-C21	-6.02	107.84	115.06
43	12	304	A86	C23-C16-C22	-6.02	98.50	107.37
45	4	308	KC2	CBD-CHA-C1A	6.02	140.09	128.88
43	5	301	A86	C17-C16-C15	6.01	115.30	109.16
42	7	314	KC1	C2C-C1C-NC	6.01	117.14	110.57
43	19	301	A86	O4-C34-C33	6.01	122.56	107.59
43	4	301	A86	C17-C16-C15	6.01	115.29	109.16
42	16	315	KC1	CHB-C4A-C3A	-6.01	115.59	124.98
43	11	302	A86	C19-C18-C17	-6.00	99.18	110.77
42	4	313	KC1	CAC-C3C-C4C	6.00	132.59	124.81
42	16	315	KC1	CHC-C1C-NC	-6.00	114.76	124.20
42	16	315	KC1	C3C-C4C-NC	6.00	115.52	109.88
43	5	303	A86	C23-C16-C17	-5.99	98.57	108.98
43	8	304	A86	C41-C32-C40	-5.99	90.14	108.53
45	2	310	KC2	CHC-C4B-C3B	-5.99	115.01	125.26
43	10	304	A86	C19-C18-C17	-5.99	99.21	110.77
43	19	303	A86	O1-C20-C21	-5.99	107.88	115.06
42	p	609	KC1	CMD-C2D-C1D	-5.99	119.26	128.46
43	12	303	A86	C3-C2-C1	-5.99	118.77	127.31
44	p	612	DD6	C12-C11-C10	-5.99	114.54	122.92
43	10	306	A86	C3-C2-C1	-5.99	118.77	127.31
42	19	314	KC1	C2C-C1C-NC	5.98	117.11	110.57
43	9	301	A86	O4-C34-C33	5.98	122.49	107.59
43	3	302	A86	C25-C26-C27	-5.98	118.78	127.31
43	11	320	A86	C25-C26-C27	-5.98	118.78	127.31
43	5	304	A86	O4-C34-C35	5.98	122.48	107.59
43	1	303	A86	O4-C34-C33	-5.98	92.71	107.59
45	8	308	KC2	C2C-C1C-NC	5.98	117.10	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	16	310	KC2	CHC-C1C-NC	-5.97	114.79	124.20
31	b	617	CLA	C4A-NA-C1A	5.97	109.39	106.71
43	11	302	A86	C23-C16-C22	-5.97	98.56	107.37
43	11	303	A86	C21-C20-C19	-5.97	107.57	114.28
31	4	307	CLA	C4A-NA-C1A	5.97	109.39	106.71
42	18	313	KC1	CHC-C1C-NC	-5.97	114.81	124.20
45	16	310	KC2	C2C-C1C-NC	5.96	117.08	110.57
43	12	301	A86	C19-C18-C17	-5.96	99.26	110.77
31	W	202	CLA	C4A-NA-C1A	5.96	109.39	106.71
43	10	306	A86	C41-C32-C31	5.96	115.80	110.47
43	8	305	A86	C41-C32-C40	-5.96	90.25	108.53
45	15	308	KC2	CBD-CHA-C1A	5.95	139.98	128.88
43	13	303	A86	C17-C16-C15	5.95	115.23	109.16
43	7	301	A86	C4-C5-C6	-5.95	118.82	127.31
43	2	302	A86	C23-C16-C22	-5.95	98.60	107.37
45	15	308	KC2	CHC-C4B-C3B	-5.95	115.09	125.26
43	0	304	A86	C19-C18-C17	-5.95	99.29	110.77
31	P	602	CLA	C4A-NA-C1A	5.95	109.38	106.71
31	w	203	CLA	C4A-NA-C1A	5.95	109.38	106.71
45	1	311	KC2	CMD-C2D-C3D	5.94	135.80	124.68
45	7	311	KC2	C4C-C3C-C2C	-5.94	102.40	107.11
43	1	302	A86	O4-C34-C35	-5.94	92.80	107.59
31	B	616	CLA	C4A-NA-C1A	5.93	109.37	106.71
45	11	309	KC2	CHC-C4B-C3B	-5.93	115.11	125.26
42	7	314	KC1	CAB-C3B-C2B	-5.93	109.06	128.60
42	11	314	KC1	CHC-C1C-NC	-5.93	114.86	124.20
42	p	609	KC1	CHB-C4A-C3A	-5.93	115.72	124.98
31	12	308	CLA	CMB-C2B-C1B	-5.92	119.36	128.46
42	P	609	KC1	CHB-C4A-C3A	-5.92	115.72	124.98
45	8	308	KC2	CHC-C4B-C3B	-5.92	115.13	125.26
43	14	304	A86	C40-C32-C31	5.92	115.77	110.47
42	18	313	KC1	CHC-C4B-C3B	-5.92	115.14	125.26
43	18	304	A86	C41-C32-C40	-5.91	90.38	108.53
31	7	308	CLA	C4A-NA-C1A	5.91	109.36	106.71
31	B	614	CLA	C4A-NA-C1A	5.91	109.36	106.71
45	14	308	KC2	C2C-C1C-NC	5.91	117.02	110.57
31	12	307	CLA	CMB-C2B-C3B	5.91	135.73	124.68
43	16	305	A86	O1-C20-C19	5.91	117.82	113.38
45	12	309	KC2	CHB-C4A-C3A	-5.90	115.76	124.98
43	6	301	A86	C17-C16-C15	5.90	115.18	109.16
45	19	309	KC2	CHB-C4A-C3A	-5.89	115.78	124.98
45	17	311	KC2	CHC-C1C-NC	-5.89	114.93	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	403	CLA	C4A-NA-C1A	5.88	109.35	106.71
43	14	305	A86	C17-C16-C15	5.88	115.16	109.16
43	18	301	A86	C23-C16-C22	-5.88	98.70	107.37
45	1	311	KC2	C4C-C3C-C2C	-5.88	102.45	107.11
45	0	310	KC2	C1A-C2A-C3A	-5.87	102.45	107.11
45	12	309	KC2	C2C-C1C-NC	5.87	116.98	110.57
43	11	302	A86	C25-C26-C27	-5.87	118.94	127.31
43	0	304	A86	C23-C16-C22	-5.86	98.73	107.37
31	a	403	CLA	C4A-NA-C1A	5.85	109.34	106.71
45	14	308	KC2	CHC-C4B-C3B	-5.85	115.25	125.26
42	p	609	KC1	CHC-C1C-NC	-5.85	114.99	124.20
43	16	303	A86	C4-C5-C6	-5.85	118.96	127.31
43	1	302	A86	O4-C34-C33	5.85	122.16	107.59
43	6	302	A86	C4-C5-C6	-5.85	118.96	127.31
45	10	310	KC2	CMD-C2D-C1D	-5.84	119.48	128.46
43	10	304	A86	C23-C16-C22	-5.84	98.75	107.37
42	6	315	KC1	CHD-C4C-NC	5.84	133.06	124.20
45	7	309	KC2	CHC-C1C-NC	-5.84	115.01	124.20
31	7	307	CLA	CED-O2D-CGD	5.83	129.13	115.94
43	8	301	A86	O1-C20-C19	-5.83	109.00	113.38
45	18	308	KC2	CHC-C1C-NC	-5.83	115.02	124.20
45	16	310	KC2	CHC-C4B-C3B	-5.83	115.28	125.26
43	6	301	A86	C4-C5-C6	-5.83	118.99	127.31
42	13	314	KC1	OBD-CAD-CBD	5.83	134.22	125.89
42	10	315	KC1	CHB-C4A-NA	5.83	133.38	124.20
42	14	313	KC1	CHC-C1C-NC	-5.83	115.03	124.20
43	18	301	A86	C4-C5-C6	-5.82	119.00	127.31
43	17	304	A86	C41-C32-C31	5.82	115.68	110.47
42	P	609	KC1	CHC-C1C-NC	-5.82	115.03	124.20
42	1	314	KC1	OBD-CAD-C3D	-5.82	118.32	127.98
45	18	308	KC2	CHD-C4C-NC	-5.82	115.38	124.20
43	13	304	A86	C25-C26-C27	-5.82	119.01	127.31
45	18	308	KC2	CHC-C4B-C3B	-5.82	115.31	125.26
43	0	306	A86	C41-C32-C31	5.81	115.67	110.47
31	0	309	CLA	C4A-NA-C1A	5.81	109.32	106.71
42	17	314	KC1	CHC-C1C-NC	-5.81	115.05	124.20
42	19	314	KC1	CHC-C1C-NC	-5.81	115.06	124.20
43	1	302	A86	C25-C26-C27	-5.81	119.03	127.31
31	18	306	CLA	CED-O2D-CGD	5.80	129.06	115.94
31	19	313	CLA	CHB-C4A-NA	5.80	132.53	124.51
45	7	311	KC2	CHC-C1C-NC	-5.80	115.07	124.20
42	8	313	KC1	CAC-C3C-C4C	5.80	132.33	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	7	303	A86	C25-C26-C27	-5.79	119.04	127.31
45	12	309	KC2	C1A-NA-C4A	-5.79	104.10	106.71
43	13	302	A86	C4-C5-C6	-5.79	119.04	127.31
43	12	301	A86	C23-C16-C22	-5.78	98.84	107.37
43	19	301	A86	C23-C16-C22	-5.78	98.84	107.37
31	B	604	CLA	CAC-C3C-C4C	-5.78	117.31	124.81
43	6	306	A86	O4-C38-O5	-5.78	111.48	122.96
45	12	309	KC2	CHC-C4B-C3B	-5.78	115.38	125.26
31	18	309	CLA	CMB-C2B-C1B	-5.78	119.59	128.46
43	19	301	A86	C19-C18-C17	-5.78	99.62	110.77
43	4	302	A86	C23-C16-C17	-5.78	98.95	108.98
42	14	313	KC1	CHB-C4A-C3A	-5.78	115.96	124.98
43	6	303	A86	O1-C20-C21	-5.77	108.14	115.06
45	14	310	KC2	C4C-C3C-C2C	-5.77	102.53	107.11
31	b	605	CLA	CAC-C3C-C4C	-5.77	117.32	124.81
42	4	313	KC1	CHC-C1C-NC	-5.77	115.12	124.20
43	15	303	A86	C35-C34-C33	-5.77	99.81	109.88
45	17	309	KC2	CHC-C1C-NC	-5.77	115.12	124.20
43	5	318	A86	C17-C16-C15	5.77	115.05	109.16
45	16	312	KC2	C1A-NA-C4A	-5.76	104.11	106.71
42	9	314	KC1	CHC-C1C-NC	-5.76	115.13	124.20
43	7	302	A86	C17-C16-C15	5.76	115.04	109.16
43	15	303	A86	C23-C16-C17	-5.76	98.98	108.98
43	9	302	A86	C17-C16-C15	5.76	115.04	109.16
45	8	310	KC2	CHC-C1C-NC	-5.76	115.13	124.20
43	9	301	A86	C19-C18-C17	-5.76	99.66	110.77
45	17	311	KC2	CAA-C2A-C1A	5.76	151.20	124.75
43	19	304	A86	C19-C18-C17	-5.75	99.66	110.77
43	18	304	A86	C23-C16-C22	-5.75	98.89	107.37
45	9	309	KC2	CHB-C4A-C3A	-5.75	116.00	124.98
43	10	318	A86	C41-C32-C40	-5.75	90.89	108.53
31	5	306	CLA	C4A-NA-C1A	5.74	109.29	106.71
42	8	313	KC1	C4B-CHC-C1C	-5.74	113.67	126.06
42	12	314	KC1	CHC-C1C-NC	-5.74	115.16	124.20
45	15	310	KC2	CHB-C4A-C3A	-5.74	116.01	124.98
45	6	310	KC2	CHC-C1C-NC	-5.74	115.17	124.20
43	10	318	A86	O1-C20-C19	5.73	117.69	113.38
31	11	313	CLA	C4A-NA-C1A	5.73	109.28	106.71
31	c	503	CLA	CMC-C2C-C1C	-5.73	116.31	125.04
43	18	301	A86	O2-C18-C17	5.73	121.19	109.80
45	3	309	KC2	CHB-C4A-C3A	-5.73	116.03	124.98
42	7	314	KC1	CHB-C4A-C3A	-5.73	116.03	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	2	313	KC1	CHC-C1C-NC	-5.73	115.19	124.20
42	5	313	KC1	C4B-CHC-C1C	-5.72	113.72	126.06
31	C	503	CLA	CMC-C2C-C1C	-5.71	116.34	125.04
43	17	302	A86	C4-C5-C6	-5.71	119.16	127.31
45	1	311	KC2	C1A-NA-C4A	-5.71	104.14	106.71
43	9	306	A86	C28-C27-C26	-5.71	114.93	122.92
45	16	312	KC2	CHD-C4C-NC	5.70	132.86	124.20
43	16	306	A86	O4-C38-C39	5.70	121.58	111.09
43	11	306	A86	C3-C2-C1	-5.70	119.17	127.31
43	16	306	A86	C41-C32-C31	5.70	115.58	110.47
31	14	307	CLA	C4A-NA-C1A	5.70	109.27	106.71
43	10	305	A86	C25-C26-C27	-5.70	119.17	127.31
45	1	309	KC2	CHC-C4B-C3B	-5.70	115.51	125.26
45	17	309	KC2	C2C-C1C-NC	5.69	116.79	110.57
45	7	309	KC2	C2C-C1C-NC	5.69	116.79	110.57
43	7	302	A86	C4-C5-C6	-5.69	119.19	127.31
43	12	304	A86	C25-C26-C27	-5.69	119.19	127.31
42	13	314	KC1	CHC-C4B-C3B	-5.69	115.52	125.26
31	13	308	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
42	7	314	KC1	CHC-C1C-NC	-5.69	115.25	124.20
43	10	304	A86	C41-C32-C31	5.69	115.56	110.47
45	4	308	KC2	CHC-C4B-C3B	-5.68	115.54	125.26
43	16	302	A86	C25-C26-C27	-5.68	119.20	127.31
31	17	308	CLA	C4A-NA-C1A	5.68	109.26	106.71
45	18	310	KC2	CHC-C1C-NC	-5.68	115.26	124.20
43	19	305	A86	O1-C15-C20	-5.68	53.85	59.40
45	19	309	KC2	O2D-CGD-CBD	5.68	121.36	111.27
43	19	302	A86	C17-C16-C15	5.67	114.95	109.16
42	17	314	KC1	CHB-C1B-NB	5.67	129.67	124.45
42	5	313	KC1	CHC-C1C-NC	-5.67	115.27	124.20
45	5	310	KC2	C1A-NA-C4A	-5.67	104.16	106.71
43	7	301	A86	C25-C26-C27	-5.67	119.22	127.31
45	17	309	KC2	O2D-CGD-CBD	5.67	121.34	111.27
45	2	308	KC2	CHC-C1C-NC	-5.67	115.28	124.20
45	4	308	KC2	C4C-C3C-C2C	-5.67	102.62	107.11
42	4	313	KC1	CBD-CHA-C1A	5.66	139.44	128.88
42	4	313	KC1	C1A-C2A-C3A	-5.66	102.62	107.11
43	0	305	A86	O4-C38-C39	5.66	121.51	111.09
43	9	303	A86	O1-C20-C21	-5.66	108.27	115.06
43	9	305	A86	O1-C15-C20	-5.66	53.86	59.40
45	6	310	KC2	C2C-C1C-NC	5.66	116.75	110.57
43	14	304	A86	C25-C26-C27	-5.66	119.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	8	308	KC2	CHC-C1C-NC	-5.66	115.30	124.20
31	18	306	CLA	C4A-NA-C1A	5.65	109.25	106.71
45	14	308	KC2	CBD-CHA-C1A	5.65	139.42	128.88
31	8	306	CLA	CED-O2D-CGD	5.65	128.72	115.94
43	12	301	A86	C4-C5-C6	-5.65	119.24	127.31
43	14	301	A86	C36-C31-C32	5.65	125.30	119.70
45	3	311	KC2	C4C-C3C-C2C	-5.65	102.63	107.11
31	B	608	CLA	CMB-C2B-C1B	-5.64	119.79	128.46
43	12	305	A86	C3-C2-C1	-5.64	119.26	127.31
43	18	302	A86	O1-C20-C19	-5.64	109.15	113.38
45	7	309	KC2	O2D-CGD-CBD	5.64	121.28	111.27
43	18	301	A86	C17-C16-C15	5.64	114.91	109.16
43	1	319	A86	C34-O4-C38	-5.63	107.39	117.90
45	3	311	KC2	CHB-C4A-C3A	-5.63	116.18	124.98
43	3	303	A86	C3-C2-C1	-5.63	119.27	127.31
45	11	311	KC2	CAA-C2A-C1A	5.63	150.64	124.75
43	17	304	A86	C25-C26-C27	-5.63	119.27	127.31
43	6	305	A86	O1-C15-C20	-5.63	53.89	59.40
45	1	311	KC2	CAA-C2A-C1A	5.63	150.63	124.75
43	1	319	A86	C36-C31-C32	5.63	125.28	119.70
45	11	309	KC2	CHC-C1C-NC	-5.63	115.34	124.20
43	18	301	A86	C40-C32-C31	5.63	115.51	110.47
43	0	304	A86	C28-C27-C26	-5.63	115.04	122.92
45	0	310	KC2	CHC-C1C-NC	-5.62	115.34	124.20
45	6	312	KC2	C4C-C3C-C2C	-5.62	102.65	107.11
43	19	304	A86	C23-C16-C22	-5.62	99.08	107.37
45	3	311	KC2	CBD-CHA-C1A	5.62	139.36	128.88
31	b	609	CLA	CMB-C2B-C1B	-5.62	119.83	128.46
45	3	311	KC2	CHC-C1C-NC	-5.62	115.36	124.20
31	P	606	CLA	CHB-C4A-NA	5.62	132.28	124.51
43	15	304	A86	C36-C31-C32	-5.62	114.12	119.70
42	18	313	KC1	CAC-C3C-C4C	5.62	132.10	124.81
43	12	305	A86	O1-C20-C21	-5.62	108.33	115.06
31	9	313	CLA	CHB-C4A-NA	5.62	132.28	124.51
45	10	310	KC2	C1A-C2A-C3A	-5.62	102.66	107.11
45	1	311	KC2	CHD-C4C-C3C	-5.61	105.76	126.11
43	0	301	A86	C19-C18-C17	-5.61	99.93	110.77
45	3	311	KC2	CHD-C4C-C3C	-5.61	105.77	126.11
42	8	313	KC1	CHB-C4A-NA	5.61	133.04	124.20
43	9	304	A86	C19-C18-C17	-5.61	99.94	110.77
45	13	311	KC2	C4B-CHC-C1C	-5.61	113.95	126.06
31	p	606	CLA	CHB-C4A-NA	5.61	132.27	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	4	313	KC1	CHB-C4A-C3A	-5.61	116.22	124.98
43	18	301	A86	C25-C26-C27	-5.60	119.31	127.31
43	9	304	A86	C23-C16-C22	-5.60	99.10	107.37
42	9	314	KC1	CBD-CHA-C1A	5.60	139.32	128.88
45	5	310	KC2	CHB-C4A-C3A	-5.60	116.23	124.98
43	13	302	A86	C3-C2-C1	-5.60	119.32	127.31
43	3	301	A86	C22-C16-C17	5.59	118.70	108.98
31	5	312	CLA	C4A-NA-C1A	5.59	109.22	106.71
45	1	311	KC2	CHC-C1C-NC	-5.59	115.40	124.20
42	19	314	KC1	CHB-C4A-C3A	-5.59	116.25	124.98
43	2	304	A86	C19-C18-C17	-5.59	99.99	110.77
42	10	315	KC1	C4B-CHC-C1C	-5.58	114.02	126.06
43	5	301	A86	C25-C26-C27	-5.58	119.34	127.31
43	8	302	A86	C17-C16-C15	5.58	114.86	109.16
45	17	309	KC2	CHC-C4B-C3B	-5.58	115.71	125.26
43	16	304	A86	O1-C20-C21	-5.58	108.37	115.06
45	6	312	KC2	CHC-C1C-NC	-5.58	115.42	124.20
45	11	311	KC2	C2A-C3A-C4A	5.58	110.62	106.49
45	7	309	KC2	CHC-C4B-C3B	-5.58	115.72	125.26
42	2	313	KC1	CHB-C4A-NA	5.58	132.99	124.20
43	1	320	A86	C41-C32-C31	5.58	115.46	110.47
43	4	301	A86	C4-C5-C6	-5.58	119.35	127.31
31	8	309	CLA	CMB-C2B-C1B	-5.58	119.89	128.46
43	14	305	A86	O4-C38-C39	5.57	121.34	111.09
43	3	302	A86	C3-C2-C1	-5.57	119.36	127.31
45	10	310	KC2	CHC-C1C-NC	-5.57	115.42	124.20
42	5	313	KC1	C2A-C3A-C4A	5.57	110.62	106.49
43	14	303	A86	O1-C20-C21	-5.57	108.38	115.06
43	19	304	A86	C35-C34-C33	-5.57	100.16	109.88
31	10	311	CLA	CMB-C2B-C1B	-5.57	119.91	128.46
45	3	309	KC2	O2D-CGD-CBD	5.56	121.16	111.27
43	1	306	A86	O2-C18-C17	5.56	120.86	109.80
43	9	301	A86	C23-C16-C22	-5.56	99.17	107.37
42	5	313	KC1	CAA-C2A-C1A	5.56	150.30	124.75
31	0	311	CLA	CMB-C2B-C1B	-5.56	119.92	128.46
31	14	306	CLA	CAA-C2A-C3A	-5.56	97.56	112.78
43	0	306	A86	C3-C2-C1	-5.55	119.38	127.31
45	16	310	KC2	C4B-CHC-C1C	-5.55	114.08	126.06
43	5	303	A86	O4-C38-C39	5.55	121.30	111.09
42	10	315	KC1	CHC-C1C-NC	-5.55	115.46	124.20
45	14	308	KC2	CHC-C1C-NC	-5.55	115.47	124.20
43	3	305	A86	C41-C32-C40	-5.55	91.51	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	314	CLA	C4A-NA-C1A	5.54	109.20	106.71
45	16	312	KC2	CHC-C1C-NC	-5.54	115.47	124.20
45	13	309	KC2	CHB-C4A-C3A	-5.54	116.32	124.98
43	6	306	A86	O1-C20-C19	5.54	117.55	113.38
43	2	304	A86	C23-C16-C22	-5.54	99.20	107.37
31	8	306	CLA	CMB-C2B-C1B	-5.54	119.95	128.46
45	0	310	KC2	C4B-CHC-C1C	-5.54	114.11	126.06
43	14	301	A86	O4-C38-C39	5.54	121.28	111.09
45	4	310	KC2	CHB-C4A-C3A	-5.54	116.33	124.98
44	P	612	DD6	C9-C10-C11	-5.54	119.41	127.31
45	10	310	KC2	C4B-CHC-C1C	-5.54	114.11	126.06
45	16	312	KC2	C4C-C3C-C2C	-5.54	102.72	107.11
31	8	312	CLA	C2D-C1D-ND	-5.53	106.03	110.10
42	3	314	KC1	C4D-C3D-CAD	5.53	116.75	107.81
43	1	306	A86	C17-C16-C15	5.53	114.81	109.16
43	6	307	A86	C3-C2-C1	-5.53	119.42	127.31
43	7	304	A86	O4-C34-C35	5.53	121.36	107.59
45	10	310	KC2	O2D-CGD-CBD	5.53	121.09	111.27
43	3	303	A86	C4-C5-C6	-5.52	119.43	127.31
43	17	301	A86	C4-C5-C6	-5.52	119.43	127.31
31	p	606	CLA	C3A-C2A-C1A	5.52	109.61	101.34
45	4	308	KC2	C2C-C1C-NC	5.52	116.60	110.57
43	16	307	A86	O1-C20-C19	5.52	117.53	113.38
45	13	309	KC2	CHC-C1C-NC	-5.52	115.51	124.20
45	16	312	KC2	CHD-C4C-C3C	-5.52	106.12	126.11
45	13	311	KC2	C4C-C3C-C2C	-5.51	102.74	107.11
43	10	304	A86	C28-C27-C26	-5.51	115.21	122.92
43	10	301	A86	C23-C16-C22	-5.51	99.25	107.37
43	1	319	A86	C21-C20-C19	-5.50	108.09	114.28
45	2	310	KC2	CHC-C1C-NC	-5.50	115.54	124.20
31	P	606	CLA	C3A-C2A-C1A	5.50	109.58	101.34
43	17	303	A86	O1-C15-C14	-5.50	102.17	113.21
45	11	311	KC2	CBD-CHA-C1A	5.50	139.13	128.88
45	1	311	KC2	CHB-C4A-NA	5.49	132.86	124.20
45	16	312	KC2	CBD-CHA-C1A	5.49	139.12	128.88
43	8	304	A86	O4-C38-C39	5.49	121.19	111.09
43	11	320	A86	C40-C32-C31	5.49	115.39	110.47
43	13	306	A86	C4-C5-C6	-5.49	119.47	127.31
43	16	306	A86	O1-C15-C20	-5.49	54.03	59.40
43	11	304	A86	C23-C16-C22	-5.49	99.27	107.37
43	12	304	A86	C19-C18-C17	-5.49	100.17	110.77
45	14	310	KC2	CHB-C4A-C3A	-5.49	116.41	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	16	301	KC1	CHC-C1C-NC	-5.48	115.57	124.20
43	2	302	A86	C25-C26-C27	-5.48	119.49	127.31
45	6	312	KC2	CHD-C4C-C3C	-5.48	106.25	126.11
43	6	304	A86	O1-C20-C19	5.48	117.50	113.38
43	19	303	A86	O3-C36-C37	-5.48	99.64	109.39
42	16	301	KC1	CAA-C2A-C1A	5.48	149.92	124.75
45	6	310	KC2	CHC-C4B-C3B	-5.48	115.89	125.26
45	0	310	KC2	CHD-C4C-C3C	-5.47	106.28	126.11
43	17	303	A86	C4-C5-C6	-5.47	119.50	127.31
45	2	308	KC2	C2C-C1C-NC	5.47	116.55	110.57
43	6	301	A86	C3-C2-C1	-5.47	119.50	127.31
45	3	309	KC2	CHC-C4B-C3B	-5.47	115.90	125.26
39	C	520	DGD	O3G-C3G-C2G	-5.47	97.70	110.90
45	11	311	KC2	CHB-C4A-NA	5.47	132.82	124.20
43	2	305	A86	C4-C5-C6	-5.47	119.51	127.31
45	19	309	KC2	CHC-C1C-NC	-5.47	115.59	124.20
42	17	314	KC1	C4B-CHC-C1C	-5.46	114.27	126.06
45	4	310	KC2	CHC-C1C-NC	-5.46	115.60	124.20
43	18	304	A86	C19-C18-C17	-5.46	100.22	110.77
39	c	520	DGD	O3G-C3G-C2G	-5.46	97.72	110.90
31	7	310	CLA	CMB-C2B-C1B	-5.46	120.07	128.46
43	5	305	A86	C3-C2-C1	-5.46	119.52	127.31
31	14	312	CLA	CMB-C2B-C3B	5.46	134.89	124.68
45	14	310	KC2	CHB-C1B-NB	5.46	129.47	124.45
45	2	308	KC2	C1A-C2A-C3A	-5.45	102.79	107.11
45	9	309	KC2	CHC-C1C-NC	-5.45	115.62	124.20
45	18	310	KC2	CHD-C4C-C3C	-5.45	106.37	126.11
45	6	310	KC2	C4B-CHC-C1C	-5.44	114.31	126.06
43	p	613	A86	O4-C34-C33	5.44	121.15	107.59
45	7	311	KC2	CHD-C4C-C3C	-5.44	106.38	126.11
45	16	310	KC2	C1A-C2A-C3A	-5.44	102.79	107.11
45	3	309	KC2	C2C-C1C-NC	5.44	116.51	110.57
45	8	308	KC2	CMD-C2D-C3D	5.44	134.86	124.68
31	14	315	CLA	CMA-C3A-C4A	-5.44	97.16	111.77
45	11	309	KC2	CHD-C4C-C3C	-5.44	106.40	126.11
43	14	305	A86	O4-C34-C33	5.44	121.13	107.59
45	12	309	KC2	CHC-C1C-NC	-5.44	115.64	124.20
31	0	309	CLA	CMB-C2B-C1B	-5.43	120.11	128.46
43	1	304	A86	C23-C16-C22	-5.43	99.36	107.37
43	13	305	A86	O4-C38-C39	5.43	121.08	111.09
42	9	314	KC1	CHB-C4A-C3A	-5.43	116.50	124.98
31	c	506	CLA	CMB-C2B-C1B	-5.43	120.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	8	310	KC2	CHD-C4C-C3C	-5.42	106.45	126.11
43	12	302	A86	C34-O4-C38	-5.42	107.79	117.90
43	7	304	A86	C40-C32-C33	-5.42	84.70	109.05
45	14	308	KC2	C4C-C3C-C2C	-5.42	102.81	107.11
45	8	308	KC2	C1A-C2A-C3A	-5.42	102.81	107.11
43	P	613	A86	O4-C34-C33	5.42	121.09	107.59
43	4	302	A86	O4-C38-C39	5.42	121.06	111.09
45	12	309	KC2	CBD-CHA-C1A	5.42	138.98	128.88
43	5	303	A86	C3-C2-C1	-5.42	119.58	127.31
45	6	310	KC2	O2D-CGD-CBD	5.42	120.90	111.27
45	18	308	KC2	CHB-C4A-C3A	-5.42	116.52	124.98
42	0	315	KC1	O2D-CGD-CBD	5.41	120.89	111.27
43	17	302	A86	C12-C11-C13	5.41	125.11	116.02
31	C	506	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
42	0	315	KC1	C4B-CHC-C1C	-5.41	114.39	126.06
31	1	308	CLA	C4A-NA-C1A	5.41	109.14	106.71
43	0	301	A86	C23-C16-C22	-5.41	99.39	107.37
43	14	305	A86	C25-C26-C27	-5.41	119.59	127.31
43	8	302	A86	O4-C38-O5	-5.41	112.22	122.96
42	0	315	KC1	CHB-C4A-NA	5.41	132.72	124.20
31	13	315	CLA	C4A-NA-C1A	5.40	109.14	106.71
42	0	315	KC1	CHC-C1C-NC	-5.40	115.70	124.20
43	10	301	A86	C25-C26-C27	-5.40	119.60	127.31
45	18	310	KC2	CAA-C2A-C1A	5.40	149.56	124.75
43	1	304	A86	C25-C26-C27	-5.40	119.61	127.31
31	1	308	CLA	CMB-C2B-C3B	5.40	134.77	124.68
45	14	310	KC2	CHC-C1C-NC	-5.39	115.71	124.20
42	3	314	KC1	CHB-C4A-C3A	-5.39	116.56	124.98
42	12	314	KC1	CAB-C3B-C2B	-5.39	110.84	128.60
45	8	310	KC2	C4B-CHC-C1C	-5.39	114.43	126.06
43	1	306	A86	C25-C26-C27	-5.39	119.62	127.31
45	8	308	KC2	CMD-C2D-C1D	-5.38	120.19	128.46
45	1	309	KC2	CHB-C4A-C3A	-5.38	116.57	124.98
42	19	314	KC1	CBD-CHA-C1A	5.38	138.91	128.88
45	16	310	KC2	O2D-CGD-CBD	5.38	120.83	111.27
45	6	312	KC2	CBD-CHA-C1A	5.38	138.91	128.88
43	17	301	A86	O4-C38-C39	5.38	120.99	111.09
31	11	315	CLA	C4A-NA-C1A	5.38	109.12	106.71
42	18	313	KC1	C3C-C4C-NC	5.38	114.94	109.88
45	18	310	KC2	C4B-CHC-C1C	-5.38	114.45	126.06
43	18	302	A86	C25-C26-C27	-5.38	119.64	127.31
42	6	315	KC1	CHB-C4A-C3A	-5.38	116.58	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	301	A86	C3-C2-C1	-5.37	119.65	127.31
45	8	308	KC2	O2D-CGD-CBD	5.37	120.81	111.27
45	12	311	KC2	O2D-CGD-CBD	5.37	120.81	111.27
45	1	309	KC2	O2D-CGD-CBD	5.37	120.80	111.27
45	4	310	KC2	C4C-C3C-C2C	-5.37	102.86	107.11
43	19	304	A86	C17-C16-C15	-5.36	103.69	109.16
45	8	308	KC2	CHB-C4A-C3A	-5.36	116.60	124.98
31	C	513	CLA	CMB-C2B-C1B	-5.36	120.23	128.46
43	4	301	A86	C25-C26-C27	-5.36	119.66	127.31
43	12	301	A86	O4-C34-C33	5.36	120.94	107.59
45	5	308	KC2	C4B-CHC-C1C	-5.36	114.50	126.06
43	13	306	A86	C3-C2-C1	-5.35	119.67	127.31
45	15	308	KC2	CHB-C4A-C3A	-5.35	116.61	124.98
43	19	302	A86	O3-C36-C37	-5.35	99.86	109.39
45	12	309	KC2	CHB-C1B-C2B	-5.35	114.26	125.48
43	15	305	A86	C34-O4-C38	5.35	127.87	117.90
31	C	507	CLA	CMB-C2B-C1B	-5.35	120.25	128.46
31	15	312	CLA	CMB-C2B-C1B	-5.35	120.25	128.46
31	c	513	CLA	CMB-C2B-C1B	-5.35	120.25	128.46
31	c	507	CLA	CMB-C2B-C1B	-5.34	120.25	128.46
43	3	303	A86	O4-C38-O5	-5.34	112.36	122.96
31	18	311	CLA	C4A-NA-C1A	5.34	109.11	106.71
43	17	301	A86	C40-C32-C31	5.34	115.25	110.47
45	15	308	KC2	C4B-CHC-C1C	-5.34	114.54	126.06
45	11	311	KC2	CHC-C1C-NC	-5.34	115.80	124.20
43	3	305	A86	O1-C15-C20	-5.34	54.18	59.40
43	15	305	A86	C3-C2-C1	-5.34	119.69	127.31
39	c	518	DGD	O3G-C3G-C2G	-5.34	98.03	110.90
43	10	303	A86	C35-C34-C33	-5.34	100.57	109.88
43	8	301	A86	C4-C5-C6	-5.34	119.70	127.31
43	16	307	A86	O4-C38-O5	-5.33	112.37	122.96
45	4	308	KC2	CHC-C1C-NC	-5.33	115.81	124.20
39	C	518	DGD	O3G-C3G-C2G	-5.33	98.04	110.90
43	17	302	A86	C25-C26-C27	-5.33	119.70	127.31
43	7	304	A86	O4-C38-C39	5.33	120.89	111.09
43	11	303	A86	O4-C34-C33	-5.33	94.32	107.59
43	18	303	A86	C17-C16-C15	5.33	114.60	109.16
31	14	306	CLA	C1-C2-C3	-5.33	116.83	126.04
31	10	307	CLA	CMB-C2B-C3B	5.33	134.64	124.68
42	P	609	KC1	C4B-CHC-C1C	-5.33	114.57	126.06
43	15	304	A86	C21-C20-C19	-5.32	108.29	114.28
43	13	301	A86	C23-C16-C17	-5.32	99.73	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	16	301	KC1	C4B-CHC-C1C	-5.32	114.58	126.06
45	13	311	KC2	O2D-CGD-CBD	5.32	120.72	111.27
43	4	304	A86	C35-C34-C33	-5.32	100.60	109.88
45	2	308	KC2	C4B-CHC-C1C	-5.32	114.59	126.06
45	3	309	KC2	CHC-C1C-NC	-5.32	115.83	124.20
42	13	314	KC1	CAA-C2A-C1A	5.32	149.18	124.75
43	13	303	A86	C4-C5-C6	-5.32	119.72	127.31
43	13	306	A86	C23-C16-C17	5.32	118.22	108.98
43	9	304	A86	C17-C16-C15	-5.31	103.74	109.16
31	d	401	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
42	p	609	KC1	C4B-CHC-C1C	-5.31	114.60	126.06
45	14	310	KC2	CHC-C4B-C3B	-5.31	116.17	125.26
42	10	315	KC1	C3D-CAD-CBD	-5.31	100.61	107.61
45	3	309	KC2	C4B-CHC-C1C	-5.31	114.60	126.06
43	10	305	A86	O4-C38-C39	5.31	120.86	111.09
31	D	401	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
45	16	312	KC2	CHB-C4A-C3A	-5.31	116.69	124.98
31	17	310	CLA	CMB-C2B-C1B	-5.31	120.31	128.46
45	12	309	KC2	C4B-CHC-C1C	-5.31	114.61	126.06
31	17	313	CLA	C4A-NA-C1A	5.31	109.09	106.71
43	5	301	A86	C12-C11-C13	5.31	124.93	116.02
31	10	309	CLA	CMB-C2B-C1B	-5.30	120.31	128.46
42	9	314	KC1	CAC-C3C-C4C	5.30	131.69	124.81
45	11	311	KC2	CMD-C2D-C1D	-5.30	120.31	128.46
43	18	302	A86	O1-C20-C21	-5.30	108.71	115.06
45	6	312	KC2	CHB-C4A-C3A	-5.30	116.70	124.98
43	11	320	A86	C3-C2-C1	-5.30	119.75	127.31
43	13	302	A86	C21-C20-C19	-5.30	108.32	114.28
43	19	302	A86	C4-C5-C6	-5.30	119.75	127.31
43	2	302	A86	O4-C34-C33	5.30	120.78	107.59
43	4	306	A86	C25-C26-C27	-5.29	119.75	127.31
43	15	301	A86	C12-C11-C13	5.29	124.91	116.02
45	2	308	KC2	O2D-CGD-CBD	5.29	120.67	111.27
43	3	303	A86	O4-C34-C35	5.29	120.76	107.59
31	17	307	CLA	CED-O2D-CGD	5.29	127.89	115.94
45	14	310	KC2	CHD-C4C-C3C	-5.28	106.97	126.11
43	17	303	A86	C25-C26-C27	-5.28	119.78	127.31
45	3	311	KC2	C4B-CHC-C1C	-5.28	114.67	126.06
45	12	311	KC2	C4B-CHC-C1C	-5.28	114.68	126.06
43	1	303	A86	O1-C20-C19	5.27	117.34	113.38
45	8	310	KC2	O2D-CGD-CBD	5.27	120.64	111.27
43	8	304	A86	C19-C18-C17	-5.27	100.60	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	13	311	KC2	CHB-C4A-C3A	-5.27	116.75	124.98
45	6	312	KC2	O2D-CGD-CBD	5.27	120.63	111.27
43	1	319	A86	O4-C34-C35	5.27	120.71	107.59
45	4	310	KC2	C2C-C1C-NC	5.26	116.32	110.57
45	5	310	KC2	C4B-CHC-C1C	-5.26	114.70	126.06
45	4	310	KC2	CHC-C4B-C3B	-5.26	116.26	125.26
43	4	303	A86	O1-C20-C21	-5.26	108.75	115.06
45	17	311	KC2	C1B-CHB-C4A	-5.26	114.71	126.06
43	1	306	A86	C19-C18-C17	-5.26	100.61	110.77
45	1	309	KC2	C1B-CHB-C4A	-5.26	114.71	126.06
45	18	308	KC2	O2D-CGD-CBD	5.26	120.61	111.27
43	6	307	A86	O1-C20-C19	5.26	117.33	113.38
31	1	321	CLA	CAA-C2A-C3A	-5.26	98.38	112.78
31	0	307	CLA	CMB-C2B-C3B	5.26	134.51	124.68
43	4	305	A86	O1-C20-C21	5.26	121.35	115.06
45	2	308	KC2	CHC-C4B-C3B	-5.25	116.27	125.26
45	16	312	KC2	O2D-CGD-CBD	5.25	120.60	111.27
43	8	302	A86	C34-O4-C38	-5.25	108.11	117.90
45	15	310	KC2	C4B-CHC-C1C	-5.25	114.73	126.06
42	16	315	KC1	C4B-CHC-C1C	-5.25	114.73	126.06
31	5	314	CLA	C4A-NA-C1A	5.25	109.07	106.71
37	A	412	BCT	O2-C-O1	5.25	133.16	119.55
37	a	411	BCT	O2-C-O1	5.25	133.16	119.55
45	17	309	KC2	C4B-CHC-C1C	-5.25	114.74	126.06
45	9	309	KC2	CHD-C4C-C3C	-5.24	107.10	126.11
45	19	309	KC2	CHD-C4C-C3C	-5.24	107.11	126.11
43	0	303	A86	C23-C16-C22	-5.24	99.64	107.37
42	3	314	KC1	C4B-CHC-C1C	-5.24	114.75	126.06
45	11	311	KC2	CHD-C4C-C3C	-5.24	107.12	126.11
45	18	310	KC2	CHB-C4A-NA	5.24	132.46	124.20
43	8	303	A86	C3-C2-C1	-5.24	119.84	127.31
43	10	302	A86	C25-C26-C27	-5.23	119.84	127.31
42	4	313	KC1	C1B-CHB-C4A	-5.23	114.77	126.06
43	5	301	A86	C3-C2-C1	-5.23	119.85	127.31
45	7	311	KC2	CBD-CHA-C1A	5.23	138.62	128.88
45	9	309	KC2	O2D-CGD-CBD	5.23	120.56	111.27
42	11	314	KC1	CHB-C4A-C3A	-5.22	116.82	124.98
45	12	311	KC2	CHD-C4C-C3C	-5.22	107.19	126.11
45	10	310	KC2	CHD-C4C-C3C	-5.22	107.19	126.11
43	13	301	A86	O4-C34-C33	5.22	120.59	107.59
43	18	303	A86	C3-C2-C1	-5.22	119.86	127.31
43	0	302	A86	O2-C18-C17	5.21	120.17	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	11	309	KC2	CHB-C4A-NA	5.21	132.42	124.20
45	7	309	KC2	C4B-CHC-C1C	-5.21	114.81	126.06
43	14	305	A86	C3-C2-C1	-5.21	119.88	127.31
43	16	302	A86	C4-C5-C6	-5.21	119.88	127.31
43	4	302	A86	O4-C34-C35	-5.21	94.63	107.59
43	10	302	A86	O1-C20-C21	-5.21	108.82	115.06
43	11	305	A86	C17-C16-C15	5.21	114.47	109.16
45	11	309	KC2	C4B-CHC-C1C	-5.20	114.83	126.06
45	2	310	KC2	CHD-C4C-C3C	-5.20	107.26	126.11
43	15	303	A86	C3-C2-C1	-5.20	119.89	127.31
43	13	305	A86	C25-C26-C27	-5.20	119.89	127.31
43	9	304	A86	C35-C34-C33	-5.19	100.81	109.88
31	2	312	CLA	C2D-C1D-ND	-5.19	106.28	110.10
43	11	319	A86	C34-O4-C38	5.19	127.58	117.90
43	17	301	A86	C17-C16-C15	5.19	114.46	109.16
45	1	309	KC2	CAC-C3C-C4C	5.19	148.66	124.47
42	3	314	KC1	C3D-CAD-CBD	-5.19	100.77	107.61
42	11	314	KC1	C1A-NA-C4A	-5.19	104.37	106.71
43	16	305	A86	C4-C5-C6	-5.19	119.90	127.31
45	7	311	KC2	O2D-CGD-CBD	5.19	120.49	111.27
43	P	613	A86	C17-C16-C15	5.19	114.46	109.16
45	6	312	KC2	C4B-CHC-C1C	-5.19	114.86	126.06
43	p	613	A86	C17-C16-C15	5.19	114.46	109.16
45	4	310	KC2	CHD-C4C-C3C	-5.19	107.32	126.11
43	0	303	A86	C25-C26-C27	-5.18	119.91	127.31
45	14	310	KC2	C2C-C1C-NC	5.18	116.22	110.57
43	4	304	A86	C25-C26-C27	-5.17	119.93	127.31
43	2	301	A86	O4-C38-O5	-5.17	112.69	122.96
43	11	304	A86	C25-C26-C27	-5.17	119.93	127.31
45	12	311	KC2	CHB-C4A-NA	5.17	132.34	124.20
43	p	613	A86	O4-C38-C39	5.16	120.59	111.09
31	a	404	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
42	6	315	KC1	C4B-CHC-C1C	-5.16	114.93	126.06
42	12	314	KC1	CMD-C2D-C1D	-5.16	120.54	128.46
43	5	304	A86	C17-C16-C15	5.16	114.42	109.16
42	2	313	KC1	C1A-C2A-C3A	-5.16	103.02	107.11
43	P	613	A86	O4-C38-C39	5.16	120.58	111.09
31	P	606	CLA	C2A-C3A-C4A	-5.16	93.54	101.87
43	11	302	A86	C12-C11-C13	5.16	124.68	116.02
45	13	309	KC2	C4B-CHC-C1C	-5.16	114.94	126.06
43	8	302	A86	C25-C26-C27	-5.15	119.95	127.31
31	p	606	CLA	CMB-C2B-C3B	5.15	134.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	302	A86	O4-C38-O5	-5.15	112.73	122.96
31	15	312	CLA	CMA-C3A-C2A	-5.15	93.06	113.83
45	16	312	KC2	C4B-CHC-C1C	-5.15	114.96	126.06
31	P	606	CLA	CMB-C2B-C3B	5.15	134.31	124.68
42	0	315	KC1	C2A-C3A-C4A	5.15	110.30	106.49
31	C	510	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
43	7	301	A86	C12-C11-C13	5.14	124.66	116.02
45	5	308	KC2	CHC-C1C-NC	-5.14	116.11	124.20
45	9	309	KC2	C4B-CHC-C1C	-5.14	114.97	126.06
45	17	311	KC2	C4B-CHC-C1C	-5.14	114.97	126.06
45	17	311	KC2	CHB-C4A-NA	5.14	132.30	124.20
45	12	309	KC2	CHD-C4C-C3C	-5.14	107.49	126.11
42	9	314	KC1	C4B-CHC-C1C	-5.14	114.98	126.06
43	9	303	A86	C41-C32-C31	5.13	115.07	110.47
45	8	308	KC2	C4B-CHC-C1C	-5.13	115.00	126.06
31	A	404	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
31	c	510	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
45	17	311	KC2	CHD-C4C-C3C	-5.13	107.53	126.11
43	p	611	A86	C3-C2-C1	-5.12	120.00	127.31
31	p	606	CLA	C2A-C3A-C4A	-5.12	93.59	101.87
45	6	310	KC2	C1A-C2A-C3A	-5.12	103.05	107.11
43	9	303	A86	C34-O4-C38	5.12	127.44	117.90
45	2	310	KC2	O2D-CGD-CBD	5.12	120.36	111.27
43	16	302	A86	C3-C2-C1	-5.12	120.00	127.31
43	3	302	A86	C23-C16-C17	-5.12	100.09	108.98
43	10	305	A86	O1-C20-C21	-5.12	108.93	115.06
31	b	603	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
31	18	309	CLA	CMB-C2B-C3B	5.11	134.24	124.68
42	17	314	KC1	C3C-C4C-NC	5.11	114.69	109.88
31	11	308	CLA	CMB-C2B-C3B	5.11	134.24	124.68
43	5	304	A86	C21-C20-C19	-5.11	108.53	114.28
31	P	610	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
31	4	309	CLA	CMB-C2B-C1B	-5.11	120.62	128.46
43	1	303	A86	C36-C31-C32	5.11	124.76	119.70
45	3	309	KC2	CHB-C4A-NA	5.10	132.24	124.20
43	10	301	A86	C4-C5-C6	-5.10	120.03	127.31
43	14	304	A86	O1-C20-C21	5.10	121.17	115.06
31	19	310	CLA	CMB-C2B-C1B	-5.10	120.62	128.46
43	8	301	A86	C23-C16-C17	-5.10	100.12	108.98
43	3	304	A86	C4-C5-C6	-5.10	120.03	127.31
45	7	311	KC2	C4B-CHC-C1C	-5.10	115.06	126.06
42	16	315	KC1	C2A-C3A-C4A	5.10	110.27	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	602	CLA	CMB-C2B-C1B	-5.10	120.63	128.46
43	16	304	A86	C3-C2-C1	-5.10	120.03	127.31
45	5	310	KC2	O2D-CGD-CBD	5.10	120.33	111.27
43	14	301	A86	C3-C2-C1	5.10	134.59	127.31
42	13	314	KC1	C4B-CHC-C1C	-5.10	115.06	126.06
42	8	313	KC1	CHB-C1B-C2B	-5.10	114.79	125.48
45	15	308	KC2	CHC-C1C-NC	-5.10	116.18	124.20
42	19	314	KC1	C4B-CHC-C1C	-5.10	115.06	126.06
42	16	315	KC1	C2A-C1A-NA	5.10	117.57	109.40
43	13	304	A86	O1-C15-C20	-5.09	54.42	59.40
43	P	611	A86	C3-C2-C1	-5.09	120.04	127.31
31	p	610	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
45	3	311	KC2	O2D-CGD-CBD	5.09	120.32	111.27
43	5	303	A86	C4-C5-C6	-5.09	120.05	127.31
43	11	304	A86	C4-C5-C6	-5.09	120.05	127.31
42	11	314	KC1	CAB-C3B-C2B	-5.09	111.84	128.60
31	3	307	CLA	CED-O2D-CGD	5.09	127.45	115.94
42	11	314	KC1	C4B-CHC-C1C	-5.09	115.08	126.06
45	11	309	KC2	CMD-C2D-C1D	-5.09	120.65	128.46
43	0	301	A86	C4-C5-C6	-5.08	120.06	127.31
42	9	314	KC1	O2D-CGD-CBD	5.08	120.30	111.27
45	1	311	KC2	C4B-CHC-C1C	-5.08	115.09	126.06
31	4	307	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
42	7	314	KC1	C4B-CHC-C1C	-5.07	115.11	126.06
45	19	309	KC2	C4B-CHC-C1C	-5.07	115.12	126.06
45	18	308	KC2	CMD-C2D-C3D	5.07	134.16	124.68
45	4	310	KC2	CAA-C2A-C1A	5.07	148.04	124.75
43	16	303	A86	C12-C11-C13	5.07	124.53	116.02
43	15	302	A86	O1-C20-C19	5.06	117.19	113.38
45	13	311	KC2	CHC-C4B-C3B	-5.06	116.60	125.26
45	18	308	KC2	C4B-CHC-C1C	-5.06	115.14	126.06
42	18	313	KC1	C4B-CHC-C1C	-5.06	115.14	126.06
43	16	303	A86	C3-C2-C1	-5.06	120.09	127.31
43	13	304	A86	C34-O4-C38	-5.06	108.47	117.90
42	12	314	KC1	CAC-C3C-C4C	5.06	131.37	124.81
43	19	303	A86	C3-C2-C1	-5.06	120.09	127.31
43	0	304	A86	O4-C34-C33	5.06	120.19	107.59
42	1	314	KC1	OBD-CAD-CBD	5.05	133.12	125.89
43	14	303	A86	C25-C26-C27	-5.05	120.10	127.31
42	19	314	KC1	C1A-NA-C4A	-5.05	104.44	106.71
43	11	304	A86	C35-C34-C33	-5.05	101.07	109.88
31	1	307	CLA	C4A-NA-C1A	5.04	108.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	310	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
42	14	313	KC1	CAA-C2A-C1A	5.04	147.91	124.75
43	15	304	A86	C17-C16-C15	5.04	114.30	109.16
43	13	302	A86	O4-C34-C35	5.04	120.14	107.59
42	12	314	KC1	C4B-CHC-C1C	-5.04	115.19	126.06
42	16	301	KC1	C2A-C3A-C4A	5.04	110.22	106.49
43	6	303	A86	O4-C34-C33	5.04	120.14	107.59
45	4	310	KC2	CHB-C1B-NB	5.04	129.08	124.45
45	18	308	KC2	C1B-CHB-C4A	-5.04	115.19	126.06
43	4	301	A86	C3-C2-C1	-5.04	120.12	127.31
31	B	604	CLA	CMC-C2C-C1C	-5.03	117.37	125.04
43	7	306	A86	O3-C36-C37	-5.03	100.44	109.39
43	14	301	A86	C4-C3-C2	5.03	133.78	123.47
31	B	612	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
43	13	303	A86	C35-C34-C33	-5.03	101.10	109.88
43	14	305	A86	C3-C4-C5	-5.03	113.17	123.47
42	19	314	KC1	O2D-CGD-CBD	5.03	120.20	111.27
31	15	313	CLA	C4A-NA-C1A	5.03	108.97	106.71
43	18	305	A86	O1-C20-C21	-5.03	109.03	115.06
45	13	309	KC2	CHD-C4C-C3C	-5.02	107.90	126.11
45	7	311	KC2	C1B-CHB-C4A	-5.02	115.22	126.06
45	12	311	KC2	CAA-C2A-C1A	5.02	147.83	124.75
42	0	315	KC1	C1B-CHB-C4A	-5.02	115.22	126.06
45	13	311	KC2	CHC-C1C-NC	-5.02	116.30	124.20
45	14	310	KC2	CHB-C4A-NA	5.02	132.11	124.20
31	b	605	CLA	CMC-C2C-C1C	-5.02	117.39	125.04
43	15	301	A86	C23-C16-C17	-5.02	100.26	108.98
31	b	613	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
45	11	311	KC2	O2D-CGD-CBD	5.02	120.19	111.27
43	16	304	A86	C4-C5-C6	-5.02	120.15	127.31
43	1	319	A86	O-C13-C11	-5.02	110.07	121.15
43	11	304	A86	C3-C2-C1	-5.01	120.15	127.31
43	6	301	A86	O3-C36-C37	-5.01	100.47	109.39
42	2	313	KC1	C4B-CHC-C1C	-5.01	115.26	126.06
43	5	318	A86	C12-C11-C13	5.01	124.43	116.02
43	3	304	A86	C17-C16-C15	5.00	114.27	109.16
42	1	314	KC1	CAC-C3C-C4C	5.00	131.30	124.81
34	B	623	SQD	O7-S-C6	5.00	112.88	106.94
34	b	601	SQD	O7-S-C6	5.00	112.88	106.94
45	15	310	KC2	CHD-C4C-C3C	-5.00	108.00	126.11
31	19	308	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
43	6	305	A86	C41-C32-C31	5.00	114.94	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	302	A86	O4-C34-C33	5.00	120.03	107.59
45	4	310	KC2	CHB-C4A-NA	4.99	132.07	124.20
45	11	311	KC2	C4B-CHC-C1C	-4.99	115.29	126.06
31	B	616	CLA	CAA-C2A-C3A	-4.99	99.12	112.78
42	5	313	KC1	CHB-C4A-NA	4.99	132.06	124.20
43	16	302	A86	C40-C32-C31	4.98	114.93	110.47
45	1	309	KC2	CHB-C4A-NA	4.98	132.05	124.20
43	1	319	A86	O4-C38-O5	-4.98	113.07	122.96
45	14	310	KC2	CAA-C2A-C1A	4.98	147.64	124.75
45	3	309	KC2	C1B-CHB-C4A	-4.98	115.31	126.06
43	9	302	A86	C35-C34-C33	-4.98	101.19	109.88
43	0	303	A86	C35-C34-C33	-4.98	101.19	109.88
43	12	303	A86	C28-C27-C26	-4.98	115.95	122.92
43	14	303	A86	C35-C34-C33	-4.98	101.19	109.88
43	6	304	A86	C4-C5-C6	-4.98	120.21	127.31
45	0	310	KC2	C4C-C3C-C2C	-4.98	103.16	107.11
45	4	308	KC2	CHB-C4A-C3A	-4.98	117.20	124.98
43	0	303	A86	C3-C2-C1	-4.97	120.21	127.31
43	2	301	A86	C25-C26-C27	-4.97	120.21	127.31
43	7	305	A86	C4-C5-C6	-4.97	120.22	127.31
31	18	312	CLA	C4A-NA-C1A	4.97	108.94	106.71
45	11	309	KC2	CAA-C2A-C1A	4.97	147.59	124.75
31	3	313	CLA	CMB-C2B-C3B	4.97	133.97	124.68
45	1	309	KC2	C1A-C2A-C3A	-4.97	103.17	107.11
43	13	304	A86	O4-C38-C39	4.97	120.22	111.09
43	13	306	A86	O3-C36-C37	-4.97	100.55	109.39
42	7	314	KC1	CAC-C3C-C4C	4.96	131.25	124.81
43	2	305	A86	O1-C20-C19	4.96	117.11	113.38
43	9	305	A86	O4-C38-C39	4.96	120.22	111.09
43	0	302	A86	C25-C26-C27	-4.96	120.23	127.31
45	14	308	KC2	C4B-CHC-C1C	-4.96	115.36	126.06
45	14	310	KC2	CBD-CHA-C1A	4.96	138.12	128.88
45	11	309	KC2	CHB-C1B-C2B	-4.95	115.09	125.48
43	5	302	A86	C3-C2-C1	-4.95	120.24	127.31
42	5	313	KC1	C2A-C1A-NA	4.95	117.34	109.40
45	4	310	KC2	C1B-CHB-C4A	-4.95	115.38	126.06
31	p	604	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
43	3	301	A86	C9-C8-C6	-4.95	112.52	126.42
43	17	303	A86	C12-C11-C13	4.94	124.33	116.02
45	8	308	KC2	C1B-CHB-C4A	-4.94	115.39	126.06
42	13	314	KC1	CHB-C4A-NA	4.94	131.99	124.20
31	b	617	CLA	CAA-C2A-C3A	-4.94	99.26	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	310	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
31	12	307	CLA	C4A-NA-C1A	4.94	108.92	106.71
31	P	604	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
43	10	303	A86	C3-C2-C1	-4.93	120.27	127.31
45	18	310	KC2	O2D-CGD-CBD	4.93	120.04	111.27
31	p	606	CLA	CHA-C1A-NA	4.93	137.69	126.40
31	P	606	CLA	CHA-C1A-NA	4.93	137.69	126.40
42	7	314	KC1	CHB-C1B-NB	4.93	128.99	124.45
43	15	301	A86	C33-C32-C31	4.93	114.00	109.21
43	1	303	A86	C21-C20-C19	-4.93	108.73	114.28
42	14	313	KC1	C4B-CHC-C1C	-4.93	115.43	126.06
43	5	318	A86	C3-C2-C1	-4.93	120.28	127.31
31	1	313	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
45	1	311	KC2	CMD-C2D-C1D	-4.93	120.89	128.46
42	4	313	KC1	CHB-C1B-C2B	-4.92	115.15	125.48
43	1	303	A86	C4-C5-C6	-4.92	120.28	127.31
43	3	302	A86	O4-C34-C33	4.92	119.85	107.59
43	1	306	A86	O4-C38-C39	4.92	120.14	111.09
43	1	304	A86	C17-C16-C15	4.92	114.18	109.16
42	7	314	KC1	C4D-C3D-CAD	4.92	115.76	107.81
45	5	310	KC2	CHD-C4C-C3C	-4.92	108.29	126.11
45	4	308	KC2	C4B-CHC-C1C	-4.91	115.46	126.06
45	14	308	KC2	CHB-C4A-C3A	-4.91	117.31	124.98
43	16	302	A86	O4-C38-C39	4.91	120.12	111.09
42	16	301	KC1	CHB-C4A-NA	4.91	131.94	124.20
45	15	308	KC2	CAC-C3C-C4C	4.91	147.33	124.47
43	3	301	A86	O4-C38-C39	4.91	120.12	111.09
42	4	313	KC1	C4B-CHC-C1C	-4.90	115.48	126.06
43	6	306	A86	C4-C5-C6	-4.90	120.31	127.31
43	2	303	A86	O4-C38-C39	4.90	120.11	111.09
43	10	301	A86	O4-C34-C33	4.90	119.80	107.59
43	11	306	A86	O4-C38-C39	4.90	120.11	111.09
43	17	306	A86	C4-C5-C6	-4.90	120.32	127.31
43	9	305	A86	C3-C2-C1	-4.90	120.32	127.31
42	14	313	KC1	C1B-CHB-C4A	-4.89	115.50	126.06
42	0	315	KC1	CHB-C1B-C2B	-4.89	115.22	125.48
31	14	309	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
43	6	306	A86	C41-C32-C40	-4.89	93.53	108.53
43	6	301	A86	C25-C26-C27	-4.89	120.33	127.31
43	4	305	A86	C23-C16-C17	-4.89	100.49	108.98
31	8	309	CLA	CMB-C2B-C3B	4.89	133.82	124.68
43	11	305	A86	O4-C38-C39	4.89	120.08	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	7	314	KC1	C3D-CAD-CBD	-4.89	101.17	107.61
43	8	303	A86	C4-C5-C6	-4.89	120.34	127.31
43	6	302	A86	C12-C11-C13	4.89	124.23	116.02
43	5	304	A86	O4-C38-C39	4.89	120.08	111.09
31	2	309	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
43	3	301	A86	C36-C31-C32	-4.88	114.85	119.70
45	14	310	KC2	C1B-CHB-C4A	-4.88	115.53	126.06
43	17	304	A86	C3-C2-C1	-4.88	120.35	127.31
31	10	312	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
43	8	304	A86	C33-C32-C31	-4.88	104.47	109.21
43	4	304	A86	C3-C2-C1	-4.88	120.35	127.31
45	18	308	KC2	C1A-C2A-C3A	-4.87	103.25	107.11
43	19	302	A86	C3-C2-C1	-4.87	120.36	127.31
43	5	304	A86	C41-C32-C40	-4.87	93.59	108.53
45	0	310	KC2	CHB-C1B-C2B	-4.86	115.28	125.48
43	5	303	A86	C28-C27-C26	-4.86	116.11	122.92
43	13	301	A86	C12-C11-C13	4.86	124.19	116.02
34	A	411	SQD	C1-O5-C5	4.86	123.23	113.69
34	0	318	SQD	O7-S-C6	4.86	112.72	106.94
43	16	307	A86	C4-C5-C6	-4.86	120.37	127.31
31	C	504	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
43	6	307	A86	O1-C20-C21	-4.86	109.23	115.06
43	11	303	A86	C4-C5-C6	-4.86	120.38	127.31
45	16	310	KC2	CHB-C4A-C3A	-4.86	117.39	124.98
45	12	309	KC2	C1B-CHB-C4A	-4.85	115.59	126.06
42	13	314	KC1	O2D-CGD-CBD	4.85	119.89	111.27
42	12	314	KC1	C1B-CHB-C4A	-4.85	115.59	126.06
42	11	314	KC1	CAC-C3C-C4C	4.85	131.11	124.81
31	c	504	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
43	0	301	A86	O4-C34-C33	4.85	119.67	107.59
31	2	315	CLA	CMC-C2C-C1C	-4.84	117.66	125.04
31	C	511	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
31	c	511	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
42	13	314	KC1	C2A-C3A-C4A	4.84	110.08	106.49
31	14	306	CLA	O2A-C1-C2	4.84	121.35	108.64
45	10	310	KC2	C1B-CHB-C4A	-4.84	115.62	126.06
43	6	303	A86	O4-C38-O5	-4.84	113.36	122.96
43	0	306	A86	O1-C20-C21	-4.84	109.26	115.06
43	10	306	A86	O1-C20-C21	-4.84	109.26	115.06
43	3	304	A86	C3-C2-C1	-4.84	120.41	127.31
45	2	308	KC2	CHB-C4A-C3A	-4.84	117.42	124.98
45	1	309	KC2	CHB-C1B-C2B	-4.83	115.34	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	P	609	KC1	O2D-CGD-CBD	4.83	119.86	111.27
42	p	609	KC1	O2D-CGD-CBD	4.83	119.85	111.27
31	11	307	CLA	CAC-C3C-C4C	4.83	131.08	124.81
43	7	301	A86	O4-C34-C33	4.83	119.62	107.59
43	19	302	A86	C25-C26-C27	4.83	134.20	127.31
34	i	101	SQD	C1-O5-C5	4.83	123.16	113.69
31	9	308	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
45	1	311	KC2	CHB-C1B-C2B	-4.82	115.37	125.48
43	1	302	A86	C17-C16-C15	4.82	114.08	109.16
43	1	302	A86	C3-C2-C1	-4.82	120.43	127.31
43	2	303	A86	O1-C20-C19	4.82	117.00	113.38
43	6	302	A86	C3-C2-C1	-4.82	120.44	127.31
45	2	310	KC2	CAA-C2A-C1A	4.82	146.88	124.75
45	14	308	KC2	O2D-CGD-CBD	4.82	119.83	111.27
43	9	301	A86	C21-C20-C19	-4.82	108.86	114.28
45	13	311	KC2	C2C-C1C-NC	4.82	115.83	110.57
43	14	304	A86	C23-C16-C17	-4.81	100.62	108.98
31	0	309	CLA	CMB-C2B-C3B	4.81	133.68	124.68
42	16	301	KC1	O2D-CGD-CBD	4.81	119.82	111.27
43	10	303	A86	C25-C26-C27	-4.81	120.44	127.31
31	B	613	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
43	11	306	A86	O-C13-C11	-4.81	110.53	121.15
42	10	315	KC1	C3C-C4C-NC	4.80	114.40	109.88
38	15	315	LMG	O6-C5-C4	4.80	118.41	109.69
42	7	314	KC1	C3C-C4C-NC	4.80	114.40	109.88
45	1	311	KC2	O2D-CGD-CBD	4.79	119.79	111.27
43	10	304	A86	O4-C34-C33	4.79	119.53	107.59
31	b	614	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
45	10	310	KC2	C4C-C3C-C2C	-4.79	103.31	107.11
43	1	305	A86	O4-C38-C39	4.79	119.91	111.09
45	1	309	KC2	C2C-C1C-NC	4.79	115.80	110.57
45	2	310	KC2	C4B-CHC-C1C	-4.79	115.73	126.06
45	10	310	KC2	CHB-C1B-C2B	-4.79	115.44	125.48
34	b	601	SQD	C1-O5-C5	4.79	123.09	113.69
45	5	308	KC2	CAC-C3C-C4C	4.79	146.78	124.47
43	17	303	A86	C35-C34-C33	-4.78	101.53	109.88
43	15	303	A86	C4-C5-C6	-4.78	120.48	127.31
43	0	304	A86	C35-C34-C33	-4.78	101.53	109.88
43	19	305	A86	O4-C38-C39	4.78	119.89	111.09
43	2	302	A86	C12-C11-C13	4.78	124.05	116.02
43	14	303	A86	C3-C2-C1	-4.78	120.49	127.31
45	1	311	KC2	C1B-CHB-C4A	-4.78	115.75	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	7	302	A86	O4-C38-C39	4.78	119.88	111.09
43	3	301	A86	C25-C24-C1	-4.77	113.00	126.42
34	B	623	SQD	C1-O5-C5	4.77	123.06	113.69
42	p	609	KC1	CHB-C4A-NA	4.77	131.72	124.20
45	1	309	KC2	C4B-CHC-C1C	-4.77	115.77	126.06
43	5	305	A86	C17-C16-C15	4.77	114.03	109.16
43	1	302	A86	C22-C16-C17	-4.77	100.70	108.98
43	5	305	A86	C41-C32-C31	4.77	114.74	110.47
42	P	609	KC1	CHB-C4A-NA	4.77	131.72	124.20
43	3	306	A86	C4-C5-C6	-4.77	120.51	127.31
43	5	302	A86	C23-C16-C22	4.77	114.40	107.37
45	15	308	KC2	CHB-C1B-C2B	-4.77	115.48	125.48
43	16	307	A86	C33-C32-C31	-4.76	104.58	109.21
43	1	305	A86	C17-C16-C15	4.76	114.02	109.16
45	12	311	KC2	CHC-C1C-NC	-4.76	116.70	124.20
43	2	302	A86	C4-C5-C6	-4.76	120.52	127.31
31	18	307	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
43	4	302	A86	C3-C2-C1	-4.76	120.52	127.31
45	6	310	KC2	C1B-CHB-C4A	-4.76	115.79	126.06
43	5	301	A86	C23-C16-C17	-4.76	100.71	108.98
43	3	306	A86	C23-C16-C22	4.76	114.39	107.37
31	C	509	CLA	CMB-C2B-C3B	4.76	133.58	124.68
45	5	310	KC2	CHB-C1B-C2B	-4.76	115.50	125.48
42	1	314	KC1	C3C-C4C-NC	4.75	114.35	109.88
45	6	310	KC2	CHB-C4A-C3A	-4.75	117.55	124.98
43	11	303	A86	O1-C15-C20	-4.75	54.75	59.40
31	1	313	CLA	C4A-NA-C1A	4.75	108.84	106.71
43	12	302	A86	C20-C19-C18	4.75	122.15	112.75
45	13	309	KC2	O2D-CGD-CBD	4.75	119.71	111.27
43	5	305	A86	C41-C32-C40	-4.75	93.95	108.53
31	p	606	CLA	C4D-CHA-C1A	-4.75	115.47	121.25
31	14	307	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
43	16	302	A86	O3-C36-C37	-4.75	100.94	109.39
43	12	301	A86	C25-C26-C27	-4.75	120.53	127.31
45	5	310	KC2	CHC-C1C-NC	-4.75	116.73	124.20
43	16	303	A86	O4-C34-C33	4.75	119.42	107.59
34	10	320	SQD	O7-S-C6	4.75	112.58	106.94
42	2	313	KC1	CAC-C3C-C4C	4.75	130.97	124.81
45	0	310	KC2	C1B-CHB-C4A	-4.75	115.82	126.06
45	11	311	KC2	C1A-NA-C4A	-4.75	104.57	106.71
45	18	310	KC2	C2A-C3A-C4A	4.75	110.01	106.49
42	17	314	KC1	CAC-C3C-C4C	4.75	130.97	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	509	CLA	CMB-C2B-C3B	4.75	133.56	124.68
44	P	612	DD6	C4-C5-C6	-4.74	120.54	127.31
43	19	305	A86	C3-C2-C1	-4.74	120.55	127.31
43	1	319	A86	O1-C15-C20	-4.74	54.77	59.40
31	10	311	CLA	CMB-C2B-C3B	4.74	133.54	124.68
42	9	314	KC1	CHB-C1B-C2B	-4.74	115.54	125.48
31	P	606	CLA	C4D-CHA-C1A	-4.74	115.48	121.25
45	19	309	KC2	CHB-C1B-C2B	-4.74	115.54	125.48
43	0	302	A86	C19-C18-C17	-4.74	101.62	110.77
43	1	320	A86	C3-C2-C1	-4.74	120.55	127.31
45	7	311	KC2	CHB-C1B-C2B	-4.73	115.55	125.48
45	11	311	KC2	C1B-CHB-C4A	-4.73	115.85	126.06
45	2	310	KC2	C1B-CHB-C4A	-4.73	115.85	126.06
43	16	305	A86	C25-C26-C27	-4.73	120.56	127.31
43	8	301	A86	C3-C2-C1	-4.73	120.56	127.31
31	18	312	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
31	7	310	CLA	CMB-C2B-C3B	4.73	133.53	124.68
43	1	303	A86	O1-C15-C20	-4.73	54.78	59.40
43	14	302	A86	C4-C5-C6	-4.73	120.56	127.31
45	1	311	KC2	CBD-CHA-C1A	4.73	137.69	128.88
42	1	314	KC1	C1B-CHB-C4A	-4.73	115.86	126.06
45	6	310	KC2	CHB-C1B-C2B	-4.72	115.57	125.48
43	9	306	A86	C41-C32-C31	4.72	114.70	110.47
43	P	611	A86	O3-C36-C37	-4.72	100.99	109.39
45	12	309	KC2	C4C-C3C-C2C	-4.72	103.37	107.11
31	B	607	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
43	p	611	A86	O3-C36-C37	-4.72	100.99	109.39
43	18	305	A86	C25-C26-C27	-4.72	120.58	127.31
43	6	304	A86	C25-C26-C27	-4.72	120.58	127.31
43	3	303	A86	C20-C19-C18	4.72	122.08	112.75
31	a	403	CLA	CMB-C2B-C3B	4.72	133.50	124.68
31	0	311	CLA	CMB-C2B-C3B	4.71	133.50	124.68
31	A	403	CLA	CMB-C2B-C3B	4.71	133.50	124.68
31	b	608	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
31	b	615	CLA	CAA-C2A-C3A	-4.71	99.88	112.78
42	19	314	KC1	CHB-C1B-C2B	-4.71	115.60	125.48
43	5	302	A86	C4-C5-C6	-4.71	120.59	127.31
45	16	310	KC2	C1B-CHB-C4A	-4.71	115.90	126.06
43	16	305	A86	O4-C38-C39	4.71	119.75	111.09
43	6	301	A86	O4-C38-C39	4.70	119.74	111.09
43	10	304	A86	C35-C34-C33	-4.70	101.67	109.88
45	18	308	KC2	CHB-C1B-C2B	-4.70	115.62	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	311	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
43	13	304	A86	C3-C4-C5	-4.70	113.84	123.47
43	7	303	A86	C35-C34-C33	-4.70	101.67	109.88
42	1	314	KC1	C4B-CHC-C1C	-4.70	115.92	126.06
43	17	303	A86	C34-O4-C38	4.70	126.65	117.90
43	12	302	A86	C4-C5-C6	-4.70	120.61	127.31
38	D	403	LMG	O1-C1-C2	-4.69	100.97	108.30
31	p	606	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
42	18	313	KC1	CHB-C1B-C2B	-4.69	115.64	125.48
45	13	309	KC2	CBD-CHA-C1A	4.69	137.62	128.88
43	14	301	A86	C24-C1-C2	-4.69	111.75	118.94
45	3	311	KC2	C1B-CHB-C4A	-4.69	115.94	126.06
31	10	309	CLA	CMB-C2B-C3B	4.69	133.45	124.68
45	15	310	KC2	O2D-CGD-CBD	4.69	119.60	111.27
45	18	308	KC2	CMD-C2D-C1D	-4.69	121.26	128.46
43	8	302	A86	O4-C34-C33	4.69	119.26	107.59
45	9	309	KC2	CHB-C1B-C2B	-4.68	115.65	125.48
43	10	318	A86	C36-C31-C32	-4.68	115.05	119.70
45	12	311	KC2	CHB-C1B-C2B	-4.68	115.66	125.48
43	10	301	A86	C21-C20-C19	-4.68	109.01	114.28
31	16	314	CLA	CMB-C2B-C3B	4.68	133.44	124.68
45	8	310	KC2	CAA-C2A-C1A	4.68	146.27	124.75
31	P	606	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
43	6	304	A86	O4-C38-C39	4.68	119.70	111.09
43	12	303	A86	C35-C34-C33	-4.68	101.71	109.88
43	16	307	A86	C41-C32-C40	-4.68	94.18	108.53
43	10	304	A86	C25-C26-C27	-4.67	120.64	127.31
42	8	313	KC1	C1B-CHB-C4A	-4.67	115.98	126.06
43	12	302	A86	O4-C34-C35	4.67	119.22	107.59
43	7	302	A86	C12-C11-C13	4.67	123.86	116.02
43	3	305	A86	C25-C26-C27	-4.67	120.65	127.31
43	10	302	A86	C40-C32-C31	-4.66	106.30	110.47
42	3	314	KC1	CAC-C3C-C4C	4.66	130.86	124.81
43	9	303	A86	C3-C2-C1	-4.66	120.66	127.31
45	15	310	KC2	CHB-C1B-C2B	-4.66	115.70	125.48
45	15	310	KC2	CAA-C2A-C1A	4.66	146.17	124.75
43	12	302	A86	O1-C15-C20	-4.66	54.84	59.40
31	0	312	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
31	a	406	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
31	14	311	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
43	5	305	A86	C33-C32-C31	-4.66	104.68	109.21
43	5	305	A86	O4-C38-C39	4.66	119.66	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	406	CLA	CMB-C2B-C1B	-4.66	121.31	128.46
42	19	314	KC1	CAC-C3C-C4C	4.66	130.85	124.81
45	5	310	KC2	C1B-CHB-C4A	-4.66	116.02	126.06
42	14	313	KC1	CHB-C1B-C2B	-4.66	115.72	125.48
43	3	304	A86	C35-C34-C33	-4.66	101.75	109.88
43	5	302	A86	C35-C34-C33	-4.66	101.75	109.88
43	4	304	A86	C4-C5-C6	-4.65	120.67	127.31
45	7	309	KC2	CHB-C4A-C3A	-4.65	117.71	124.98
45	15	308	KC2	CAA-C2A-C1A	4.65	146.12	124.75
31	17	310	CLA	CMB-C2B-C3B	4.65	133.38	124.68
31	17	307	CLA	CAC-C3C-C4C	4.65	130.84	124.81
43	12	302	A86	O4-C38-O5	-4.65	113.72	122.96
43	19	301	A86	C21-C20-C19	-4.64	109.06	114.28
43	13	302	A86	C20-C19-C18	4.64	121.94	112.75
44	p	612	DD6	C7-C6-C5	-4.64	116.42	122.92
45	15	310	KC2	CHC-C1C-NC	-4.64	116.89	124.20
43	12	302	A86	C21-C20-C19	-4.64	109.06	114.28
45	13	311	KC2	CHD-C4C-C3C	-4.64	109.29	126.11
45	18	310	KC2	C1B-CHB-C4A	-4.64	116.05	126.06
42	8	313	KC1	C4C-C3C-C2C	-4.64	100.14	106.90
43	11	302	A86	O-C13-C14	-4.64	112.23	121.66
43	p	613	A86	C41-C32-C33	4.64	129.88	109.05
45	16	310	KC2	CHB-C1B-C2B	-4.64	115.75	125.48
33	Y	101	BCR	C24-C23-C22	-4.64	119.23	126.23
33	y	101	BCR	C24-C23-C22	-4.64	119.23	126.23
43	P	613	A86	C41-C32-C33	4.64	129.88	109.05
43	17	316	A86	O4-C38-O5	-4.64	113.75	122.96
43	3	301	A86	C17-C16-C15	4.63	113.89	109.16
43	7	302	A86	C3-C2-C1	-4.63	120.70	127.31
43	19	301	A86	C41-C32-C31	-4.63	106.33	110.47
43	13	302	A86	O1-C15-C20	-4.63	54.87	59.40
45	5	308	KC2	O2D-CGD-CBD	4.63	119.50	111.27
43	12	305	A86	C17-C16-C15	4.63	113.89	109.16
45	2	310	KC2	CHB-C4A-NA	4.63	131.50	124.20
42	9	314	KC1	C3C-C4C-NC	4.63	114.23	109.88
43	10	303	A86	C23-C16-C22	-4.63	100.54	107.37
43	13	306	A86	C19-C18-C17	-4.63	101.84	110.77
43	16	303	A86	C25-C26-C27	-4.63	120.71	127.31
43	12	301	A86	C3-C2-C1	-4.63	120.71	127.31
43	7	305	A86	C41-C32-C40	-4.63	94.33	108.53
45	11	311	KC2	CHB-C1B-C2B	-4.63	115.78	125.48
43	19	302	A86	C23-C16-C22	-4.62	100.55	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	303	A86	C3-C2-C1	-4.62	120.71	127.31
43	3	303	A86	O1-C15-C20	-4.62	54.88	59.40
45	3	309	KC2	CMD-C2D-C3D	4.62	133.32	124.68
43	4	305	A86	C4-C3-C2	-4.62	114.01	123.47
43	1	302	A86	C14-C15-C16	4.62	136.44	118.75
41	v	201	HEM	CBA-CAA-C2A	4.62	120.50	112.62
43	19	303	A86	C40-C32-C31	4.61	114.60	110.47
45	3	309	KC2	CHB-C1B-C2B	-4.61	115.80	125.48
45	8	308	KC2	CHB-C1B-C2B	-4.61	115.80	125.48
31	B	614	CLA	CAA-C2A-C3A	-4.61	100.15	112.78
43	1	305	A86	C3-C4-C5	-4.61	114.03	123.47
43	19	306	A86	C3-C2-C1	-4.61	120.73	127.31
45	8	310	KC2	C1B-CHB-C4A	-4.61	116.11	126.06
43	0	305	A86	O1-C20-C21	-4.61	109.53	115.06
43	6	303	A86	C17-C16-C15	4.61	113.86	109.16
38	5	316	LMG	O1-C7-C8	-4.61	99.78	110.90
31	C	513	CLA	CMB-C2B-C3B	4.61	133.29	124.68
43	11	303	A86	O-C13-C11	-4.60	110.98	121.15
43	9	301	A86	C34-O4-C38	4.60	126.48	117.90
43	9	306	A86	O4-C38-C39	4.60	119.56	111.09
45	6	312	KC2	CAA-C2A-C1A	4.60	145.89	124.75
43	18	302	A86	O4-C38-C39	4.60	119.55	111.09
42	7	314	KC1	CHB-C4A-NA	4.60	131.45	124.20
42	17	314	KC1	CHB-C4A-NA	4.60	131.45	124.20
42	10	315	KC1	CAC-C3C-C4C	4.60	130.78	124.81
31	c	506	CLA	CMB-C2B-C3B	4.60	133.28	124.68
43	1	319	A86	C20-C19-C18	4.60	121.84	112.75
43	19	306	A86	O4-C38-C39	4.60	119.55	111.09
43	0	305	A86	C4-C5-C6	-4.60	120.75	127.31
31	19	307	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
45	4	308	KC2	CHB-C1B-C2B	-4.59	115.85	125.48
45	14	308	KC2	CHD-C4C-C3C	-4.59	109.47	126.11
45	4	308	KC2	CHD-C4C-C3C	-4.59	109.47	126.11
42	8	313	KC1	O2D-CGD-CBD	4.59	119.43	111.27
43	17	316	A86	O1-C15-C20	-4.59	54.91	59.40
41	V	201	HEM	CBA-CAA-C2A	4.59	120.45	112.62
43	11	303	A86	C36-C31-C32	4.59	124.25	119.70
31	7	307	CLA	CAC-C3C-C4C	4.59	130.76	124.81
31	7	313	CLA	C4A-NA-C1A	4.59	108.77	106.71
43	7	304	A86	O1-C15-C20	-4.59	54.92	59.40
45	4	310	KC2	CBD-CHA-C1A	4.59	137.43	128.88
45	12	309	KC2	O2D-CGD-CBD	4.58	119.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	306	A86	C41-C32-C40	-4.58	94.46	108.53
43	7	304	A86	C25-C26-C27	-4.58	120.77	127.31
42	1	314	KC1	CHB-C4A-C3A	-4.58	117.82	124.98
31	1	321	CLA	C1-C2-C3	-4.58	118.12	126.04
43	11	303	A86	O1-C20-C19	4.58	116.83	113.38
31	b	615	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
43	4	306	A86	C3-C2-C1	-4.58	120.78	127.31
43	9	306	A86	C35-C34-C33	-4.58	101.89	109.88
31	c	503	CLA	CMC-C2C-C3C	4.57	138.53	126.12
43	6	305	A86	C25-C26-C27	-4.57	120.78	127.31
43	17	316	A86	C4-C5-C6	-4.57	120.78	127.31
31	C	506	CLA	CMB-C2B-C3B	4.57	133.24	124.68
43	19	304	A86	C3-C2-C1	-4.57	120.79	127.31
42	1	314	KC1	CAB-C3B-C2B	-4.57	113.55	128.60
45	11	309	KC2	C2A-C3A-C4A	4.57	109.88	106.49
43	3	304	A86	C23-C16-C22	-4.57	100.63	107.37
42	9	314	KC1	C1A-NA-C4A	-4.57	104.65	106.71
42	5	313	KC1	CHD-C4C-NC	4.57	131.13	124.20
45	8	310	KC2	CHB-C4A-NA	4.57	131.40	124.20
45	5	308	KC2	C1B-CHB-C4A	-4.57	116.21	126.06
31	b	610	CLA	CMB-C2B-C1B	-4.57	121.45	128.46
31	d	404	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
31	c	513	CLA	CMB-C2B-C3B	4.56	133.22	124.68
43	8	301	A86	C19-C18-C17	4.56	119.58	110.77
31	C	503	CLA	CMC-C2C-C3C	4.56	138.50	126.12
45	1	311	KC2	C2A-C3A-C4A	4.56	109.87	106.49
31	5	309	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
45	15	308	KC2	C4B-C3B-C2B	-4.56	103.01	106.75
43	15	304	A86	O4-C34-C33	4.56	118.94	107.59
43	11	305	A86	C12-C11-C13	4.55	123.67	116.02
43	14	303	A86	C4-C5-C6	-4.55	120.81	127.31
43	7	304	A86	C28-C27-C26	-4.55	116.55	122.92
31	B	614	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
31	5	312	CLA	CMA-C3A-C2A	-4.55	95.47	113.83
43	6	303	A86	C41-C32-C31	4.55	114.55	110.47
43	14	301	A86	C10-C9-C8	4.55	137.42	123.22
45	2	308	KC2	C1B-CHB-C4A	-4.55	116.25	126.06
43	2	303	A86	C28-C27-C26	-4.54	116.56	122.92
43	7	306	A86	C4-C5-C6	-4.54	120.83	127.31
42	5	313	KC1	CHB-C1B-C2B	-4.54	115.95	125.48
43	1	303	A86	C20-C19-C18	4.54	121.74	112.75
45	11	309	KC2	C1B-CHB-C4A	-4.54	116.26	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	302	A86	O4-C34-C33	4.54	118.90	107.59
45	16	312	KC2	CAA-C2A-C1A	4.54	145.62	124.75
38	0	317	LMG	O6-C5-C4	4.54	117.94	109.69
45	15	308	KC2	O2D-CGD-CBD	4.54	119.33	111.27
43	4	301	A86	O1-C15-C14	-4.54	104.11	113.21
42	0	315	KC1	CAA-C2A-C1A	4.54	145.60	124.75
43	11	319	A86	O4-C38-O5	-4.54	113.95	122.96
31	D	404	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
43	6	303	A86	C35-C34-C33	-4.53	101.97	109.88
43	16	304	A86	C35-C34-C33	-4.53	101.97	109.88
43	18	305	A86	O4-C38-C39	4.53	119.43	111.09
31	B	609	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
31	12	308	CLA	CMB-C2B-C3B	4.53	133.16	124.68
43	5	305	A86	C3-C4-C5	-4.53	114.19	123.47
43	12	305	A86	C23-C16-C17	-4.53	101.11	108.98
45	2	308	KC2	CHB-C1B-C2B	-4.53	115.98	125.48
42	0	315	KC1	CAC-C3C-C4C	4.53	130.68	124.81
43	17	316	A86	O4-C34-C35	4.53	118.86	107.59
45	19	309	KC2	C4C-C3C-C2C	-4.52	103.52	107.11
43	0	304	A86	C25-C26-C27	-4.52	120.86	127.31
35	A	409	PL9	C7-C3-C4	4.52	120.55	116.88
43	3	302	A86	C12-C11-C13	4.52	123.61	116.02
45	11	309	KC2	O2D-CGD-CBD	4.51	119.29	111.27
43	8	301	A86	C34-O4-C38	4.51	126.31	117.90
43	17	316	A86	C4-C3-C2	-4.51	114.23	123.47
45	3	311	KC2	C1A-NA-C4A	-4.51	104.68	106.71
31	15	307	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
43	15	302	A86	O4-C34-C33	4.50	118.81	107.59
43	2	304	A86	C25-C26-C27	-4.50	120.89	127.31
43	16	304	A86	O4-C34-C35	-4.50	96.38	107.59
43	8	305	A86	O1-C20-C19	4.50	116.76	113.38
45	16	312	KC2	C1B-CHB-C4A	-4.50	116.35	126.06
43	19	304	A86	O1-C20-C21	-4.50	109.67	115.06
45	6	312	KC2	C1B-CHB-C4A	-4.50	116.36	126.06
43	4	303	A86	C4-C5-C6	-4.50	120.89	127.31
31	16	311	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
45	1	309	KC2	CHC-C1C-NC	-4.49	117.13	124.20
43	12	305	A86	C35-C34-C33	-4.49	102.04	109.88
43	6	302	A86	C41-C32-C31	-4.49	106.45	110.47
43	11	304	A86	C17-C16-C15	4.49	113.74	109.16
43	19	306	A86	C35-C34-C33	-4.49	102.04	109.88
42	6	315	KC1	C4C-C3C-C2C	-4.49	100.36	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	4	308	KC2	C1B-CHB-C4A	-4.49	116.38	126.06
43	4	303	A86	O4-C38-C39	4.49	119.34	111.09
43	10	304	A86	C17-C16-C15	-4.49	104.59	109.16
45	18	308	KC2	CHB-C4A-NA	4.49	131.27	124.20
43	1	302	A86	O-C13-C14	-4.48	112.55	121.66
31	4	309	CLA	CMB-C2B-C3B	4.48	133.07	124.68
45	14	308	KC2	CHB-C1B-C2B	-4.48	116.08	125.48
44	p	612	DD6	C9-C8-C6	4.48	139.01	126.42
43	4	303	A86	C17-C16-C15	4.48	113.73	109.16
31	9	307	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
43	3	304	A86	C41-C32-C31	4.48	114.48	110.47
43	6	307	A86	O-C13-C14	4.48	130.76	121.66
31	2	312	CLA	CMB-C2B-C3B	4.48	133.06	124.68
43	1	306	A86	C3-C2-C1	-4.48	120.92	127.31
45	7	309	KC2	C1B-CHB-C4A	-4.48	116.40	126.06
31	11	315	CLA	CBC-CAC-C3C	4.48	124.77	112.43
45	15	310	KC2	CHD-C4C-NC	4.48	130.99	124.20
31	19	311	CLA	C2A-C1A-CHA	4.47	131.68	123.86
43	4	302	A86	C40-C32-C33	4.47	129.14	109.05
31	12	310	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
43	18	301	A86	O3-C36-C37	-4.47	101.43	109.39
42	2	313	KC1	O2D-CGD-CBD	4.47	119.21	111.27
45	15	308	KC2	C1B-CHB-C4A	-4.47	116.42	126.06
43	12	301	A86	C12-C11-C13	4.47	123.53	116.02
43	7	303	A86	C3-C2-C1	-4.47	120.94	127.31
43	0	304	A86	C17-C16-C15	-4.47	104.61	109.16
31	P	606	CLA	CMC-C2C-C1C	-4.47	118.24	125.04
43	13	302	A86	O4-C38-O5	-4.46	114.09	122.96
31	p	606	CLA	CMC-C2C-C1C	-4.46	118.24	125.04
31	3	307	CLA	CMB-C2B-C1B	-4.46	121.60	128.46
31	15	309	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
45	13	309	KC2	CHB-C4A-NA	4.46	131.23	124.20
43	19	301	A86	C34-O4-C38	4.46	126.20	117.90
45	17	309	KC2	CHB-C4A-C3A	-4.46	118.02	124.98
43	0	302	A86	C17-C16-C15	4.46	113.71	109.16
32	D	402	PHO	CMB-C2B-C3B	4.45	133.01	124.68
43	11	303	A86	C20-C19-C18	4.45	121.56	112.75
45	5	308	KC2	CHB-C1B-C2B	-4.45	116.14	125.48
42	2	313	KC1	C1B-CHB-C4A	-4.45	116.46	126.06
35	a	409	PL9	C7-C3-C4	4.45	120.49	116.88
45	5	308	KC2	CHB-C4A-C3A	-4.45	118.03	124.98
43	11	305	A86	C40-C32-C31	-4.45	106.49	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	314	KC1	O2D-CGD-CBD	4.45	119.17	111.27
43	1	304	A86	C3-C2-C1	-4.45	120.97	127.31
43	6	302	A86	O-C13-C14	-4.44	112.63	121.66
45	18	310	KC2	CHB-C1B-C2B	-4.44	116.16	125.48
45	8	308	KC2	CHB-C4A-NA	4.44	131.20	124.20
31	5	307	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
42	0	315	KC1	C2A-C1A-NA	4.44	116.52	109.40
31	0	312	CLA	CBC-CAC-C3C	4.44	124.67	112.43
32	d	402	PHO	CMB-C2B-C3B	4.44	132.98	124.68
31	c	510	CLA	CMB-C2B-C3B	4.44	132.98	124.68
31	B	612	CLA	CMB-C2B-C3B	4.44	132.98	124.68
31	b	613	CLA	CMB-C2B-C3B	4.44	132.98	124.68
38	5	316	LMG	O6-C1-O1	-4.44	99.47	109.97
31	8	312	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
45	14	308	KC2	C1B-CHB-C4A	-4.43	116.50	126.06
43	12	302	A86	O-C13-C11	-4.43	111.36	121.15
31	C	510	CLA	CMB-C2B-C3B	4.43	132.97	124.68
34	A	411	SQD	C4-C3-C2	4.43	118.56	110.82
38	d	403	LMG	O1-C1-C2	-4.43	101.39	108.30
45	8	310	KC2	CHB-C1B-C2B	-4.43	116.19	125.48
31	C	502	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
43	11	320	A86	O3-C36-C37	-4.43	101.51	109.39
31	16	314	CLA	CHA-C4D-ND	4.42	141.75	132.50
45	8	308	KC2	CHD-C4C-NC	-4.42	117.49	124.20
43	17	305	A86	O1-C15-C20	-4.42	55.08	59.40
31	6	311	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
45	15	310	KC2	C1B-CHB-C4A	-4.42	116.52	126.06
31	7	313	CLA	CAA-CBA-CGA	-4.42	100.34	113.25
43	13	303	A86	C3-C2-C1	-4.42	121.00	127.31
43	0	301	A86	C41-C32-C31	-4.42	106.52	110.47
43	16	302	A86	O1-C20-C21	-4.42	109.76	115.06
43	13	304	A86	O-C13-C14	4.42	130.63	121.66
31	C	514	CLA	CMB-C2B-C1B	-4.42	121.68	128.46
45	11	311	KC2	C4B-C3B-C2B	-4.41	103.13	106.75
43	16	302	A86	O2-C18-C17	4.41	118.57	109.80
45	13	309	KC2	C1B-CHB-C4A	-4.41	116.54	126.06
43	12	306	A86	C9-C8-C6	-4.41	114.02	126.42
43	4	302	A86	C25-C26-C27	-4.41	121.02	127.31
31	19	315	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
31	c	502	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
43	11	320	A86	O1-C20-C19	4.41	116.69	113.38
34	i	101	SQD	C4-C3-C2	4.41	118.52	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	0	318	SQD	C4-C3-C2	4.41	118.52	110.82
43	18	303	A86	O4-C38-C39	4.41	119.20	111.09
43	6	307	A86	C25-C24-C1	-4.41	114.04	126.42
31	6	314	CLA	CMB-C2B-C3B	4.40	132.92	124.68
45	1	309	KC2	CAC-C3C-C2C	-4.40	114.09	128.60
43	13	304	A86	C9-C8-C6	-4.40	114.05	126.42
45	3	311	KC2	CHB-C4A-NA	4.40	131.13	124.20
43	9	304	A86	C3-C2-C1	-4.40	121.03	127.31
31	10	307	CLA	C4A-NA-C1A	4.40	108.68	106.71
42	P	609	KC1	CHB-C1B-C2B	-4.40	116.26	125.48
31	13	308	CLA	CMB-C2B-C3B	4.39	132.90	124.68
42	9	314	KC1	C1B-CHB-C4A	-4.39	116.58	126.06
43	6	303	A86	C3-C2-C1	-4.39	121.05	127.31
42	5	313	KC1	O2D-CGD-CBD	4.39	119.06	111.27
31	7	313	CLA	CMB-C2B-C3B	4.39	132.89	124.68
42	p	609	KC1	CHB-C1B-C2B	-4.39	116.28	125.48
43	1	303	A86	C25-C26-C27	-4.39	121.05	127.31
31	b	605	CLA	CAC-C3C-C2C	4.39	135.03	127.53
45	7	311	KC2	CHB-C4A-NA	4.38	131.11	124.20
31	10	316	CLA	CMB-C2B-C1B	-4.38	121.72	128.46
31	9	312	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
42	p	609	KC1	C1B-CHB-C4A	-4.38	116.60	126.06
45	13	311	KC2	C1B-CHB-C4A	-4.38	116.60	126.06
43	6	307	A86	O4-C38-C39	4.38	119.15	111.09
45	13	311	KC2	CBD-CHA-C1A	4.38	137.05	128.88
43	9	302	A86	C23-C16-C22	-4.38	100.91	107.37
45	11	309	KC2	C2A-C1A-NA	4.38	116.43	109.40
43	2	302	A86	C3-C2-C1	-4.38	121.06	127.31
31	P	604	CLA	CMB-C2B-C3B	4.38	132.87	124.68
31	19	312	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
42	P	609	KC1	C1B-CHB-C4A	-4.38	116.61	126.06
43	3	306	A86	O4-C38-O5	-4.38	114.26	122.96
45	9	309	KC2	C4C-C3C-C2C	-4.38	103.64	107.11
45	0	310	KC2	O2D-CGD-O1D	-4.38	115.28	123.84
43	18	301	A86	O1-C15-C20	-4.38	55.12	59.40
43	1	305	A86	C25-C26-C27	-4.38	121.06	127.31
31	B	604	CLA	CAC-C3C-C2C	4.38	135.02	127.53
31	p	602	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
42	2	313	KC1	C3C-C4C-NC	4.38	114.00	109.88
31	c	514	CLA	CMB-C2B-C1B	-4.38	121.74	128.46
43	0	301	A86	C25-C26-C27	-4.38	121.07	127.31
43	16	302	A86	C17-C16-C15	4.37	113.63	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	303	A86	O-C13-C14	-4.37	112.77	121.66
43	10	301	A86	C41-C32-C31	-4.37	106.56	110.47
43	7	306	A86	C36-C31-C32	-4.37	115.36	119.70
43	4	306	A86	O1-C20-C21	-4.37	109.82	115.06
43	13	302	A86	C25-C26-C27	-4.37	121.07	127.31
42	10	315	KC1	CHB-C1B-C2B	-4.37	116.31	125.48
31	15	311	CLA	O2D-CGD-O1D	-4.36	115.30	123.84
45	17	309	KC2	CHD-C4C-C3C	-4.36	110.29	126.11
45	12	311	KC2	C1B-CHB-C4A	-4.36	116.65	126.06
31	P	602	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
43	1	319	A86	O1-C20-C19	4.36	116.66	113.38
45	14	310	KC2	O2D-CGD-CBD	4.36	119.01	111.27
31	p	604	CLA	CMB-C2B-C3B	4.36	132.83	124.68
43	17	306	A86	C33-C32-C31	-4.36	104.98	109.21
43	14	302	A86	O4-C38-C39	4.35	119.10	111.09
43	10	301	A86	C17-C16-C15	-4.35	104.72	109.16
34	a	408	SQD	O7-S-C6	4.35	112.11	106.94
31	11	307	CLA	O2D-CGD-O1D	-4.35	115.33	123.84
42	1	314	KC1	CAA-C2A-C1A	4.35	144.74	124.75
45	16	310	KC2	CHD-C4C-C3C	-4.35	110.35	126.11
38	15	315	LMG	O6-C1-O1	-4.35	99.68	109.97
31	19	310	CLA	CMB-C2B-C3B	4.35	132.81	124.68
44	p	612	DD6	C14-C13-C11	-4.35	118.78	125.53
45	6	310	KC2	CHD-C4C-C3C	-4.35	110.36	126.11
43	10	305	A86	C4-C5-C6	-4.35	121.11	127.31
42	12	314	KC1	CAA-C2A-C1A	4.35	144.72	124.75
43	15	303	A86	O1-C20-C19	4.34	116.65	113.38
42	19	314	KC1	C3C-C4C-NC	4.34	113.97	109.88
43	11	320	A86	C36-C31-C32	-4.34	115.39	119.70
34	A	408	SQD	O7-S-C6	4.34	112.10	106.94
31	b	604	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
43	14	304	A86	C28-C27-C26	-4.34	116.84	122.92
31	B	608	CLA	CMB-C2B-C3B	4.34	132.80	124.68
43	11	303	A86	C3-C2-C1	-4.34	121.12	127.31
31	9	315	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
31	2	314	CLA	CAA-C2A-C3A	-4.34	105.98	116.10
45	17	311	KC2	CHB-C1B-C2B	-4.34	116.39	125.48
43	7	301	A86	O-C13-C14	-4.33	112.86	121.66
42	14	313	KC1	CHB-C4A-NA	4.33	131.03	124.20
45	17	309	KC2	C1B-CHB-C4A	-4.33	116.71	126.06
45	7	309	KC2	CHD-C4C-C3C	-4.33	110.41	126.11
43	5	305	A86	C23-C16-C22	-4.33	100.98	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	13	311	KC2	CHB-C4A-NA	4.33	131.03	124.20
42	17	314	KC1	O2D-CGD-CBD	4.33	118.96	111.27
31	B	604	CLA	CMC-C2C-C3C	4.33	137.87	126.12
43	9	301	A86	C28-C27-C26	-4.33	116.86	122.92
45	1	309	KC2	C3C-C2C-C1C	4.33	109.69	106.49
31	z	103	CLA	CMB-C2B-C1B	-4.33	121.82	128.46
43	5	303	A86	O1-C15-C20	-4.32	55.17	59.40
31	14	309	CLA	CMB-C2B-C3B	4.32	132.76	124.68
43	19	304	A86	O4-C38-O5	-4.32	114.38	122.96
45	7	309	KC2	CHB-C1B-C2B	-4.32	116.42	125.48
43	9	302	A86	C4-C5-C6	-4.32	121.15	127.31
42	11	314	KC1	C1B-CHB-C4A	-4.31	116.75	126.06
45	17	311	KC2	O2D-CGD-CBD	4.31	118.93	111.27
43	3	301	A86	C20-C19-C18	4.31	121.28	112.75
45	4	310	KC2	O2D-CGD-CBD	4.31	118.93	111.27
31	b	605	CLA	CMC-C2C-C3C	4.31	137.82	126.12
43	3	301	A86	C9-C10-C11	-4.31	113.94	126.61
43	1	320	A86	O4-C38-O5	-4.31	114.40	122.96
43	12	305	A86	C25-C26-C27	-4.31	121.16	127.31
31	B	603	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
43	9	306	A86	C28-C27-C29	4.31	128.91	118.93
38	5	316	LMG	O1-C1-C2	-4.30	101.58	108.30
36	18	316	LHG	O4-P-O5	4.30	133.50	112.24
42	13	314	KC1	OBD-CAD-C3D	-4.30	120.84	127.98
42	12	314	KC1	C3C-C4C-NC	4.30	113.92	109.88
43	11	319	A86	C25-C26-C27	-4.30	121.17	127.31
36	a	410	LHG	O4-P-O5	4.30	133.49	112.24
43	19	301	A86	C28-C27-C26	-4.30	116.91	122.92
31	6	308	CLA	CAC-C3C-C4C	4.30	130.38	124.81
31	b	609	CLA	CMB-C2B-C3B	4.30	132.72	124.68
36	A	410	LHG	O4-P-O5	4.29	133.47	112.24
43	7	305	A86	O1-C20-C19	4.29	116.61	113.38
45	2	310	KC2	CHD-C4C-NC	4.29	130.72	124.20
43	9	305	A86	C25-C26-C27	-4.29	121.19	127.31
45	1	311	KC2	C4B-C3B-C2B	-4.29	103.23	106.75
43	9	306	A86	C3-C2-C1	-4.29	121.19	127.31
43	16	305	A86	C35-C34-C33	-4.29	102.39	109.88
39	B	621	DGD	C1E-O6E-C5E	4.29	122.11	113.69
42	1	314	KC1	CHB-C4A-NA	4.29	130.96	124.20
43	19	305	A86	C35-C34-C33	-4.29	102.40	109.88
43	10	302	A86	O4-C38-C39	4.29	118.97	111.09
43	1	304	A86	C35-C34-C33	-4.29	102.40	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	1	314	KC1	O2D-CGD-CBD	4.29	118.88	111.27
42	11	314	KC1	CHB-C4A-NA	4.29	130.96	124.20
43	17	305	A86	O-C13-C11	-4.28	111.68	121.15
31	17	313	CLA	C2D-C1D-ND	-4.28	106.95	110.10
36	8	316	LHG	O4-P-O5	4.28	133.41	112.24
31	16	314	CLA	CMD-C2D-C3D	-4.28	117.76	127.61
45	13	309	KC2	CHB-C1B-C2B	-4.28	116.50	125.48
31	7	308	CLA	CAA-C2A-C3A	-4.28	106.11	116.10
43	7	303	A86	C41-C32-C31	4.28	114.30	110.47
43	13	306	A86	C14-C15-C16	4.28	135.14	118.75
31	3	310	CLA	CMB-C2B-C3B	4.28	132.68	124.68
43	0	301	A86	C3-C2-C1	-4.28	121.20	127.31
43	5	304	A86	C28-C27-C26	-4.28	116.93	122.92
42	19	314	KC1	C1B-CHB-C4A	-4.28	116.83	126.06
43	12	302	A86	C25-C26-C27	-4.28	121.21	127.31
42	11	314	KC1	CAA-C2A-C1A	4.27	144.39	124.75
42	4	313	KC1	CHB-C4A-NA	4.27	130.94	124.20
43	11	305	A86	C3-C4-C5	-4.27	114.72	123.47
34	A	411	SQD	O9-S-C6	4.27	112.02	106.94
43	4	302	A86	O1-C20-C21	4.27	120.17	115.06
31	9	310	CLA	CMB-C2B-C3B	4.27	132.67	124.68
38	10	319	LMG	O6-C5-C4	4.27	117.45	109.69
34	i	101	SQD	O9-S-C6	4.27	112.01	106.94
45	8	310	KC2	C2A-C3A-C4A	4.26	109.65	106.49
43	4	305	A86	C33-C32-C31	-4.26	105.07	109.21
43	3	306	A86	C19-C18-C17	-4.26	102.54	110.77
31	C	511	CLA	CMB-C2B-C3B	4.26	132.65	124.68
31	c	511	CLA	CMB-C2B-C3B	4.26	132.65	124.68
43	10	302	A86	C4-C5-C6	-4.26	121.23	127.31
31	11	307	CLA	O2D-CGD-CBD	4.26	118.84	111.27
45	5	308	KC2	CAA-C2A-C1A	4.26	144.31	124.75
31	B	611	CLA	CMB-C2B-C3B	4.26	132.64	124.68
43	11	306	A86	C35-C34-C33	-4.26	102.45	109.88
38	5	316	LMG	O6-C5-C4	4.26	117.42	109.69
31	18	312	CLA	CAA-C2A-C3A	-4.26	101.13	112.78
43	5	303	A86	C41-C32-C31	4.25	114.28	110.47
31	18	311	CLA	CGD-CBD-CAD	4.25	124.51	110.73
45	17	311	KC2	C2A-C3A-C4A	4.25	109.64	106.49
45	13	311	KC2	CHB-C1B-C2B	-4.25	116.56	125.48
31	0	316	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
45	12	311	KC2	C4B-C3B-C2B	-4.25	103.26	106.75
43	8	305	A86	C36-C31-C32	-4.25	115.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	302	A86	C19-C18-C17	4.25	118.98	110.77
42	14	313	KC1	C3C-C4C-NC	4.25	113.88	109.88
31	d	401	CLA	CMB-C2B-C3B	4.25	132.62	124.68
43	9	303	A86	C40-C32-C31	4.24	114.27	110.47
43	3	302	A86	C41-C32-C31	-4.24	106.67	110.47
36	4	317	LHG	O4-P-O5	4.24	133.21	112.24
43	8	302	A86	C35-C34-C33	-4.24	102.48	109.88
31	4	312	CLA	CMD-C2D-C1D	-4.24	117.24	124.71
31	D	401	CLA	CMB-C2B-C3B	4.24	132.61	124.68
43	14	304	A86	C35-C34-C33	4.24	117.27	109.88
31	P	610	CLA	CMB-C2B-C3B	4.24	132.60	124.68
36	C	521	LHG	O4-P-O5	4.24	133.18	112.24
45	11	309	KC2	C4B-C3B-C2B	-4.23	103.27	106.75
43	17	306	A86	O1-C20-C19	4.23	116.56	113.38
31	p	610	CLA	CMB-C2B-C3B	4.23	132.60	124.68
43	11	305	A86	C41-C32-C40	-4.23	95.55	108.53
36	w	202	LHG	O4-P-O5	4.23	133.14	112.24
43	7	302	A86	C4-C3-C2	-4.23	114.81	123.47
42	10	315	KC1	C1B-CHB-C4A	-4.23	116.94	126.06
31	5	309	CLA	CMB-C2B-C3B	4.23	132.58	124.68
43	19	303	A86	C41-C32-C31	4.22	114.25	110.47
42	11	314	KC1	C3C-C4C-NC	4.22	113.85	109.88
42	5	313	KC1	C1B-CHB-C4A	-4.22	116.95	126.06
43	17	302	A86	C28-C27-C26	-4.22	117.01	122.92
45	2	310	KC2	CHB-C1B-C2B	-4.22	116.62	125.48
43	9	304	A86	O1-C20-C21	-4.22	110.00	115.06
31	b	612	CLA	CMB-C2B-C3B	4.22	132.57	124.68
34	L	102	SQD	O9-S-C6	4.22	111.95	106.94
31	0	314	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
36	b	623	LHG	O4-P-O5	4.22	133.09	112.24
43	7	305	A86	C33-C32-C31	-4.22	105.11	109.21
43	11	303	A86	C25-C26-C27	-4.22	121.29	127.31
42	13	314	KC1	C1B-CHB-C4A	-4.21	116.97	126.06
43	10	305	A86	C19-C18-C17	-4.21	102.64	110.77
43	18	305	A86	C3-C2-C1	-4.21	121.30	127.31
43	15	302	A86	C4-C5-C6	-4.21	121.30	127.31
36	B	622	LHG	O4-P-O5	4.21	133.06	112.24
43	17	304	A86	C35-C34-C33	-4.21	102.53	109.88
31	10	312	CLA	CBC-CAC-C3C	4.21	124.04	112.43
42	2	313	KC1	CHB-C1B-C2B	-4.21	116.65	125.48
43	18	304	A86	O4-C34-C35	4.21	118.07	107.59
31	2	309	CLA	CMB-C2B-C3B	4.21	132.55	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	P	609	KC1	C4B-C3B-C2B	-4.21	103.30	106.75
36	14	317	LHG	O4-P-O5	4.21	133.04	112.24
43	19	304	A86	C4-C5-C6	-4.21	121.31	127.31
34	i	101	SQD	O5-C5-C4	4.21	117.33	109.69
43	14	304	A86	O4-C34-C33	4.20	118.06	107.59
42	10	315	KC1	O2D-CGD-CBD	4.20	118.74	111.27
43	4	302	A86	O-C13-C14	-4.20	113.12	121.66
42	3	314	KC1	O2D-CGD-CBD	4.20	118.74	111.27
45	8	308	KC2	CHD-C4C-C3C	-4.20	110.88	126.11
39	1	318	DGD	O3G-C3G-C2G	-4.20	100.76	110.90
31	a	404	CLA	CMB-C2B-C3B	4.20	132.54	124.68
34	A	411	SQD	O5-C5-C4	4.20	117.32	109.69
39	b	622	DGD	C1E-O6E-C5E	4.20	121.93	113.69
31	9	313	CLA	CMB-C2B-C3B	4.20	132.53	124.68
43	11	302	A86	C28-C27-C26	-4.20	117.05	122.92
43	3	302	A86	O-C13-C14	-4.20	113.13	121.66
43	4	302	A86	C35-C34-C33	-4.20	102.56	109.88
31	5	312	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
43	15	303	A86	O1-C15-C20	-4.20	55.30	59.40
43	13	303	A86	C41-C32-C31	4.19	114.23	110.47
43	8	302	A86	O1-C15-C20	-4.19	55.30	59.40
36	d	407	LHG	O4-P-O5	4.19	132.97	112.24
45	15	310	KC2	CHB-C4A-NA	4.19	130.81	124.20
43	11	302	A86	O4-C34-C33	4.19	118.03	107.59
31	4	315	CLA	CMA-C3A-C4A	-4.19	100.51	111.77
36	8	315	LHG	O4-P-O5	4.19	132.94	112.24
31	18	312	CLA	C4D-C3D-CAD	-4.19	103.16	108.10
31	0	313	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
36	18	315	LHG	O4-P-O5	4.18	132.93	112.24
36	D	407	LHG	O4-P-O5	4.18	132.93	112.24
31	p	603	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
43	1	319	A86	C4-C5-C6	-4.18	121.34	127.31
31	17	315	CLA	CAA-C2A-C3A	-4.18	106.34	116.10
39	W	203	DGD	O3G-C3G-C2G	-4.18	100.81	110.90
31	b	607	CLA	CHB-C4A-NA	4.18	130.29	124.51
43	9	301	A86	C25-C26-C27	-4.18	121.34	127.31
45	2	308	KC2	CHD-C4C-C3C	-4.18	110.96	126.11
36	p	615	LHG	O4-P-O5	4.18	132.90	112.24
31	A	404	CLA	CMB-C2B-C3B	4.18	132.50	124.68
42	p	609	KC1	C4B-C3B-C2B	-4.18	103.32	106.75
31	0	313	CLA	CAA-C2A-C1A	4.18	121.39	112.14
43	3	305	A86	O4-C38-C39	4.18	118.77	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	603	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
42	13	314	KC1	C4C-C3C-C2C	-4.18	100.81	106.90
36	15	316	LHG	O4-P-O5	4.17	132.87	112.24
31	9	311	CLA	C2A-C1A-CHA	4.17	131.15	123.86
45	17	309	KC2	CHB-C1B-C2B	-4.17	116.73	125.48
31	19	308	CLA	CMB-C2B-C3B	4.17	132.48	124.68
36	P	615	LHG	O4-P-O5	4.17	132.85	112.24
43	10	303	A86	O2-C18-C19	-4.17	101.52	109.80
43	3	301	A86	C3-C4-C5	-4.17	114.94	123.47
43	1	306	A86	C35-C34-C33	-4.16	102.61	109.88
43	14	305	A86	O4-C34-C35	-4.16	97.22	107.59
39	w	204	DGD	O3G-C3G-C2G	-4.16	100.86	110.90
43	9	305	A86	C35-C34-C33	-4.16	102.61	109.88
43	6	303	A86	C4-C5-C6	-4.16	121.37	127.31
45	19	309	KC2	C1B-CHB-C4A	-4.16	117.09	126.06
45	3	311	KC2	CHB-C1B-C2B	-4.16	116.76	125.48
43	17	302	A86	O-C13-C14	-4.16	113.21	121.66
43	0	302	A86	O4-C38-C39	4.16	118.74	111.09
42	19	314	KC1	CHB-C4A-NA	4.16	130.75	124.20
43	10	303	A86	O1-C20-C19	4.16	116.50	113.38
43	0	306	A86	C35-C34-C33	-4.16	102.62	109.88
36	5	317	LHG	O4-P-O5	4.16	132.78	112.24
45	5	310	KC2	CHB-C4A-NA	4.16	130.75	124.20
31	18	307	CLA	C7-C6-C5	-4.15	102.08	113.36
31	c	512	CLA	CMD-C2D-C1D	-4.15	117.40	124.71
43	17	304	A86	C4-C5-C6	-4.15	121.39	127.31
31	7	313	CLA	CAA-C2A-C3A	-4.15	101.42	112.78
31	10	316	CLA	CMB-C2B-C3B	4.15	132.44	124.68
44	P	612	DD6	C21-C20-C15	-4.15	115.31	122.26
42	9	314	KC1	CHB-C4A-NA	4.15	130.74	124.20
45	12	309	KC2	CHB-C4A-NA	4.15	130.74	124.20
34	10	320	SQD	C4-C3-C2	4.15	118.06	110.82
31	2	306	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
43	17	303	A86	C3-C2-C1	-4.15	121.39	127.31
43	19	304	A86	C28-C27-C26	-4.14	117.12	122.92
45	9	309	KC2	C1B-CHB-C4A	-4.14	117.12	126.06
31	4	311	CLA	CMB-C2B-C3B	4.14	132.43	124.68
31	16	314	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
36	l	102	LHG	O4-P-O5	4.14	132.72	112.24
36	L	101	LHG	O4-P-O5	4.14	132.72	112.24
43	19	301	A86	C25-C26-C27	-4.14	121.40	127.31
43	13	306	A86	C22-C16-C17	-4.14	101.79	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	302	A86	C41-C32-C31	-4.14	106.77	110.47
43	14	301	A86	C25-C26-C27	4.14	133.22	127.31
43	8	305	A86	C4-C5-C6	-4.14	121.40	127.31
43	1	303	A86	O-C13-C11	-4.14	112.01	121.15
45	3	311	KC2	CAA-C2A-C1A	4.14	143.76	124.75
43	8	305	A86	C20-C19-C18	4.14	120.94	112.75
43	10	301	A86	C3-C2-C1	-4.14	121.41	127.31
43	18	301	A86	C3-C2-C1	-4.14	121.41	127.31
43	11	306	A86	C25-C26-C27	-4.14	121.41	127.31
31	11	315	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
43	2	301	A86	C20-C19-C18	4.14	120.93	112.75
31	2	306	CLA	O2D-CGD-O1D	-4.13	115.75	123.84
43	6	306	A86	C20-C19-C18	4.13	120.93	112.75
31	B	606	CLA	CHB-C4A-NA	4.13	130.23	124.51
45	10	310	KC2	CBC-CAC-C3C	-4.13	107.06	127.62
43	6	303	A86	O1-C15-C20	-4.13	55.36	59.40
43	12	301	A86	C17-C16-C15	-4.13	104.95	109.16
43	16	304	A86	C34-O4-C38	4.13	125.59	117.90
43	7	306	A86	C25-C26-C27	-4.13	121.41	127.31
43	8	301	A86	O-C13-C11	-4.13	112.02	121.15
43	5	305	A86	O1-C20-C21	-4.13	110.11	115.06
43	2	303	A86	C3-C4-C5	-4.13	115.02	123.47
43	3	303	A86	C25-C26-C27	-4.13	121.42	127.31
44	p	612	DD6	C7-C6-C8	-4.13	111.57	118.08
43	4	305	A86	O4-C38-C39	4.13	118.68	111.09
43	13	304	A86	C19-C18-C17	4.13	118.74	110.77
43	15	302	A86	C3-C2-C1	-4.12	121.42	127.31
31	A	406	CLA	CMB-C2B-C3B	4.12	132.39	124.68
43	5	302	A86	C34-O4-C38	4.12	125.58	117.90
43	16	307	A86	C20-C19-C18	4.12	120.91	112.75
43	5	318	A86	C35-C34-C33	-4.12	102.68	109.88
43	12	302	A86	O1-C20-C19	4.12	116.48	113.38
31	9	313	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
43	19	303	A86	C4-C5-C6	-4.12	121.43	127.31
31	11	307	CLA	C2D-C1D-ND	-4.12	107.07	110.10
31	10	317	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
43	13	301	A86	C41-C32-C31	-4.12	106.79	110.47
43	1	302	A86	C9-C8-C6	-4.12	114.85	126.42
39	B	621	DGD	O6E-C5E-C4E	4.12	117.17	109.69
45	3	309	KC2	CHD-C4C-C3C	-4.11	111.20	126.11
45	5	310	KC2	CBD-CHA-C1A	4.11	136.54	128.88
43	2	302	A86	C17-C16-C15	-4.11	104.97	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	13	307	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
31	C	512	CLA	CMD-C2D-C1D	-4.11	117.47	124.71
43	3	305	A86	C4-C3-C2	-4.11	115.06	123.47
31	a	406	CLA	CMB-C2B-C3B	4.11	132.36	124.68
43	8	301	A86	C14-C15-C16	4.11	134.47	118.75
43	1	304	A86	C4-C5-C6	-4.11	121.45	127.31
45	13	311	KC2	C4B-C3B-C2B	-4.10	103.38	106.75
31	C	504	CLA	CMB-C2B-C3B	4.10	132.36	124.68
31	c	504	CLA	CMB-C2B-C3B	4.10	132.36	124.68
43	15	304	A86	C19-C18-C17	4.10	118.70	110.77
43	12	306	A86	C25-C24-C1	-4.10	114.89	126.42
43	17	316	A86	C20-C19-C18	4.10	120.86	112.75
43	0	305	A86	C19-C18-C17	-4.10	102.85	110.77
43	12	305	A86	O4-C38-C39	4.10	118.64	111.09
45	16	312	KC2	CHB-C4A-NA	4.10	130.66	124.20
45	10	310	KC2	CHB-C4A-NA	4.10	130.66	124.20
31	P	606	CLA	C3D-C4D-ND	4.10	116.87	110.24
31	10	314	CLA	C2D-C1D-ND	-4.10	107.08	110.10
43	5	318	A86	O4-C38-C39	4.10	118.63	111.09
31	14	311	CLA	CMB-C2B-C3B	4.10	132.34	124.68
36	Z	103	LHG	O4-P-O5	4.10	132.49	112.24
31	p	606	CLA	C3D-C4D-ND	4.10	116.86	110.24
31	4	312	CLA	CMD-C2D-C3D	4.10	137.03	127.61
45	5	310	KC2	C4B-C3B-C2B	-4.09	103.39	106.75
45	16	310	KC2	CHB-C4A-NA	4.09	130.65	124.20
43	19	306	A86	C25-C26-C27	-4.09	121.47	127.31
31	b	603	CLA	CMB-C2B-C3B	4.09	132.34	124.68
31	4	307	CLA	CMB-C2B-C3B	4.09	132.33	124.68
38	15	315	LMG	O1-C7-C8	-4.09	101.03	110.90
45	18	308	KC2	CHD-C4C-C3C	-4.09	111.30	126.11
45	0	310	KC2	CBC-CAC-C3C	-4.08	107.30	127.62
45	15	308	KC2	CAC-C3C-C2C	-4.08	115.15	128.60
43	8	301	A86	O2-C18-C19	-4.08	101.69	109.80
36	z	102	LHG	O4-P-O5	4.08	132.42	112.24
43	9	302	A86	C25-C26-C27	-4.08	121.48	127.31
43	12	302	A86	C3-C2-C1	-4.08	121.49	127.31
31	8	306	CLA	CMB-C2B-C3B	4.08	132.31	124.68
43	7	305	A86	C20-C19-C18	4.08	120.81	112.75
31	15	306	CLA	CAA-C2A-C3A	-4.08	104.08	114.26
43	15	301	A86	O4-C38-O5	-4.07	114.87	122.96
34	l	101	SQD	O9-S-C6	4.07	111.78	106.94
43	8	302	A86	C4-C5-C6	-4.07	121.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	13	304	A86	C40-C32-C31	-4.07	106.83	110.47
31	15	306	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
45	19	309	KC2	C4B-C3B-C2B	-4.07	103.41	106.75
31	b	617	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
43	9	305	A86	C4-C5-C6	-4.07	121.50	127.31
43	10	305	A86	O1-C15-C20	-4.07	55.42	59.40
31	B	616	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
42	13	314	KC1	CHB-C1B-C2B	-4.06	116.96	125.48
43	8	305	A86	C23-C16-C22	4.06	113.36	107.37
45	6	312	KC2	CHB-C4A-NA	4.06	130.60	124.20
43	11	305	A86	C14-C15-C16	4.06	134.31	118.75
45	6	310	KC2	CHB-C4A-NA	4.06	130.60	124.20
43	16	305	A86	C28-C27-C26	-4.06	117.24	122.92
38	P	614	LMG	O6-C5-C4	4.06	117.06	109.69
43	10	304	A86	O4-C38-O5	-4.05	114.91	122.96
42	4	313	KC1	C3C-C4C-NC	4.05	113.69	109.88
31	B	602	CLA	CMB-C2B-C3B	4.05	132.26	124.68
43	5	305	A86	C25-C26-C27	-4.05	121.53	127.31
43	13	305	A86	C4-C5-C6	-4.05	121.53	127.31
45	1	309	KC2	CHD-C4C-C3C	-4.05	111.44	126.11
31	0	316	CLA	CMB-C2B-C3B	4.05	132.25	124.68
31	B	606	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
39	b	622	DGD	O6E-C5E-C4E	4.05	117.04	109.69
31	2	306	CLA	CMB-C2B-C3B	4.04	132.25	124.68
43	0	305	A86	O1-C15-C20	-4.04	55.45	59.40
31	15	309	CLA	CMB-C2B-C3B	4.04	132.24	124.68
45	19	309	KC2	CAB-C3B-C4B	-4.04	115.14	124.90
45	5	310	KC2	CAA-C2A-C1A	4.04	143.32	124.75
43	1	305	A86	C40-C32-C31	-4.04	106.86	110.47
43	4	305	A86	C12-C11-C13	4.04	122.81	116.02
43	0	304	A86	O4-C38-O5	-4.04	114.94	122.96
43	9	301	A86	C17-C16-C15	-4.03	105.05	109.16
43	9	304	A86	C34-O4-C38	4.03	125.41	117.90
42	10	315	KC1	C3A-C4A-NA	4.03	114.98	110.57
43	P	611	A86	C26-C25-C24	-4.03	110.63	123.22
45	7	309	KC2	CHB-C4A-NA	4.03	130.56	124.20
31	15	313	CLA	CAA-C2A-C3A	-4.03	106.69	116.10
31	0	309	CLA	CBC-CAC-C3C	4.03	123.54	112.43
43	7	302	A86	O1-C15-C20	-4.03	55.46	59.40
43	1	302	A86	O4-C38-C39	4.03	118.50	111.09
43	7	305	A86	C19-C18-C17	-4.03	103.00	110.77
43	17	316	A86	C40-C32-C31	4.03	114.08	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	305	A86	O4-C34-C35	4.02	117.62	107.59
43	1	305	A86	C41-C32-C40	-4.02	96.18	108.53
43	p	611	A86	C26-C25-C24	-4.02	110.66	123.22
31	0	307	CLA	C4A-NA-C1A	4.02	108.52	106.71
44	P	612	DD6	C21-C20-C19	4.02	118.81	114.28
43	7	304	A86	O-C13-C14	4.02	129.83	121.66
43	17	306	A86	C20-C19-C18	4.02	120.70	112.75
43	3	304	A86	C28-C27-C26	-4.02	117.29	122.92
43	0	303	A86	C3-C4-C5	-4.02	115.24	123.47
33	f	101	BCR	C3-C4-C5	-4.02	106.90	114.08
43	1	302	A86	C28-C27-C26	-4.02	117.29	122.92
43	9	304	A86	C4-C5-C6	-4.02	121.57	127.31
31	7	315	CLA	CAA-C2A-C3A	-4.02	106.72	116.10
42	16	301	KC1	C1B-CHB-C4A	-4.02	117.39	126.06
31	4	312	CLA	C4D-C3D-CAD	-4.02	103.36	108.10
45	2	308	KC2	CHB-C4A-NA	4.02	130.53	124.20
43	10	318	A86	C20-C19-C18	4.02	120.70	112.75
38	11	301	LMG	O6-C5-C4	4.02	116.99	109.69
43	8	303	A86	C25-C26-C27	-4.02	121.58	127.31
43	12	306	A86	O4-C38-C39	4.02	118.48	111.09
38	p	614	LMG	O6-C5-C4	4.01	116.98	109.69
31	9	308	CLA	CMB-C2B-C3B	4.01	132.19	124.68
42	16	301	KC1	CHB-C1B-C2B	-4.01	117.06	125.48
31	d	405	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
31	16	308	CLA	CAC-C3C-C4C	4.01	130.01	124.81
43	1	305	A86	C8-C6-C5	4.01	125.09	118.94
43	9	303	A86	C28-C27-C26	-4.01	117.31	122.92
43	0	304	A86	C21-C20-C19	-4.01	109.77	114.28
31	10	314	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
31	12	313	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
43	18	303	A86	C19-C18-C17	-4.01	103.04	110.77
44	p	612	DD6	C21-C20-C15	-4.01	115.55	122.26
31	11	315	CLA	CAA-C2A-C3A	-4.00	106.76	116.10
31	17	313	CLA	C4D-C3D-CAD	4.00	112.81	108.10
43	9	302	A86	C3-C2-C1	-4.00	121.60	127.31
38	1	301	LMG	O6-C5-C4	4.00	116.96	109.69
31	7	307	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
42	18	313	KC1	CHB-C4A-NA	4.00	130.51	124.20
33	F	101	BCR	C3-C4-C5	-4.00	106.93	114.08
42	14	313	KC1	C2A-C1A-NA	4.00	115.82	109.40
31	P	610	CLA	CAA-C2A-C3A	-4.00	106.76	116.10
43	0	301	A86	C12-C11-C13	4.00	122.74	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	7	304	A86	C33-C32-C31	4.00	113.09	109.21
42	5	313	KC1	C3C-C4C-NC	4.00	113.64	109.88
31	p	610	CLA	CAA-C2A-C3A	-4.00	106.78	116.10
43	17	303	A86	C41-C32-C31	-4.00	106.90	110.47
31	19	313	CLA	CMB-C2B-C3B	4.00	132.15	124.68
43	19	306	A86	C4-C5-C6	-3.99	121.61	127.31
31	5	314	CLA	CAA-C2A-C3A	-3.99	106.78	116.10
43	10	318	A86	C4-C5-C6	-3.99	121.61	127.31
45	15	308	KC2	C2A-C3A-C4A	3.99	109.45	106.49
42	19	314	KC1	CMD-C2D-C3D	3.99	132.15	124.68
31	17	308	CLA	CAA-C2A-C3A	-3.99	106.79	116.10
42	3	314	KC1	CHB-C4A-NA	3.99	130.49	124.20
43	11	319	A86	C20-C19-C18	3.99	120.64	112.75
43	10	303	A86	C3-C4-C5	-3.99	115.30	123.47
42	16	315	KC1	O2D-CGD-CBD	3.99	118.36	111.27
31	b	614	CLA	CMB-C2B-C3B	3.99	132.14	124.68
43	11	306	A86	C4-C5-C6	-3.99	121.62	127.31
31	D	405	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
43	7	301	A86	C3-C2-C1	-3.99	121.62	127.31
45	3	309	KC2	C1A-C2A-C3A	-3.99	103.95	107.11
31	16	311	CLA	CMB-C2B-C3B	3.98	132.13	124.68
43	1	320	A86	O3-C36-C37	-3.98	102.31	109.39
31	19	307	CLA	CMB-C2B-C3B	3.98	132.12	124.68
43	19	305	A86	C4-C5-C6	-3.98	121.63	127.31
43	0	301	A86	C21-C20-C19	-3.98	109.80	114.28
43	1	306	A86	C41-C32-C31	-3.98	106.91	110.47
45	0	310	KC2	CHB-C4A-NA	3.98	130.47	124.20
45	8	310	KC2	CBD-CHA-C1A	3.98	136.29	128.88
43	10	303	A86	O4-C38-O5	-3.98	115.06	122.96
43	10	306	A86	C3-C4-C5	-3.98	115.33	123.47
42	7	314	KC1	C1B-CHB-C4A	-3.97	117.48	126.06
42	17	314	KC1	C1B-CHB-C4A	-3.97	117.49	126.06
43	13	304	A86	C9-C10-C11	-3.97	114.93	126.61
43	17	316	A86	O3-C36-C37	-3.97	102.32	109.39
31	B	613	CLA	CMB-C2B-C3B	3.97	132.11	124.68
43	18	301	A86	O-C13-C14	3.97	129.73	121.66
43	14	301	A86	C9-C8-C6	3.97	137.57	126.42
39	C	520	DGD	O6D-C1D-O3G	-3.97	100.57	109.97
34	A	408	SQD	O5-C5-C4	3.97	116.91	109.69
43	11	305	A86	C8-C6-C5	3.97	125.03	118.94
43	5	303	A86	O1-C20-C19	3.97	116.36	113.38
43	10	305	A86	C20-C19-C18	3.97	120.61	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	18	305	A86	O1-C20-C19	-3.97	110.40	113.38
31	5	311	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
45	3	309	KC2	CMD-C2D-C1D	-3.97	122.37	128.46
43	1	306	A86	C40-C32-C31	3.97	114.02	110.47
43	13	305	A86	C35-C34-C33	-3.96	102.96	109.88
34	a	408	SQD	O5-C5-C4	3.96	116.89	109.69
43	16	304	A86	O2-C18-C17	3.96	117.68	109.80
43	13	305	A86	C3-C2-C1	-3.96	121.66	127.31
42	16	315	KC1	CHB-C4A-NA	3.96	130.44	124.20
31	2	306	CLA	CAC-C3C-C4C	3.96	129.95	124.81
45	5	308	KC2	CAC-C3C-C2C	-3.96	115.56	128.60
43	9	304	A86	O4-C38-O5	-3.96	115.10	122.96
45	17	311	KC2	C3B-C2B-C1B	-3.96	103.30	107.08
43	3	306	A86	C20-C19-C18	3.96	120.58	112.75
43	1	319	A86	C3-C2-C1	-3.96	121.66	127.31
43	5	301	A86	O4-C38-O5	-3.96	115.10	122.96
43	5	304	A86	O-C13-C14	-3.95	113.62	121.66
31	11	313	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
45	5	308	KC2	C4B-C3B-C2B	-3.95	103.51	106.75
31	9	307	CLA	CAC-C3C-C4C	3.95	129.94	124.81
43	17	301	A86	O3-C36-C37	-3.95	102.36	109.39
42	P	609	KC1	CAA-C2A-C1A	3.95	142.90	124.75
43	0	303	A86	O2-C18-C19	-3.95	101.95	109.80
43	0	306	A86	C3-C4-C5	-3.95	115.39	123.47
45	9	309	KC2	C4B-C3B-C2B	-3.95	103.51	106.75
42	12	314	KC1	C3D-CAD-CBD	-3.95	102.41	107.61
43	11	305	A86	C19-C18-C17	3.95	118.39	110.77
43	17	306	A86	C19-C18-C17	-3.94	103.16	110.77
45	7	311	KC2	CAA-C2A-C1A	3.94	142.88	124.75
43	11	319	A86	C28-C27-C26	-3.94	117.40	122.92
42	10	315	KC1	CAA-C2A-C1A	3.94	142.86	124.75
43	6	303	A86	C20-C19-C18	-3.94	104.95	112.75
31	1	321	CLA	O2A-C1-C2	3.94	118.99	108.64
43	19	301	A86	C17-C16-C15	-3.94	105.14	109.16
45	18	310	KC2	CBD-CHA-C1A	3.94	136.22	128.88
39	c	520	DGD	O6D-C1D-O3G	-3.94	100.64	109.97
42	p	609	KC1	CAA-C2A-C1A	3.94	142.84	124.75
39	c	519	DGD	O6D-C1D-O3G	-3.94	100.65	109.97
43	5	304	A86	C20-C19-C18	-3.94	104.96	112.75
43	16	303	A86	O1-C20-C21	3.94	119.77	115.06
31	14	315	CLA	CHB-C4A-NA	3.93	129.95	124.51
45	15	308	KC2	C2A-C1A-NA	3.93	115.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	17	313	CLA	CMB-C2B-C3B	3.93	132.03	124.68
45	15	310	KC2	C4B-C3B-C2B	-3.93	103.52	106.75
43	1	305	A86	C20-C19-C18	-3.93	104.97	112.75
43	14	301	A86	C-C1-C24	3.93	124.27	118.08
43	1	320	A86	C33-C32-C31	-3.93	105.39	109.21
43	13	302	A86	C12-C11-C13	3.93	122.62	116.02
43	5	305	A86	C4-C5-C6	-3.93	121.70	127.31
42	5	313	KC1	CAC-C3C-C4C	3.93	129.90	124.81
31	6	311	CLA	CMB-C2B-C3B	3.93	132.02	124.68
45	19	309	KC2	C2A-C1A-NA	3.93	115.70	109.40
43	4	303	A86	C3-C2-C1	-3.92	121.71	127.31
39	C	519	DGD	O6D-C1D-O3G	-3.92	100.68	109.97
41	V	201	HEM	CMB-C2B-C1B	-3.92	119.07	125.04
43	P	613	A86	O4-C34-C35	-3.92	97.83	107.59
43	0	305	A86	C20-C19-C18	3.92	120.51	112.75
43	6	304	A86	C35-C34-C33	-3.92	103.03	109.88
43	19	302	A86	C25-C24-C1	-3.92	115.40	126.42
31	b	607	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
31	14	307	CLA	CMB-C2B-C3B	3.92	132.01	124.68
31	11	312	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
43	10	306	A86	C4-C5-C6	-3.92	121.72	127.31
31	18	311	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
43	2	304	A86	O4-C34-C35	3.92	117.35	107.59
43	11	304	A86	C28-C27-C26	-3.92	117.44	122.92
38	b	621	LMG	C1-C2-C3	-3.92	101.84	110.00
43	p	613	A86	O4-C34-C35	-3.92	97.84	107.59
31	17	307	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
43	19	301	A86	C4-C5-C6	-3.91	121.73	127.31
31	B	611	CLA	C1C-C2C-C3C	3.91	111.07	106.96
43	16	303	A86	C9-C8-C6	-3.91	115.44	126.42
43	9	301	A86	C4-C5-C6	-3.91	121.73	127.31
43	5	301	A86	C33-C32-C31	3.91	113.01	109.21
42	9	314	KC1	C4B-C3B-C2B	-3.91	103.54	106.75
43	15	304	A86	C20-C19-C18	-3.91	105.02	112.75
43	5	318	A86	C14-C15-C16	3.91	133.71	118.75
45	15	308	KC2	CHD-C4C-C3C	-3.90	111.96	126.11
34	l	101	SQD	O7-S-C6	3.90	111.58	106.94
43	12	301	A86	C41-C32-C31	-3.90	106.98	110.47
38	B	620	LMG	C1-C2-C3	-3.90	101.87	110.00
43	2	301	A86	C35-C34-C33	-3.90	103.07	109.88
45	19	309	KC2	CAB-C3B-C2B	3.90	141.45	128.60
43	18	304	A86	C14-C15-C16	-3.90	103.83	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	305	A86	C33-C32-C31	-3.90	105.42	109.21
43	16	303	A86	O4-C38-O5	-3.90	115.22	122.96
42	16	315	KC1	C4C-C3C-C2C	-3.89	101.22	106.90
43	15	305	A86	C3-C4-C5	-3.89	115.50	123.47
43	2	305	A86	C20-C19-C18	3.89	120.45	112.75
45	5	308	KC2	CHD-C4C-NC	-3.89	118.30	124.20
31	13	310	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
43	8	301	A86	C21-C20-C19	-3.89	109.90	114.28
43	17	305	A86	O4-C38-C39	3.89	118.24	111.09
43	1	302	A86	C20-C19-C18	-3.89	105.06	112.75
43	11	306	A86	C19-C18-C17	3.89	118.28	110.77
31	3	310	CLA	CAA-C2A-C3A	-3.89	107.03	116.10
45	17	309	KC2	CHB-C4A-NA	3.89	130.33	124.20
43	8	301	A86	C28-C27-C26	-3.89	117.48	122.92
31	11	315	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
43	p	613	A86	C28-C27-C26	-3.88	117.48	122.92
43	P	613	A86	O1-C15-C20	-3.88	55.60	59.40
43	1	320	A86	C4-C5-C6	-3.88	121.77	127.31
43	3	303	A86	C12-C11-C13	3.88	122.54	116.02
43	0	302	A86	C4-C5-C6	-3.88	121.77	127.31
43	10	305	A86	C33-C32-C31	-3.88	105.44	109.21
31	5	306	CLA	CAC-C3C-C4C	3.88	129.84	124.81
43	3	305	A86	C14-C15-C16	-3.88	103.91	118.75
45	16	312	KC2	CHB-C1B-C2B	-3.88	117.35	125.48
31	c	503	CLA	CHB-C4A-NA	3.88	129.87	124.51
43	19	301	A86	O4-C38-O5	-3.88	115.26	122.96
43	2	304	A86	O4-C34-C33	3.87	117.24	107.59
43	11	320	A86	C4-C5-C6	-3.87	121.78	127.31
31	10	308	CLA	CAC-C3C-C4C	3.87	129.84	124.81
42	6	315	KC1	CHB-C1B-C2B	-3.87	117.36	125.48
43	17	302	A86	C3-C2-C1	-3.87	121.78	127.31
41	v	201	HEM	CMB-C2B-C1B	-3.87	119.14	125.04
43	16	307	A86	C3-C2-C1	-3.87	121.79	127.31
31	16	314	CLA	C3D-C2D-C1D	3.87	111.11	105.83
31	c	502	CLA	CMB-C2B-C3B	3.87	131.92	124.68
45	0	310	KC2	CMD-C2D-C3D	3.87	131.92	124.68
43	1	306	A86	C4-C5-C6	-3.87	121.79	127.31
45	6	312	KC2	CHB-C1B-C2B	-3.87	117.37	125.48
43	7	306	A86	C3-C2-C1	-3.87	121.79	127.31
43	p	613	A86	O1-C15-C20	-3.87	55.62	59.40
43	7	302	A86	C35-C34-C33	-3.87	103.13	109.88
31	C	502	CLA	CMB-C2B-C3B	3.87	131.91	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	307	CLA	CAA-C2A-C3A	-3.86	102.20	112.78
31	1	313	CLA	CMB-C2B-C3B	3.86	131.91	124.68
31	9	307	CLA	CMB-C2B-C3B	3.86	131.91	124.68
43	9	303	A86	C4-C5-C6	-3.86	121.80	127.31
31	C	514	CLA	CMB-C2B-C3B	3.86	131.90	124.68
43	5	304	A86	C14-C15-C16	3.86	133.54	118.75
42	18	313	KC1	C1B-CHB-C4A	-3.86	117.73	126.06
43	9	305	A86	C19-C18-C17	3.86	118.23	110.77
43	2	303	A86	C35-C34-C33	-3.86	103.14	109.88
45	17	311	KC2	CBD-CHA-C1A	3.86	136.07	128.88
43	1	305	A86	C9-C10-C11	-3.86	115.27	126.61
43	P	613	A86	C28-C27-C26	-3.86	117.52	122.92
45	12	309	KC2	CBC-CAC-C3C	-3.86	108.43	127.62
43	15	304	A86	C12-C11-C13	3.86	122.50	116.02
34	B	623	SQD	C4-C3-C2	3.86	117.55	110.82
31	12	310	CLA	CMB-C2B-C3B	3.86	131.89	124.68
45	12	311	KC2	C2A-C3A-C4A	3.85	109.34	106.49
31	10	312	CLA	CMB-C2B-C3B	3.85	131.89	124.68
45	5	308	KC2	CHD-C4C-C3C	-3.85	112.14	126.11
31	c	514	CLA	CMB-C2B-C3B	3.85	131.89	124.68
43	5	318	A86	C41-C32-C31	3.85	113.92	110.47
43	0	303	A86	O4-C38-O5	-3.85	115.31	122.96
31	b	607	CLA	CMA-C3A-C4A	3.85	122.12	111.77
31	11	316	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
43	10	318	A86	O4-C38-O5	-3.85	115.32	122.96
31	15	306	CLA	CAC-C3C-C4C	3.84	129.79	124.81
43	10	304	A86	C40-C32-C31	3.84	113.91	110.47
31	b	612	CLA	C1C-C2C-C3C	3.84	110.99	106.96
31	0	313	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
43	2	305	A86	O1-C15-C20	-3.84	55.64	59.40
42	16	301	KC1	CBD-CHA-C1A	3.84	136.04	128.88
43	3	302	A86	O4-C38-O5	-3.84	115.33	122.96
43	12	301	A86	O4-C38-O5	-3.84	115.34	122.96
34	0	318	SQD	O9-S-O7	-3.84	100.67	113.95
31	4	312	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
31	3	316	CLA	C1C-C2C-C3C	-3.83	102.92	106.96
31	C	503	CLA	CHB-C4A-NA	3.83	129.81	124.51
31	B	611	CLA	CAC-C3C-C4C	3.83	129.78	124.81
43	8	304	A86	C14-C15-C16	-3.83	104.08	118.75
43	10	304	A86	C21-C20-C19	-3.83	109.97	114.28
43	8	301	A86	C4-C3-C2	-3.83	115.63	123.47
45	1	309	KC2	C4B-C3B-C2B	-3.83	103.61	106.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	12	307	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
43	11	319	A86	C22-C16-C17	3.83	115.63	108.98
34	b	601	SQD	C4-C3-C2	3.83	117.50	110.82
43	6	306	A86	C3-C2-C1	-3.83	121.85	127.31
39	H	102	DGD	C1D-C2D-C3D	-3.83	102.03	110.00
31	10	313	CLA	CAA-C2A-C1A	3.82	120.61	112.14
34	10	320	SQD	O9-S-O7	-3.82	100.72	113.95
42	3	314	KC1	C4C-C3C-C2C	-3.82	101.33	106.90
43	8	302	A86	C3-C2-C1	-3.82	121.86	127.31
43	1	305	A86	C14-C15-C16	3.82	133.38	118.75
39	h	102	DGD	C1D-C2D-C3D	-3.82	102.05	110.00
43	19	305	A86	C19-C18-C17	3.82	118.14	110.77
43	2	304	A86	C14-C15-C16	-3.81	104.15	118.75
43	8	301	A86	C35-C34-C33	-3.81	103.22	109.88
31	11	307	CLA	C4A-NA-C1A	3.81	108.42	106.71
31	5	306	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
43	10	306	A86	C35-C34-C33	-3.81	103.23	109.88
31	b	612	CLA	CAC-C3C-C4C	3.81	129.75	124.81
42	5	313	KC1	C4B-C3B-C2B	-3.81	103.62	106.75
43	12	304	A86	C9-C8-C6	-3.81	115.72	126.42
43	15	302	A86	O4-C38-C39	3.80	118.09	111.09
45	9	309	KC2	CAB-C3B-C4B	-3.80	115.71	124.90
42	9	314	KC1	CMD-C2D-C3D	3.80	131.79	124.68
43	12	304	A86	C9-C10-C11	-3.80	115.43	126.61
31	19	315	CLA	CMB-C2B-C3B	3.80	131.79	124.68
42	6	315	KC1	CHB-C4A-NA	3.80	130.19	124.20
45	19	309	KC2	CHB-C4A-NA	3.80	130.19	124.20
31	b	615	CLA	CMB-C2B-C3B	3.79	131.77	124.68
43	0	306	A86	C4-C5-C6	-3.79	121.90	127.31
43	11	302	A86	C36-C31-C32	3.79	123.46	119.70
43	10	301	A86	C12-C11-C13	3.79	122.38	116.02
43	3	303	A86	O-C13-C11	-3.79	112.78	121.15
43	18	305	A86	C12-C11-C13	3.79	122.38	116.02
43	15	304	A86	C14-C15-C16	3.79	133.25	118.75
43	17	306	A86	C41-C32-C31	3.79	113.86	110.47
42	10	315	KC1	C3B-C2B-C1B	-3.79	103.46	107.08
43	8	304	A86	C3-C2-C1	-3.78	121.91	127.31
31	4	315	CLA	CHB-C4A-NA	3.78	129.74	124.51
31	17	307	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
45	7	309	KC2	CAA-C2A-C1A	3.78	142.12	124.75
43	17	302	A86	O4-C34-C35	3.78	117.00	107.59
45	9	309	KC2	CHB-C4A-NA	3.78	130.16	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	p	609	KC1	C1A-NA-C4A	-3.77	105.01	106.71
43	13	304	A86	C14-C15-C16	-3.77	104.30	118.75
43	8	305	A86	O4-C38-O5	-3.77	115.47	122.96
43	3	306	A86	O4-C34-C33	-3.77	98.20	107.59
31	8	312	CLA	C4A-NA-C1A	3.77	108.40	106.71
39	B	621	DGD	O5D-C6D-C5D	-3.77	102.07	109.05
43	15	301	A86	C4-C3-C2	-3.77	115.75	123.47
43	11	319	A86	C35-C34-C33	-3.77	103.30	109.88
43	17	301	A86	C9-C8-C6	-3.77	115.83	126.42
31	B	614	CLA	CMB-C2B-C3B	3.77	131.73	124.68
31	9	315	CLA	CMB-C2B-C3B	3.77	131.73	124.68
43	14	305	A86	C41-C32-C33	3.77	125.97	109.05
45	8	308	KC2	CAC-C3C-C4C	3.77	142.02	124.47
31	19	313	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
42	14	313	KC1	C2A-C3A-C4A	3.77	109.28	106.49
43	19	305	A86	C25-C26-C27	-3.77	121.94	127.31
43	13	301	A86	O4-C38-O5	-3.76	115.48	122.96
43	18	301	A86	O1-C20-C21	-3.76	110.55	115.06
43	4	306	A86	C3-C4-C5	-3.76	115.76	123.47
42	13	314	KC1	C2A-C1A-NA	3.76	115.44	109.40
38	p	614	LMG	C1-O6-C5	3.76	121.07	113.69
43	12	306	A86	C9-C10-C11	-3.76	115.55	126.61
43	4	301	A86	C40-C32-C31	3.76	113.84	110.47
43	16	302	A86	C14-C15-C16	3.76	133.15	118.75
31	10	317	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
31	z	103	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
43	11	302	A86	C4-C3-C2	-3.76	115.78	123.47
43	12	303	A86	C3-C4-C5	-3.76	115.78	123.47
31	b	610	CLA	CMB-C2B-C3B	3.76	131.71	124.68
43	15	305	A86	C25-C26-C27	-3.75	121.95	127.31
42	1	314	KC1	CBD-CHA-C1A	3.75	135.88	128.88
43	14	302	A86	O1-C15-C20	-3.75	55.73	59.40
31	B	609	CLA	CMB-C2B-C3B	3.75	131.70	124.68
31	p	607	CLA	CAC-C3C-C4C	3.75	129.68	124.81
43	7	306	A86	O1-C15-C20	-3.75	55.73	59.40
34	L	102	SQD	O7-S-C6	3.75	111.40	106.94
31	P	607	CLA	CAC-C3C-C4C	3.75	129.68	124.81
43	8	305	A86	C19-C18-C17	-3.75	103.53	110.77
31	3	313	CLA	CAA-C2A-C3A	-3.75	102.51	112.78
43	9	301	A86	C12-C11-C13	3.75	122.32	116.02
43	6	306	A86	C41-C32-C31	3.75	113.83	110.47
45	4	310	KC2	CBC-CAC-C3C	-3.75	108.98	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	303	A86	O4-C38-O5	-3.75	115.52	122.96
43	19	304	A86	C34-O4-C38	3.75	124.88	117.90
43	10	303	A86	C36-C31-C32	-3.74	115.98	119.70
42	13	314	KC1	C3B-C2B-C1B	-3.74	103.50	107.08
42	10	315	KC1	C2B-C1B-NB	3.74	112.86	110.10
31	B	606	CLA	CMB-C2B-C3B	3.74	131.68	124.68
31	B	606	CLA	CMA-C3A-C4A	3.74	121.83	111.77
45	12	311	KC2	C2A-C1A-NA	3.74	115.40	109.40
45	4	308	KC2	CHB-C4A-NA	3.74	130.10	124.20
43	14	304	A86	C12-C11-C13	3.74	122.31	116.02
42	19	314	KC1	C4B-C3B-C2B	-3.74	103.68	106.75
38	P	614	LMG	C1-O6-C5	3.74	121.03	113.69
31	12	315	CLA	CAA-C2A-C3A	-3.74	107.38	116.10
31	6	316	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
43	7	305	A86	C41-C32-C31	3.73	113.81	110.47
43	18	304	A86	C3-C2-C1	-3.73	121.98	127.31
43	17	304	A86	C28-C27-C26	-3.73	117.70	122.92
42	11	314	KC1	CBD-CHA-C1A	3.73	135.84	128.88
43	1	305	A86	C12-C11-C13	3.73	122.29	116.02
42	P	609	KC1	C1A-NA-C4A	-3.73	105.03	106.71
43	0	306	A86	O4-C38-C39	3.73	117.95	111.09
31	15	306	CLA	CED-O2D-CGD	3.73	124.37	115.94
31	16	308	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
31	w	203	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
43	9	306	A86	C4-C5-C6	-3.72	122.00	127.31
43	16	306	A86	C14-C15-C16	-3.72	104.50	118.75
31	1	310	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
45	2	310	KC2	CBD-CHA-C1A	3.72	135.82	128.88
43	6	306	A86	C19-C18-C17	-3.72	103.59	110.77
45	15	310	KC2	C2A-C3A-C4A	3.72	109.25	106.49
43	0	301	A86	O4-C38-O5	-3.72	115.58	122.96
45	12	309	KC2	CAA-C2A-C1A	3.72	141.83	124.75
43	13	303	A86	C4-C3-C2	-3.72	115.86	123.47
31	b	607	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
31	C	507	CLA	CMB-C2B-C3B	3.72	131.63	124.68
31	15	313	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
43	19	302	A86	C41-C32-C31	3.71	113.80	110.47
43	4	303	A86	O1-C15-C20	-3.71	55.77	59.40
31	c	507	CLA	CMB-C2B-C3B	3.71	131.62	124.68
31	3	313	CLA	C2D-C1D-ND	-3.71	107.37	110.10
31	11	310	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
43	0	303	A86	O1-C20-C19	3.71	116.17	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	304	A86	C4-C3-C2	-3.71	115.88	123.47
45	8	310	KC2	C2A-C1A-NA	3.71	115.35	109.40
31	8	312	CLA	CAA-C2A-C3A	-3.71	102.63	112.78
43	10	301	A86	O4-C38-O5	-3.71	115.60	122.96
45	17	309	KC2	CAA-C2A-C1A	3.71	141.78	124.75
43	14	303	A86	O1-C20-C19	-3.71	110.60	113.38
43	6	304	A86	C23-C16-C22	-3.71	101.90	107.37
43	17	306	A86	O1-C15-C20	-3.70	55.78	59.40
31	0	308	CLA	CAC-C3C-C4C	3.70	129.62	124.81
31	W	202	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
31	6	308	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
31	2	312	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
43	18	302	A86	C4-C3-C2	-3.70	115.89	123.47
31	b	615	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
43	5	304	A86	C19-C18-C17	3.70	117.92	110.77
43	18	303	A86	C4-C5-C6	-3.70	122.03	127.31
31	10	308	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
43	16	307	A86	C19-C18-C17	-3.70	103.63	110.77
31	3	315	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
45	9	309	KC2	CAB-C3B-C2B	3.70	140.78	128.60
43	19	301	A86	C12-C11-C13	3.69	122.23	116.02
45	11	311	KC2	CAB-C3B-C2B	3.69	140.78	128.60
31	13	307	CLA	CAA-C2A-C3A	-3.69	105.03	114.26
43	8	301	A86	C25-C24-C1	-3.69	116.04	126.42
43	8	305	A86	O1-C15-C20	-3.69	55.79	59.40
38	D	403	LMG	O6-C1-C2	3.69	118.16	110.35
42	1	314	KC1	CHB-C1B-C2B	-3.69	117.74	125.48
45	10	310	KC2	C3A-C4A-NA	3.69	114.60	110.57
43	12	303	A86	C33-C32-C31	-3.69	105.63	109.21
42	9	314	KC1	CAA-C2A-C1A	3.69	141.70	124.75
43	16	306	A86	O-C13-C14	3.69	129.15	121.66
43	17	316	A86	C41-C32-C40	-3.68	97.22	108.53
31	9	312	CLA	CMB-C2B-C3B	3.68	131.57	124.68
45	7	311	KC2	C3B-C2B-C1B	-3.68	103.56	107.08
42	11	314	KC1	C2A-C3A-C4A	3.68	109.22	106.49
31	2	315	CLA	CHD-C4C-C3C	-3.68	119.43	124.84
43	1	305	A86	O-C13-C11	-3.68	113.02	121.15
31	B	606	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
39	1	318	DGD	O6D-C1D-O3G	-3.68	101.26	109.97
43	4	304	A86	O4-C38-C39	3.68	117.86	111.09
43	13	303	A86	C23-C16-C22	-3.68	101.94	107.37
34	B	623	SQD	O9-S-O7	-3.68	101.22	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	15	308	KC2	CHB-C4A-NA	3.68	130.00	124.20
34	b	601	SQD	O9-S-O7	-3.68	101.22	113.95
31	c	512	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
31	2	314	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
43	12	301	A86	C28-C27-C26	-3.68	117.77	122.92
31	0	312	CLA	CMB-C2B-C3B	3.68	131.56	124.68
43	16	306	A86	C3-C2-C1	-3.68	122.06	127.31
45	1	311	KC2	CAB-C3B-C2B	3.67	140.70	128.60
43	0	302	A86	O-C13-C11	-3.67	113.04	121.15
31	C	512	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
42	12	314	KC1	C1A-C2A-C3A	-3.67	104.20	107.11
43	6	307	A86	C34-O4-C38	-3.67	111.06	117.90
42	4	313	KC1	C3B-C2B-C1B	-3.67	103.57	107.08
43	14	305	A86	C8-C6-C5	-3.67	113.31	118.94
31	b	607	CLA	CMB-C2B-C3B	3.66	131.53	124.68
45	14	308	KC2	CHB-C4A-NA	3.66	129.98	124.20
43	17	316	A86	O-C13-C11	-3.66	113.06	121.15
43	3	306	A86	O1-C20-C19	3.66	116.13	113.38
31	3	308	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
45	9	309	KC2	CBC-CAC-C3C	-3.66	109.41	127.62
43	7	303	A86	C4-C5-C6	-3.66	122.09	127.31
43	4	305	A86	C10-C9-C8	-3.66	111.79	123.22
31	D	404	CLA	CAC-C3C-C4C	3.66	129.56	124.81
31	3	316	CLA	CAC-C3C-C2C	3.66	133.79	127.53
32	a	405	PHO	CMB-C2B-C3B	3.66	131.52	124.68
43	10	306	A86	C25-C26-C27	-3.66	122.09	127.31
32	A	405	PHO	CMB-C2B-C3B	3.66	131.52	124.68
43	6	306	A86	C33-C32-C31	-3.66	105.66	109.21
31	17	312	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
43	16	307	A86	O1-C15-C20	-3.66	55.82	59.40
31	b	604	CLA	C3C-C4C-NC	-3.66	106.47	110.57
43	7	305	A86	O1-C15-C20	-3.66	55.83	59.40
45	1	311	KC2	CAB-C3B-C4B	-3.66	116.07	124.90
45	14	310	KC2	CBC-CAC-C3C	-3.65	109.44	127.62
43	14	305	A86	C36-C31-C32	3.65	123.32	119.70
43	14	302	A86	C12-C11-C13	3.65	122.16	116.02
33	H	101	BCR	C2-C1-C6	3.65	116.11	110.48
31	3	307	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
43	16	305	A86	C23-C16-C22	-3.65	101.98	107.37
42	17	314	KC1	C4C-C3C-C2C	-3.65	101.57	106.90
42	18	313	KC1	C4C-C3C-C2C	-3.65	101.57	106.90
43	6	306	A86	O1-C15-C20	-3.65	55.83	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	14	306	CLA	C2A-C1A-CHA	3.65	130.25	123.86
31	0	314	CLA	CMB-C2B-C3B	3.65	131.51	124.68
43	16	306	A86	C19-C18-C17	3.65	117.83	110.77
43	0	305	A86	C40-C32-C31	3.65	113.74	110.47
31	b	607	CLA	C1B-CHB-C4A	-3.65	122.89	130.12
38	d	403	LMG	O6-C1-C2	3.65	118.08	110.35
43	11	319	A86	C3-C2-C1	-3.65	122.10	127.31
31	W	202	CLA	CAC-C3C-C4C	3.65	129.54	124.81
43	1	305	A86	C36-C31-C32	-3.65	116.08	119.70
43	2	301	A86	O1-C20-C21	-3.65	110.68	115.06
43	0	303	A86	O1-C15-C20	-3.65	55.83	59.40
33	h	101	BCR	C3-C4-C5	-3.65	107.56	114.08
43	8	304	A86	C25-C26-C27	-3.65	122.11	127.31
43	4	304	A86	O1-C20-C19	-3.64	110.64	113.38
45	11	311	KC2	CAB-C3B-C4B	-3.64	116.10	124.90
31	8	306	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
31	b	607	CLA	C2D-C1D-ND	-3.64	107.42	110.10
43	6	301	A86	C22-C16-C17	-3.64	102.66	108.98
42	3	314	KC1	CHB-C1B-C2B	-3.64	117.84	125.48
43	14	305	A86	C9-C10-C11	-3.64	115.90	126.61
45	4	308	KC2	O2D-CGD-O1D	-3.64	116.72	123.84
43	3	305	A86	C19-C18-C17	3.64	117.80	110.77
31	3	316	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
38	15	315	LMG	O1-C1-C2	-3.64	102.62	108.30
45	19	309	KC2	C3C-C2C-C1C	-3.64	103.79	106.49
43	7	303	A86	C28-C27-C26	-3.64	117.83	122.92
33	h	101	BCR	C2-C1-C6	3.64	116.08	110.48
43	13	301	A86	C8-C6-C5	3.64	124.52	118.94
34	A	411	SQD	O9-S-O7	-3.64	101.36	113.95
42	8	313	KC1	C3B-C2B-C1B	-3.63	103.61	107.08
43	17	302	A86	O4-C38-O5	-3.63	115.74	122.96
31	w	203	CLA	CAC-C3C-C4C	3.63	129.53	124.81
43	1	304	A86	O4-C38-C39	3.63	117.77	111.09
31	0	308	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
43	6	301	A86	C9-C8-C6	-3.63	116.21	126.42
34	i	101	SQD	O9-S-O7	-3.63	101.38	113.95
43	6	305	A86	O-C13-C14	3.63	129.04	121.66
34	10	320	SQD	O9-S-C6	3.63	111.25	106.94
43	6	301	A86	C9-C10-C11	-3.63	115.94	126.61
43	2	303	A86	C23-C16-C22	-3.63	102.02	107.37
33	H	101	BCR	C3-C4-C5	-3.63	107.60	114.08
31	B	614	CLA	O2D-CGD-O1D	-3.63	116.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	D	408	LMG	O1-C1-C2	-3.63	102.64	108.30
43	14	303	A86	C17-C16-C15	3.62	112.86	109.16
31	19	312	CLA	CMB-C2B-C3B	3.62	131.46	124.68
43	14	305	A86	O1-C20-C21	-3.62	110.71	115.06
45	6	310	KC2	CAA-C2A-C1A	3.62	141.40	124.75
31	18	307	CLA	CMB-C2B-C3B	3.62	131.46	124.68
43	6	305	A86	C14-C15-C16	-3.62	104.88	118.75
45	16	310	KC2	CAA-C2A-C1A	3.62	141.40	124.75
31	18	311	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
42	2	313	KC1	C4B-C3B-C2B	-3.62	103.78	106.75
34	a	408	SQD	C1-O5-C5	3.62	120.80	113.69
34	b	601	SQD	O5-C5-C4	3.62	116.27	109.69
42	14	313	KC1	C3B-C2B-C1B	-3.62	103.62	107.08
31	C	505	CLA	C3C-C4C-NC	-3.62	106.51	110.57
45	9	309	KC2	C3C-C2C-C1C	-3.62	103.80	106.49
45	15	310	KC2	C2A-C1A-NA	3.62	115.21	109.40
31	d	404	CLA	CAC-C3C-C4C	3.62	129.50	124.81
31	3	312	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
31	5	307	CLA	CMB-C2B-C3B	3.62	131.45	124.68
43	11	302	A86	C3-C2-C1	-3.62	122.15	127.31
43	7	301	A86	O4-C38-O5	-3.62	115.78	122.96
42	10	315	KC1	C2A-C1A-CHA	3.62	139.41	127.44
45	2	310	KC2	CAB-C3B-C4B	-3.62	116.16	124.90
43	2	305	A86	O4-C38-O5	-3.61	115.78	122.96
34	B	623	SQD	O5-C5-C4	3.61	116.26	109.69
31	18	312	CLA	CHD-C1D-ND	-3.61	121.13	124.45
38	d	408	LMG	O1-C1-C2	-3.61	102.66	108.30
42	1	314	KC1	C3B-C2B-C1B	-3.61	103.62	107.08
34	0	318	SQD	O9-S-C6	3.61	111.23	106.94
43	2	303	A86	O1-C15-C20	-3.61	55.87	59.40
31	B	603	CLA	C3C-C4C-NC	-3.61	106.52	110.57
31	19	313	CLA	C1B-CHB-C4A	-3.61	122.96	130.12
45	18	310	KC2	C2A-C1A-NA	3.61	115.19	109.40
43	7	306	A86	C20-C19-C18	-3.61	105.61	112.75
31	17	315	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
31	9	315	CLA	CAA-C2A-C3A	-3.61	107.67	116.10
45	10	310	KC2	C3C-C2C-C1C	-3.61	103.81	106.49
45	0	310	KC2	C3A-C4A-NA	3.61	114.51	110.57
31	7	315	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
43	16	306	A86	C41-C32-C40	-3.61	97.45	108.53
43	7	305	A86	C23-C16-C22	3.61	112.69	107.37
31	5	309	CLA	CHB-C4A-NA	3.61	129.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	606	CLA	CHD-C1D-ND	-3.61	121.14	124.45
43	0	301	A86	C17-C16-C15	-3.61	105.48	109.16
43	4	301	A86	C21-C20-C19	-3.61	110.22	114.28
43	0	306	A86	C25-C26-C27	-3.61	122.16	127.31
34	L	102	SQD	O9-S-O7	-3.61	101.47	113.95
43	0	303	A86	C36-C31-C32	-3.61	116.12	119.70
42	10	315	KC1	C2A-C1A-NA	3.60	115.18	109.40
31	13	310	CLA	CMB-C2B-C3B	3.60	131.42	124.68
31	16	311	CLA	CAA-C2A-C3A	-3.60	107.69	116.10
34	l	101	SQD	O9-S-O7	-3.60	101.48	113.95
31	c	505	CLA	CHB-C4A-NA	3.60	129.49	124.51
43	15	304	A86	C28-C27-C26	-3.60	117.88	122.92
43	12	303	A86	O4-C38-C39	3.60	117.71	111.09
42	7	314	KC1	C4C-C3C-C2C	-3.60	101.65	106.90
43	1	305	A86	C19-C18-C17	3.60	117.73	110.77
34	A	408	SQD	C1-O5-C5	3.60	120.75	113.69
31	b	611	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
31	18	306	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
31	13	313	CLA	C1-O2A-CGA	3.60	125.88	116.44
43	11	305	A86	C25-C26-C27	-3.60	122.18	127.31
43	7	304	A86	O-C13-C11	-3.60	113.21	121.15
43	6	302	A86	O4-C38-O5	-3.59	115.82	122.96
43	0	305	A86	C25-C24-C1	-3.59	116.32	126.42
31	6	311	CLA	CAA-C2A-C3A	-3.59	107.71	116.10
43	6	302	A86	C9-C8-C6	-3.59	116.33	126.42
31	p	606	CLA	CHD-C1D-ND	-3.59	121.15	124.45
42	12	314	KC1	CHB-C1B-C2B	-3.59	117.95	125.48
43	17	302	A86	C40-C32-C31	-3.59	107.26	110.47
45	16	312	KC2	C4B-C3B-C2B	-3.59	103.80	106.75
43	18	302	A86	C34-O4-C38	-3.59	111.21	117.90
42	3	314	KC1	C4B-C3B-C2B	-3.59	103.81	106.75
31	5	311	CLA	C4A-NA-C1A	3.59	108.32	106.71
42	6	315	KC1	C1B-CHB-C4A	-3.59	118.32	126.06
43	12	306	A86	O-C13-C14	3.58	128.94	121.66
42	6	315	KC1	O2D-CGD-CBD	3.58	117.64	111.27
43	15	303	A86	C25-C26-C27	-3.58	122.19	127.31
34	a	408	SQD	O9-S-O7	-3.58	101.55	113.95
43	14	303	A86	O4-C38-C39	3.58	117.68	111.09
31	19	307	CLA	CAC-C3C-C4C	3.58	129.46	124.81
45	1	309	KC2	CMD-C2D-C3D	3.58	131.38	124.68
42	8	313	KC1	C2B-C1B-NB	3.58	112.74	110.10
43	6	305	A86	C19-C18-C17	3.58	117.69	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	13	313	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
31	B	606	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
45	18	308	KC2	CAC-C3C-C4C	3.58	141.14	124.47
31	1	321	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
42	18	313	KC1	C4B-C3B-C2B	-3.58	103.81	106.75
31	14	315	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
43	1	304	A86	C28-C27-C26	-3.57	117.92	122.92
31	16	308	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
31	12	316	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
31	2	311	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
31	B	610	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
43	2	305	A86	C19-C18-C17	-3.57	103.88	110.77
43	17	302	A86	C9-C8-C6	-3.57	116.39	126.42
34	A	408	SQD	O9-S-O7	-3.57	101.59	113.95
31	c	505	CLA	C3C-C4C-NC	-3.57	106.57	110.57
45	11	309	KC2	CBC-CAC-C3C	-3.57	109.86	127.62
45	9	309	KC2	C2A-C1A-NA	3.57	115.12	109.40
34	A	411	SQD	O47-C7-C8	3.57	119.19	111.50
43	16	304	A86	C22-C16-C17	-3.57	102.78	108.98
42	2	313	KC1	C4D-C3D-CAD	3.57	113.57	107.81
34	i	101	SQD	O47-C7-C8	3.57	119.19	111.50
43	6	303	A86	C12-C11-C13	3.56	122.00	116.02
43	17	301	A86	C9-C10-C11	-3.56	116.14	126.61
44	P	612	DD6	C12-C11-C10	-3.56	117.94	122.92
31	10	314	CLA	CMB-C2B-C3B	3.56	131.33	124.68
31	C	505	CLA	CHB-C4A-NA	3.56	129.43	124.51
31	11	307	CLA	CAC-C3C-C2C	-3.56	121.45	127.53
31	10	309	CLA	CBC-CAC-C3C	3.55	122.23	112.43
43	14	303	A86	C28-C27-C26	-3.55	117.95	122.92
45	15	310	KC2	CBC-CAC-C3C	-3.55	109.96	127.62
45	2	310	KC2	C3B-C2B-C1B	-3.55	103.69	107.08
31	3	316	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
43	10	305	A86	O3-C36-C37	-3.55	103.08	109.39
43	10	318	A86	O1-C15-C20	-3.55	55.93	59.40
43	15	301	A86	C9-C8-C6	-3.55	116.46	126.42
43	5	303	A86	C34-O4-C38	3.54	124.50	117.90
31	15	309	CLA	CHB-C4A-NA	3.54	129.41	124.51
43	11	302	A86	C17-C16-C15	-3.54	105.55	109.16
45	19	309	KC2	CBC-CAC-C3C	-3.54	110.00	127.62
43	1	303	A86	C12-C11-C13	3.54	121.97	116.02
45	4	308	KC2	CBC-CAC-C3C	-3.54	110.00	127.62
43	11	305	A86	C20-C19-C18	-3.54	105.74	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	13	309	KC2	CAA-C2A-C1A	3.54	141.02	124.75
45	6	312	KC2	C2A-C3A-C4A	3.54	109.11	106.49
43	5	301	A86	C21-C20-C19	3.54	118.26	114.28
31	14	314	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
43	14	302	A86	O1-C20-C21	-3.54	110.82	115.06
43	13	304	A86	C3-C2-C1	-3.54	122.26	127.31
43	5	301	A86	C9-C8-C6	-3.54	116.48	126.42
33	Y	101	BCR	C15-C14-C13	-3.54	122.26	127.31
31	19	311	CLA	CHB-C4A-NA	3.54	129.40	124.51
42	4	313	KC1	CAA-C2A-C1A	3.54	141.00	124.75
31	1	310	CLA	CMB-C2B-C3B	3.54	131.29	124.68
44	P	612	DD6	C37-C36-C35	3.54	120.91	114.36
39	W	203	DGD	O6D-C1D-O3G	-3.54	101.60	109.97
43	2	301	A86	C33-C32-C31	-3.53	105.78	109.21
42	16	301	KC1	C2A-C1A-NA	3.53	115.07	109.40
31	C	502	CLA	CAA-C2A-C3A	-3.53	103.10	112.78
43	6	305	A86	C4-C3-C2	-3.53	116.24	123.47
45	14	310	KC2	C4B-C3B-C2B	-3.53	103.85	106.75
43	2	302	A86	O-C13-C14	-3.53	114.49	121.66
43	14	305	A86	C7-C6-C8	3.53	123.64	118.08
31	12	307	CLA	CAA-C2A-C3A	-3.53	105.44	114.26
43	6	301	A86	C25-C24-C1	-3.53	116.50	126.42
43	8	301	A86	C40-C32-C33	3.53	124.89	109.05
43	10	305	A86	C25-C24-C1	-3.53	116.51	126.42
42	6	315	KC1	C2A-C1A-NA	3.53	115.06	109.40
39	w	204	DGD	O6D-C1D-O3G	-3.53	101.62	109.97
31	c	502	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
43	7	302	A86	C20-C19-C18	-3.53	105.77	112.75
31	4	309	CLA	CHB-C4A-NA	3.53	129.39	124.51
43	15	304	A86	O-C13-C14	-3.52	114.50	121.66
45	4	308	KC2	C4B-C3B-C2B	-3.52	103.86	106.75
43	7	306	A86	C21-C20-C19	-3.52	110.32	114.28
44	p	612	DD6	C37-C36-C35	3.52	120.88	114.36
43	11	320	A86	C3-C4-C5	-3.52	116.26	123.47
43	11	320	A86	C34-O4-C38	3.52	124.46	117.90
43	17	305	A86	O-C13-C14	3.52	128.82	121.66
43	8	302	A86	C4-C3-C2	-3.52	116.26	123.47
43	17	316	A86	C19-C18-C17	-3.52	103.97	110.77
42	12	314	KC1	C3B-C2B-C1B	-3.52	103.72	107.08
31	6	314	CLA	C4A-NA-C1A	3.52	108.29	106.71
43	5	301	A86	C28-C27-C26	-3.52	118.00	122.92
43	18	305	A86	C33-C32-C31	-3.52	105.79	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	11	314	KC1	CHB-C1B-C2B	-3.52	118.10	125.48
31	4	314	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
31	19	315	CLA	CAA-C2A-C3A	-3.52	107.89	116.10
43	6	307	A86	O3-C36-C37	-3.51	103.14	109.39
31	12	313	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
43	11	319	A86	C3-C4-C5	-3.51	116.28	123.47
45	2	308	KC2	CAA-C2A-C1A	3.51	140.89	124.75
45	0	310	KC2	C3B-C2B-C1B	-3.51	103.72	107.08
43	7	305	A86	O4-C38-O5	-3.51	115.99	122.96
43	5	318	A86	C9-C8-C6	-3.51	116.55	126.42
43	18	305	A86	C14-C15-C16	3.51	132.20	118.75
31	18	309	CLA	CHB-C4A-NA	3.51	129.37	124.51
31	9	311	CLA	CHB-C4A-NA	3.51	129.36	124.51
43	12	304	A86	C14-C15-C16	-3.51	105.32	118.75
43	17	303	A86	O4-C34-C33	3.51	116.33	107.59
43	10	303	A86	O1-C15-C20	-3.51	55.97	59.40
31	B	606	CLA	C2D-C1D-ND	-3.51	107.52	110.10
42	3	314	KC1	C1A-NA-C4A	-3.51	105.13	106.71
31	16	309	CLA	CAA-C2A-C3A	-3.51	103.17	112.78
45	3	309	KC2	CAA-C2A-C1A	3.51	140.87	124.75
42	11	314	KC1	C3B-C2B-C1B	-3.51	103.73	107.08
31	B	612	CLA	CHB-C4A-NA	3.51	129.36	124.51
31	b	613	CLA	CHB-C4A-NA	3.50	129.36	124.51
31	B	614	CLA	CBA-CAA-C2A	3.50	124.20	113.86
31	p	606	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
42	19	314	KC1	CAA-C2A-C1A	3.50	140.84	124.75
31	19	311	CLA	CAA-C2A-C1A	3.50	123.44	111.97
31	9	312	CLA	C2D-C1D-ND	-3.50	107.53	110.10
43	1	319	A86	C25-C26-C27	-3.50	122.32	127.31
31	9	313	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
45	14	308	KC2	CBC-CAC-C3C	-3.50	110.22	127.62
43	17	303	A86	C4-C3-C2	-3.50	116.31	123.47
31	14	309	CLA	CHB-C4A-NA	3.50	129.34	124.51
31	3	316	CLA	CHD-C4C-NC	3.49	129.71	124.20
43	0	305	A86	O4-C38-O5	-3.49	116.02	122.96
43	16	304	A86	C33-C32-C31	-3.49	105.82	109.21
45	10	310	KC2	C3B-C2B-C1B	-3.49	103.74	107.08
42	3	314	KC1	C1B-CHB-C4A	-3.49	118.53	126.06
31	13	315	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
43	8	301	A86	O4-C34-C35	-3.49	98.90	107.59
33	y	101	BCR	C15-C14-C13	-3.49	122.33	127.31
43	18	303	A86	C25-C26-C27	-3.49	122.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	304	A86	C28-C27-C26	-3.49	118.04	122.92
31	P	608	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
45	12	309	KC2	C4B-C3B-C2B	-3.49	103.89	106.75
31	15	312	CLA	CMB-C2B-C3B	3.49	131.20	124.68
43	2	301	A86	C10-C9-C8	-3.49	112.34	123.22
43	3	306	A86	O1-C15-C20	-3.49	55.99	59.40
43	4	302	A86	C12-C11-C13	3.49	121.88	116.02
31	1	307	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
31	19	313	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
31	12	315	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
31	16	314	CLA	CMD-C2D-C1D	3.48	130.85	124.71
31	11	308	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
43	2	302	A86	O4-C38-O5	-3.48	116.04	122.96
43	12	306	A86	O1-C15-C20	-3.48	55.99	59.40
42	12	314	KC1	C4D-C3D-CAD	3.48	113.44	107.81
43	19	303	A86	C34-O4-C38	3.48	124.38	117.90
31	B	611	CLA	C2C-C1C-NC	-3.48	106.71	109.97
31	11	315	CLA	CMC-C2C-C1C	-3.48	119.74	125.04
31	8	311	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
31	p	602	CLA	CMB-C2B-C3B	3.48	131.19	124.68
38	F	102	LMG	C1-C2-C3	-3.48	102.75	110.00
43	11	306	A86	C3-C4-C5	-3.48	116.35	123.47
39	c	518	DGD	O6D-C5D-C6D	-3.48	99.65	106.67
31	16	316	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
31	7	313	CLA	C2D-C1D-ND	-3.48	107.54	110.10
43	10	303	A86	C34-O4-C38	3.47	124.37	117.90
45	6	312	KC2	C4B-C3B-C2B	-3.47	103.90	106.75
31	P	603	CLA	CMB-C2B-C3B	3.47	131.18	124.68
31	13	307	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
43	9	302	A86	O1-C15-C20	-3.47	56.00	59.40
31	3	313	CLA	C4A-NA-C1A	3.47	108.27	106.71
45	15	308	KC2	CAB-C3B-C2B	3.47	140.04	128.60
38	f	102	LMG	C1-C2-C3	-3.47	102.77	110.00
33	B	618	BCR	C15-C14-C13	-3.47	122.36	127.31
31	5	314	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
43	16	302	A86	C9-C10-C11	-3.47	116.41	126.61
43	12	305	A86	C3-C4-C5	-3.47	116.37	123.47
31	P	606	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
45	4	310	KC2	CAB-C3B-C4B	-3.47	116.52	124.90
39	C	518	DGD	O6D-C5D-C6D	-3.47	99.67	106.67
31	p	608	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
42	16	315	KC1	C4B-C3B-C2B	-3.47	103.91	106.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	313	CLA	CAA-C2A-C3A	-3.47	103.29	112.78
31	2	306	CLA	O2D-CGD-CBD	3.47	117.43	111.27
45	5	310	KC2	CBC-CAC-C3C	-3.46	110.39	127.62
31	1	321	CLA	CBA-CAA-C2A	3.46	124.08	113.86
42	6	315	KC1	C2A-C1A-CHA	-3.46	115.99	127.44
43	1	320	A86	C34-O4-C38	3.46	124.35	117.90
43	4	302	A86	C40-C32-C31	3.46	113.57	110.47
43	12	304	A86	C3-C4-C5	-3.46	116.38	123.47
31	15	307	CLA	CMB-C2B-C3B	3.46	131.15	124.68
43	7	302	A86	C41-C32-C31	3.46	113.57	110.47
43	17	306	A86	O4-C38-O5	-3.46	116.09	122.96
45	0	310	KC2	C3C-C2C-C1C	-3.46	103.92	106.49
31	p	603	CLA	CMB-C2B-C3B	3.46	131.15	124.68
43	19	306	A86	O1-C15-C20	-3.46	56.02	59.40
33	b	619	BCR	C15-C14-C13	-3.45	122.38	127.31
43	4	302	A86	C21-C20-C19	3.45	118.17	114.28
31	Z	101	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
31	13	310	CLA	CAA-C2A-C3A	-3.45	108.04	116.10
31	z	101	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
43	14	302	A86	C3-C2-C1	-3.45	122.39	127.31
43	12	305	A86	O1-C15-C20	-3.45	56.03	59.40
42	16	315	KC1	CHB-C1B-C2B	-3.44	118.25	125.48
43	7	304	A86	C19-C18-C17	3.44	117.42	110.77
31	4	312	CLA	C1-O2A-CGA	3.44	125.48	116.44
43	7	301	A86	C9-C8-C6	-3.44	116.74	126.42
38	5	315	LMG	O6-C1-O1	-3.44	101.82	109.97
43	11	305	A86	C23-C16-C17	-3.44	103.00	108.98
42	0	315	KC1	C4B-C3B-C2B	-3.44	103.92	106.75
31	17	307	CLA	CAC-C3C-C2C	-3.44	121.64	127.53
31	5	306	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
31	P	602	CLA	CMB-C2B-C3B	3.44	131.11	124.68
31	11	310	CLA	CMB-C2B-C3B	3.44	131.11	124.68
45	16	312	KC2	C2A-C3A-C4A	3.44	109.04	106.49
43	10	306	A86	O4-C38-C39	3.44	117.42	111.09
31	b	612	CLA	C2C-C1C-NC	-3.44	106.75	109.97
31	7	307	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
43	11	319	A86	C4-C5-C6	-3.44	122.41	127.31
43	11	305	A86	O-C13-C11	-3.44	113.56	121.15
42	17	314	KC1	C4B-C3B-C2B	-3.44	103.93	106.75
43	4	304	A86	C17-C16-C15	3.43	112.67	109.16
33	C	516	BCR	C28-C27-C26	-3.43	107.94	114.08
43	15	302	A86	C19-C18-C17	-3.43	104.14	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	313	CLA	CMA-C3A-C4A	-3.43	102.55	111.77
33	F	101	BCR	C7-C8-C9	-3.43	121.05	126.23
43	7	301	A86	C4-C3-C2	-3.43	116.44	123.47
42	16	301	KC1	C4B-C3B-C2B	-3.43	103.93	106.75
42	10	315	KC1	C2A-C3A-C4A	3.43	109.03	106.49
45	3	311	KC2	C4B-C3B-C2B	-3.43	103.94	106.75
43	19	303	A86	O1-C15-C20	-3.43	56.05	59.40
31	9	311	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
31	b	612	CLA	CHC-C1C-NC	3.43	129.40	124.20
43	12	303	A86	O1-C20-C19	3.43	115.95	113.38
31	8	309	CLA	CHB-C4A-NA	3.42	129.25	124.51
31	18	311	CLA	O1D-CGD-CBD	3.42	131.49	124.48
31	10	313	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
31	10	314	CLA	CHB-C4A-NA	3.42	129.25	124.51
45	4	310	KC2	C4B-C3B-C2B	-3.42	103.94	106.75
31	12	312	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
31	6	314	CLA	CHA-C4D-ND	3.42	139.66	132.50
31	12	312	CLA	O2A-CGA-O1A	-3.42	114.77	123.30
31	2	315	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
43	15	302	A86	C41-C32-C33	3.42	124.41	109.05
31	15	312	CLA	C1B-CHB-C4A	-3.42	123.35	130.12
33	f	101	BCR	C7-C8-C9	-3.42	121.07	126.23
43	6	306	A86	C23-C16-C22	3.42	112.41	107.37
43	18	305	A86	C20-C19-C18	-3.41	105.99	112.75
43	9	301	A86	O4-C34-C35	3.41	116.09	107.59
31	12	307	CLA	C2D-C1D-ND	-3.41	107.59	110.10
43	5	301	A86	O1-C20-C21	3.41	119.14	115.06
39	w	204	DGD	O5D-C1E-C2E	3.41	113.63	108.30
43	4	303	A86	C19-C18-C17	-3.41	104.18	110.77
39	W	203	DGD	O5D-C1E-C2E	3.41	113.63	108.30
43	18	304	A86	O4-C38-C39	3.41	117.36	111.09
43	19	302	A86	O1-C15-C20	-3.41	56.07	59.40
45	13	311	KC2	CAA-C2A-C1A	3.41	140.42	124.75
43	12	304	A86	C17-C16-C15	-3.41	105.68	109.16
43	9	301	A86	O4-C38-O5	-3.41	116.19	122.96
31	13	313	CLA	C1-C2-C3	3.41	131.94	126.04
31	13	316	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
43	7	306	A86	O1-C15-C14	-3.41	106.37	113.21
42	16	301	KC1	CAC-C3C-C4C	3.41	129.23	124.81
43	9	303	A86	O1-C15-C20	-3.41	56.07	59.40
39	B	621	DGD	C1D-O6D-C5D	-3.40	107.01	113.69
45	14	308	KC2	C4B-C3B-C2B	-3.40	103.96	106.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	0	302	A86	C35-C34-C33	-3.40	103.94	109.88
33	c	516	BCR	C28-C27-C26	-3.40	108.00	114.08
31	13	316	CLA	CHB-C4A-NA	3.40	129.22	124.51
45	13	309	KC2	CBC-CAC-C3C	-3.40	110.70	127.62
31	18	314	CLA	CBC-CAC-C3C	3.40	121.81	112.43
43	8	301	A86	O-C13-C14	-3.40	114.75	121.66
42	7	314	KC1	C3B-C2B-C1B	-3.40	103.83	107.08
31	d	405	CLA	CMB-C2B-C3B	3.40	131.03	124.68
42	9	314	KC1	C4C-C3C-C2C	-3.40	101.95	106.90
31	C	509	CLA	C1C-C2C-C3C	3.40	110.53	106.96
34	i	101	SQD	C3-C4-C5	3.39	116.29	110.24
31	B	611	CLA	CHC-C1C-NC	3.39	129.35	124.20
43	2	302	A86	O4-C34-C35	3.39	116.04	107.59
31	C	509	CLA	C2C-C1C-NC	-3.39	106.79	109.97
39	B	621	DGD	O2D-C2D-C1D	-3.39	101.81	110.05
43	1	302	A86	C36-C31-C32	3.39	123.06	119.70
42	8	313	KC1	C4D-C3D-CAD	3.39	113.28	107.81
43	3	301	A86	C40-C32-C31	3.38	113.50	110.47
42	0	315	KC1	C3C-C4C-NC	3.38	113.06	109.88
31	c	509	CLA	C1C-C2C-C3C	3.38	110.51	106.96
31	12	307	CLA	CAC-C3C-C4C	3.38	129.20	124.81
34	A	411	SQD	O7-S-C6	3.38	110.95	106.94
31	10	313	CLA	C2A-C1A-CHA	3.38	129.77	123.86
43	p	613	A86	C4-C5-C6	-3.38	122.49	127.31
43	6	303	A86	C25-C26-C27	-3.38	122.49	127.31
31	D	405	CLA	CMB-C2B-C3B	3.38	131.00	124.68
42	10	315	KC1	C4B-C3B-C2B	-3.38	103.98	106.75
31	c	509	CLA	C2C-C1C-NC	-3.38	106.81	109.97
43	10	302	A86	C3-C2-C1	-3.38	122.49	127.31
43	13	306	A86	C23-C16-C22	-3.38	102.39	107.37
41	v	201	HEM	C3B-C2B-C1B	3.38	108.99	106.49
42	14	313	KC1	C4C-C3C-C2C	-3.37	101.98	106.90
43	11	304	A86	C4-C3-C2	-3.37	116.56	123.47
42	12	314	KC1	C4C-C3C-C2C	-3.37	101.98	106.90
39	c	518	DGD	O6D-C1D-O3G	-3.37	101.99	109.97
31	8	312	CLA	CHA-C4D-ND	3.37	139.55	132.50
43	5	304	A86	C36-C31-C32	-3.37	116.35	119.70
42	2	313	KC1	C3D-CAD-CBD	-3.37	103.17	107.61
31	19	313	CLA	CMA-C3A-C4A	-3.37	102.72	111.77
43	13	301	A86	C34-O4-C38	3.37	124.17	117.90
43	16	307	A86	C23-C16-C22	3.37	112.34	107.37
45	2	310	KC2	CAB-C3B-C2B	3.37	139.70	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	303	A86	O1-C15-C20	-3.37	56.11	59.40
31	19	313	CLA	CHD-C1D-ND	-3.37	121.36	124.45
43	17	304	A86	O4-C38-C39	3.37	117.28	111.09
38	P	614	LMG	O6-C1-C2	3.37	117.47	110.35
44	p	612	DD6	O1-C20-C21	3.37	119.09	115.06
31	1	315	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
43	9	304	A86	C12-C11-C13	3.36	121.67	116.02
43	P	611	A86	C3-C4-C5	-3.36	116.58	123.47
31	4	315	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
31	14	306	CLA	CHA-C1A-NA	-3.36	118.70	126.40
39	C	518	DGD	O6D-C1D-O3G	-3.36	102.01	109.97
43	P	613	A86	C4-C5-C6	-3.36	122.51	127.31
45	14	310	KC2	CAB-C3B-C4B	-3.36	116.78	124.90
43	6	303	A86	O3-C36-C37	-3.36	103.41	109.39
38	p	614	LMG	O6-C1-C2	3.36	117.46	110.35
31	3	307	CLA	CMB-C2B-C3B	3.36	130.96	124.68
39	11	318	DGD	O3G-C3G-C2G	-3.36	102.79	110.90
43	15	301	A86	C36-C31-C32	3.36	123.03	119.70
43	1	303	A86	C4-C3-C2	-3.36	116.59	123.47
38	1	317	LMG	C1-C2-C3	-3.36	103.00	110.00
43	1	305	A86	C9-C8-C6	-3.36	116.98	126.42
31	b	608	CLA	CMB-C2B-C3B	3.36	130.96	124.68
42	2	313	KC1	C3B-C2B-C1B	-3.36	103.87	107.08
43	p	611	A86	C3-C4-C5	-3.36	116.60	123.47
31	9	311	CLA	CMB-C2B-C3B	3.35	130.95	124.68
43	4	306	A86	O1-C15-C20	-3.35	56.12	59.40
31	c	512	CLA	CMD-C2D-C3D	3.35	135.33	127.61
41	V	201	HEM	C3B-C2B-C1B	3.35	108.97	106.49
43	1	305	A86	C3-C2-C1	-3.35	122.53	127.31
34	A	411	SQD	C3-C4-C5	3.35	116.22	110.24
31	19	311	CLA	CMB-C2B-C3B	3.35	130.95	124.68
43	14	302	A86	O1-C20-C19	-3.35	110.86	113.38
33	c	515	BCR	C3-C4-C5	-3.35	108.09	114.08
43	16	306	A86	C25-C26-C27	-3.35	122.53	127.31
31	c	505	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
31	8	314	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
31	19	311	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
43	12	301	A86	C34-O4-C38	3.35	124.13	117.90
31	C	512	CLA	CMD-C2D-C3D	3.35	135.31	127.61
31	7	312	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
45	2	308	KC2	C4B-C3B-C2B	-3.34	104.00	106.75
31	19	312	CLA	C2D-C1D-ND	-3.34	107.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	301	A86	C25-C24-C1	-3.34	117.03	126.42
31	b	604	CLA	CMB-C2B-C3B	3.34	130.92	124.68
31	B	603	CLA	CMB-C2B-C3B	3.34	130.92	124.68
45	8	310	KC2	C4B-C3B-C2B	-3.34	104.01	106.75
31	1	312	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
43	12	306	A86	C41-C32-C33	-3.34	94.07	109.05
43	2	301	A86	C17-C16-C15	3.34	112.57	109.16
43	10	302	A86	C41-C32-C31	3.34	113.46	110.47
31	1	321	CLA	C1D-ND-C4D	3.34	108.70	106.33
43	2	301	A86	C22-C16-C17	3.33	114.78	108.98
43	12	305	A86	C4-C5-C6	-3.33	122.55	127.31
43	1	305	A86	O4-C38-O5	-3.33	116.34	122.96
33	f	101	BCR	C2-C1-C6	3.33	115.61	110.48
31	13	313	CLA	C2D-C1D-ND	-3.33	107.65	110.10
31	6	313	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
45	17	311	KC2	C2A-C1A-NA	3.33	114.74	109.40
31	b	615	CLA	CBA-CAA-C2A	3.33	123.69	113.86
42	12	314	KC1	C1A-NA-C4A	3.33	108.20	106.71
43	9	303	A86	C33-C32-C31	-3.33	105.97	109.21
33	C	515	BCR	C3-C4-C5	-3.33	108.13	114.08
43	11	320	A86	O-C13-C14	3.33	128.42	121.66
43	16	302	A86	C9-C8-C6	-3.33	117.06	126.42
43	16	306	A86	C-C1-C2	-3.33	118.26	122.92
43	7	302	A86	C9-C8-C6	-3.33	117.07	126.42
45	2	310	KC2	CBC-CAC-C3C	-3.33	111.07	127.62
42	14	313	KC1	O2D-CGD-O1D	-3.33	117.33	123.84
42	0	315	KC1	C3B-C2B-C1B	-3.33	103.90	107.08
43	5	318	A86	O-C13-C14	-3.33	114.90	121.66
31	B	607	CLA	CMB-C2B-C3B	3.32	130.90	124.68
31	1	321	CLA	C2A-C1A-CHA	3.32	129.67	123.86
34	i	101	SQD	O7-S-C6	3.32	110.89	106.94
43	4	306	A86	O1-C20-C19	3.32	115.88	113.38
31	c	509	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
31	18	314	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
43	2	305	A86	C4-C3-C2	-3.32	116.67	123.47
43	13	301	A86	C36-C31-C32	3.32	122.99	119.70
43	3	302	A86	C9-C8-C6	-3.32	117.09	126.42
43	12	303	A86	O1-C15-C20	-3.32	56.15	59.40
45	4	310	KC2	CAB-C3B-C2B	3.32	139.54	128.60
31	c	506	CLA	O2D-CGD-CBD	3.32	117.16	111.27
45	16	312	KC2	CBC-CAC-C3C	-3.32	111.12	127.62
31	C	505	CLA	CMB-C2B-C1B	-3.32	123.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	316	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
43	4	303	A86	C34-O4-C38	-3.31	111.72	117.90
43	13	301	A86	C25-C24-C1	-3.31	117.11	126.42
43	P	613	A86	C4-C3-C2	-3.31	116.69	123.47
43	p	613	A86	C4-C3-C2	-3.31	116.69	123.47
31	B	606	CLA	CMD-C2D-C1D	3.31	130.55	124.71
43	12	302	A86	C19-C18-C17	-3.31	104.38	110.77
43	11	305	A86	C36-C31-C32	-3.31	116.41	119.70
42	1	314	KC1	C4C-C3C-C2C	-3.31	102.08	106.90
43	3	303	A86	C19-C18-C17	-3.31	104.39	110.77
31	3	313	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
33	F	101	BCR	C2-C1-C6	3.30	115.57	110.48
31	C	509	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
31	c	508	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
43	14	304	A86	C41-C32-C31	-3.30	107.52	110.47
43	15	302	A86	C20-C19-C18	3.30	119.28	112.75
43	8	303	A86	C4-C3-C2	-3.30	116.71	123.47
45	11	309	KC2	CAA-CBA-CGA	-3.30	110.29	127.26
42	4	313	KC1	C4C-C3C-C2C	-3.30	102.09	106.90
43	13	301	A86	C7-C6-C5	-3.30	118.30	122.92
43	15	303	A86	C28-C27-C26	-3.30	118.30	122.92
31	C	506	CLA	O2D-CGD-CBD	3.30	117.13	111.27
45	18	310	KC2	C4B-C3B-C2B	-3.30	104.04	106.75
43	12	303	A86	C23-C16-C22	-3.30	102.50	107.37
31	1	307	CLA	CAC-C3C-C4C	3.30	129.09	124.81
43	12	304	A86	C41-C32-C31	-3.30	107.52	110.47
43	P	613	A86	C12-C11-C13	3.30	121.56	116.02
43	7	303	A86	O4-C38-C39	3.30	117.16	111.09
45	5	308	KC2	C2A-C3A-C4A	3.30	108.93	106.49
43	11	303	A86	C4-C3-C2	-3.30	116.72	123.47
45	15	308	KC2	CAB-C3B-C4B	-3.29	116.94	124.90
45	6	310	KC2	C4B-C3B-C2B	-3.29	104.05	106.75
31	7	307	CLA	CAC-C3C-C2C	-3.29	121.90	127.53
38	F	102	LMG	O1-C1-C2	-3.29	103.16	108.30
34	B	623	SQD	O9-S-C6	3.29	110.85	106.94
34	b	601	SQD	O9-S-C6	3.29	110.85	106.94
31	2	315	CLA	C1D-ND-C4D	-3.29	104.00	106.33
43	1	319	A86	O4-C34-C33	-3.29	99.40	107.59
43	0	304	A86	O1-C20-C21	-3.29	111.11	115.06
42	6	315	KC1	C4B-C3B-C2B	-3.29	104.05	106.75
31	C	504	CLA	C1-C2-C3	-3.29	120.35	126.04
43	4	306	A86	O4-C38-C39	3.29	117.14	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	320	A86	O4-C38-O5	-3.29	116.43	122.96
45	4	310	KC2	C2A-C3A-C4A	3.29	108.92	106.49
45	14	308	KC2	CAA-C2A-C1A	3.29	139.84	124.75
43	14	304	A86	C10-C9-C8	-3.28	112.97	123.22
43	5	318	A86	C19-C18-C17	-3.28	104.43	110.77
43	0	305	A86	C3-C4-C5	-3.28	116.75	123.47
31	14	315	CLA	CMB-C2B-C3B	3.28	130.82	124.68
43	5	301	A86	C4-C3-C2	-3.28	116.75	123.47
43	9	306	A86	O1-C15-C20	-3.28	56.19	59.40
43	13	306	A86	C25-C24-C1	-3.28	117.20	126.42
38	f	102	LMG	O1-C1-C2	-3.28	103.18	108.30
43	4	304	A86	C14-C15-C16	3.28	131.31	118.75
45	1	311	KC2	CBC-CAC-C3C	-3.28	111.31	127.62
45	8	308	KC2	CAA-C2A-C1A	3.28	139.82	124.75
43	14	303	A86	C14-C15-C16	3.28	131.31	118.75
45	4	310	KC2	C3B-C2B-C1B	-3.28	103.95	107.08
31	1	321	CLA	CAC-C3C-C4C	3.28	129.06	124.81
31	C	508	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
31	3	307	CLA	CAC-C3C-C4C	3.28	129.06	124.81
43	p	613	A86	C12-C11-C13	3.27	121.52	116.02
43	12	306	A86	C3-C4-C5	-3.27	116.77	123.47
43	7	301	A86	C41-C32-C31	-3.27	107.54	110.47
43	8	303	A86	O1-C15-C20	-3.27	56.20	59.40
43	16	306	A86	C3-C4-C5	-3.27	116.77	123.47
31	9	311	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
43	17	316	A86	C35-C34-C33	-3.27	104.17	109.88
31	c	504	CLA	C1-C2-C3	-3.27	120.39	126.04
31	15	311	CLA	C4D-C3D-CAD	-3.27	104.24	108.10
42	6	315	KC1	C2A-C3A-C4A	3.27	108.91	106.49
31	18	312	CLA	CMB-C2B-C3B	3.27	130.80	124.68
42	14	313	KC1	CGD-CBD-CAD	-3.27	100.14	110.73
43	10	306	A86	O1-C20-C19	3.27	115.84	113.38
43	8	302	A86	C41-C32-C40	-3.27	98.50	108.53
45	14	310	KC2	CAB-C3B-C2B	3.27	139.37	128.60
31	18	312	CLA	O2A-CGA-O1A	-3.27	115.35	123.59
31	13	316	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
43	14	302	A86	C34-O4-C38	-3.27	111.81	117.90
43	17	301	A86	C25-C24-C1	-3.26	117.25	126.42
41	V	201	HEM	CMC-C2C-C3C	3.26	130.78	124.68
43	4	301	A86	C19-C18-C17	3.26	117.08	110.77
43	15	302	A86	C25-C26-C27	-3.26	122.65	127.31
45	3	309	KC2	CAC-C3C-C4C	3.26	139.67	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	302	A86	C19-C18-C17	-3.26	104.47	110.77
31	10	313	CLA	CHB-C4A-NA	3.26	129.02	124.51
43	9	301	A86	C36-C31-C32	3.26	122.93	119.70
43	6	304	A86	O1-C15-C20	-3.26	56.21	59.40
45	13	311	KC2	CBC-CAC-C3C	-3.26	111.39	127.62
31	d	404	CLA	CMB-C2B-C3B	3.26	130.78	124.68
41	v	201	HEM	CMC-C2C-C3C	3.26	130.78	124.68
31	B	610	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
42	p	609	KC1	C1C-C2C-C3C	-3.26	103.53	106.96
42	P	609	KC1	C1C-C2C-C3C	-3.26	103.53	106.96
43	15	302	A86	C22-C16-C17	-3.26	103.32	108.98
31	6	309	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
31	1	315	CLA	CAA-C2A-C3A	-3.26	108.50	116.10
42	17	314	KC1	C3A-C4A-NA	3.26	114.13	110.57
45	11	309	KC2	C3A-C4A-NA	3.26	114.13	110.57
43	p	611	A86	C34-O4-C38	-3.26	111.83	117.90
43	3	301	A86	C23-C16-C22	3.25	112.17	107.37
31	13	313	CLA	O2A-C1-C2	3.25	117.19	108.64
31	3	308	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
31	D	405	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
31	D	404	CLA	CMB-C2B-C3B	3.25	130.76	124.68
43	0	303	A86	C34-O4-C38	3.25	123.96	117.90
43	5	305	A86	C9-C10-C11	-3.25	117.05	126.61
31	16	314	CLA	CAA-C2A-C3A	-3.25	106.14	114.26
45	18	310	KC2	C3B-C2B-C1B	-3.25	103.97	107.08
31	11	312	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
31	3	316	CLA	CHD-C1D-ND	-3.25	121.47	124.45
43	4	305	A86	O1-C20-C19	3.25	115.82	113.38
31	13	312	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
43	2	301	A86	O1-C15-C20	-3.25	56.22	59.40
45	6	312	KC2	CBC-CAC-C3C	-3.25	111.46	127.62
43	10	318	A86	C23-C16-C22	3.25	112.16	107.37
31	2	306	CLA	C3A-C2A-C1A	3.25	106.20	101.34
31	16	313	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
34	b	601	SQD	C3-C4-C5	3.25	116.03	110.24
43	13	303	A86	O4-C38-C39	3.25	117.06	111.09
45	2	310	KC2	C2A-C1A-NA	3.25	114.61	109.40
43	0	302	A86	O2-C18-C19	-3.25	103.35	109.80
42	7	314	KC1	O2D-CGD-CBD	3.25	117.04	111.27
43	1	304	A86	C4-C3-C2	-3.25	116.83	123.47
31	P	605	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
43	7	303	A86	O1-C15-C20	-3.24	56.23	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	505	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	2	307	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
31	d	405	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
34	i	101	SQD	C44-O6-C1	3.24	120.07	113.74
44	P	612	DD6	C13-C11-C10	3.24	123.91	118.94
45	1	309	KC2	CAA-CBA-CGA	-3.24	110.62	127.26
31	9	313	CLA	CHD-C1D-ND	-3.24	121.48	124.45
31	C	505	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
34	A	411	SQD	C44-O6-C1	3.24	120.06	113.74
43	16	305	A86	O1-C15-C20	-3.23	56.24	59.40
43	19	303	A86	C25-C26-C27	-3.23	122.69	127.31
43	6	304	A86	C3-C4-C5	-3.23	116.85	123.47
45	5	308	KC2	CHB-C4A-NA	3.23	129.30	124.20
31	11	313	CLA	CAA-C2A-C3A	-3.23	103.93	112.78
43	P	611	A86	C34-O4-C38	-3.23	111.87	117.90
43	2	303	A86	C4-C5-C6	-3.23	122.70	127.31
43	17	305	A86	C19-C18-C17	3.23	117.02	110.77
42	10	315	KC1	C4C-C3C-C2C	-3.23	102.19	106.90
31	11	313	CLA	CMB-C2B-C3B	3.23	130.72	124.68
43	10	305	A86	C3-C4-C5	-3.23	116.86	123.47
31	1	321	CLA	CHA-C1A-NA	-3.23	119.00	126.40
31	17	307	CLA	CAA-C2A-C3A	-3.23	108.56	116.10
31	6	316	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
43	4	306	A86	C14-C15-C16	-3.23	106.39	118.75
34	B	623	SQD	C3-C4-C5	3.23	116.00	110.24
31	b	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
45	16	310	KC2	C4B-C3B-C2B	-3.23	104.10	106.75
43	3	302	A86	O1-C20-C21	3.23	118.92	115.06
38	1	301	LMG	O1-C7-C8	-3.23	103.12	110.90
43	6	301	A86	O-C13-C14	3.22	128.21	121.66
45	14	310	KC2	C2A-C3A-C4A	3.22	108.88	106.49
43	5	301	A86	C25-C24-C1	-3.22	117.36	126.42
42	7	314	KC1	CMA-C3A-C4A	-3.22	120.13	125.04
43	0	302	A86	C3-C2-C1	-3.22	122.71	127.31
43	2	303	A86	C25-C26-C27	-3.22	122.71	127.31
43	1	304	A86	C3-C4-C5	-3.22	116.87	123.47
31	3	316	CLA	CHB-C4A-NA	3.22	128.97	124.51
31	8	307	CLA	CHB-C4A-NA	3.22	128.97	124.51
31	1	316	CLA	CAA-C2A-C1A	-3.22	105.01	112.14
42	17	314	KC1	CHB-C1B-C2B	-3.22	118.72	125.48
45	14	310	KC2	CHB-C1B-C2B	-3.22	118.73	125.48
38	4	316	LMG	C9-C8-C7	-3.22	104.17	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	304	A86	O1-C15-C20	-3.22	56.25	59.40
45	17	311	KC2	C4D-C3D-CAD	3.22	113.01	107.81
45	7	311	KC2	C4D-C3D-CAD	3.22	113.01	107.81
43	6	301	A86	O1-C15-C20	-3.22	56.25	59.40
38	1	301	LMG	O6-C1-O1	-3.22	102.35	109.97
38	11	301	LMG	O1-C7-C8	-3.22	103.14	110.90
43	15	304	A86	C10-C9-C8	-3.22	113.18	123.22
43	11	306	A86	C20-C19-C18	-3.22	106.39	112.75
31	16	309	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
43	2	301	A86	C4-C3-C2	-3.21	116.89	123.47
31	13	313	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
31	C	510	CLA	CHB-C4A-NA	3.21	128.96	124.51
31	p	601	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
43	7	306	A86	C19-C18-C17	3.21	116.98	110.77
43	13	306	A86	C9-C8-C6	-3.21	117.39	126.42
31	18	306	CLA	C1-C2-C3	-3.21	121.56	126.75
31	p	605	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
45	3	311	KC2	CBC-CAC-C3C	-3.21	111.65	127.62
43	12	303	A86	C23-C16-C17	-3.21	103.41	108.98
43	13	304	A86	O4-C34-C35	3.21	115.58	107.59
43	15	301	A86	O1-C20-C21	3.21	118.90	115.06
43	3	305	A86	C3-C4-C5	-3.21	116.90	123.47
31	8	306	CLA	O2D-CGD-CBD	3.21	116.97	111.27
31	c	506	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
31	7	315	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
42	18	313	KC1	C3A-C4A-NA	3.21	114.07	110.57
43	16	303	A86	C41-C32-C31	-3.21	107.60	110.47
43	9	303	A86	O4-C38-O5	-3.21	116.59	122.96
43	0	305	A86	C22-C16-C17	-3.21	103.41	108.98
42	12	314	KC1	C4B-C3B-C2B	-3.20	104.12	106.75
38	11	301	LMG	O6-C1-O1	-3.20	102.39	109.97
31	14	306	CLA	C1D-ND-C4D	3.20	108.61	106.33
43	11	304	A86	C41-C32-C31	3.20	113.34	110.47
31	11	316	CLA	CAA-C2A-C3A	-3.20	108.62	116.10
45	14	308	KC2	C1A-NA-C4A	-3.20	105.27	106.71
31	B	607	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
39	C	519	DGD	O3G-C3G-C2G	-3.20	103.17	110.90
39	c	519	DGD	O3G-C3G-C2G	-3.20	103.17	110.90
43	6	304	A86	C28-C27-C26	-3.20	118.44	122.92
31	3	315	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
31	c	503	CLA	C3B-C4B-NB	3.20	113.35	109.21
43	17	301	A86	C22-C16-C17	-3.20	103.42	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	320	A86	C25-C24-C1	-3.20	117.43	126.42
31	b	608	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
43	1	319	A86	C40-C32-C33	3.20	123.41	109.05
31	7	308	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
31	19	311	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
43	3	306	A86	C34-O4-C38	3.20	123.85	117.90
35	d	406	PL9	C36-C34-C33	-3.20	114.65	121.12
43	3	305	A86	O-C13-C14	3.20	128.15	121.66
31	15	311	CLA	C2D-C1D-ND	-3.20	107.75	110.10
39	b	622	DGD	O5D-C6D-C5D	-3.20	103.13	109.05
31	C	503	CLA	C3B-C4B-NB	3.19	113.34	109.21
31	15	306	CLA	CMB-C2B-C3B	3.19	130.65	124.68
43	2	305	A86	C3-C2-C1	-3.19	122.75	127.31
31	9	313	CLA	C3C-C4C-NC	-3.19	106.99	110.57
43	8	303	A86	C28-C27-C26	-3.19	118.45	122.92
31	P	601	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
43	5	302	A86	C20-C19-C18	3.19	119.06	112.75
31	b	616	CLA	CAC-C3C-C4C	3.19	128.95	124.81
31	z	101	CLA	CHB-C4A-NA	3.19	128.92	124.51
43	15	302	A86	O1-C15-C20	-3.19	56.28	59.40
43	15	302	A86	O1-C20-C21	3.19	118.87	115.06
45	2	310	KC2	C4B-C3B-C2B	-3.19	104.14	106.75
31	18	311	CLA	CMB-C2B-C3B	3.18	130.64	124.68
45	18	308	KC2	CAA-C2A-C1A	3.18	139.38	124.75
35	D	406	PL9	C36-C34-C33	-3.18	114.67	121.12
31	b	605	CLA	C1-C2-C3	-3.18	120.54	126.04
39	c	518	DGD	C1E-O6E-C5E	3.18	119.94	113.69
43	11	305	A86	O4-C34-C35	3.18	115.52	107.59
31	C	506	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
31	16	316	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
33	y	101	BCR	C3-C4-C5	-3.18	108.40	114.08
31	2	314	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
43	8	304	A86	C4-C3-C2	-3.18	116.97	123.47
31	13	316	CLA	CMB-C2B-C3B	3.18	130.62	124.68
31	9	311	CLA	CBA-CAA-C2A	-3.18	104.48	113.86
45	3	309	KC2	C3B-C2B-C1B	-3.18	104.04	107.08
38	D	403	LMG	O3-C3-C2	-3.18	103.00	110.35
45	3	311	KC2	C4D-C3D-CAD	3.18	112.94	107.81
43	11	304	A86	O1-C20-C21	-3.18	111.25	115.06
43	4	302	A86	O-C13-C11	-3.18	114.13	121.15
45	17	311	KC2	CBC-CAC-C3C	-3.18	111.82	127.62
43	7	305	A86	C3-C2-C1	-3.17	122.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	308	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
31	c	508	CLA	CHB-C4A-NA	3.17	128.90	124.51
31	C	508	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
45	1	309	KC2	O2D-CGD-O1D	-3.17	117.63	123.84
43	16	305	A86	C3-C4-C5	-3.17	116.97	123.47
43	15	304	A86	O4-C38-C39	3.17	116.93	111.09
43	4	306	A86	C41-C32-C40	-3.17	98.79	108.53
45	19	309	KC2	C3A-C4A-NA	3.17	114.03	110.57
43	11	304	A86	O4-C38-C39	3.17	116.92	111.09
43	1	304	A86	C41-C32-C31	3.17	113.31	110.47
31	15	311	CLA	CMA-C3A-C4A	3.17	120.29	111.77
43	14	301	A86	C12-C11-C10	-3.17	115.75	123.42
31	10	307	CLA	C2A-C1A-CHA	3.17	129.40	123.86
38	n	701	LMG	O3-C3-C2	-3.17	103.02	110.35
42	17	314	KC1	C3B-C2B-C1B	-3.17	104.05	107.08
43	3	303	A86	C3-C4-C5	-3.17	116.99	123.47
31	13	307	CLA	CMB-C2B-C3B	3.17	130.60	124.68
43	10	302	A86	O1-C15-C20	-3.16	56.31	59.40
31	3	313	CLA	CAA-CBA-CGA	-3.16	104.01	113.25
31	14	306	CLA	CAA-CBA-CGA	-3.16	104.01	113.25
39	C	518	DGD	O2D-C2D-C1D	-3.16	102.36	110.05
31	7	313	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
31	5	309	CLA	C1-C2-C3	-3.16	120.57	126.04
31	c	510	CLA	CHB-C4A-NA	3.16	128.88	124.51
43	4	302	A86	C4-C3-C2	-3.16	117.00	123.47
45	14	310	KC2	C3B-C2B-C1B	-3.16	104.06	107.08
31	p	606	CLA	CMA-C3A-C4A	3.16	120.27	111.77
33	c	517	BCR	C15-C16-C17	-3.16	117.00	123.47
42	8	313	KC1	C4B-C3B-C2B	-3.16	104.16	106.75
33	Y	101	BCR	C3-C4-C5	-3.16	108.44	114.08
39	C	518	DGD	C1E-O6E-C5E	3.16	119.89	113.69
31	15	312	CLA	CHD-C1D-ND	-3.16	121.55	124.45
43	0	304	A86	C40-C32-C31	3.16	113.30	110.47
31	9	311	CLA	CAA-C2A-C1A	3.16	122.33	111.97
31	P	606	CLA	CMA-C3A-C4A	3.16	120.26	111.77
43	P	613	A86	C25-C26-C27	-3.16	122.80	127.31
31	B	604	CLA	C1-C2-C3	-3.16	120.58	126.04
31	15	309	CLA	C1-C2-C3	-3.16	120.58	126.04
43	11	306	A86	C14-C15-C16	-3.16	106.67	118.75
45	8	308	KC2	C4B-C3B-C2B	-3.16	104.16	106.75
31	b	612	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
31	19	307	CLA	O2D-CGD-O1D	-3.16	117.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	518	DGD	O2D-C2D-C1D	-3.15	102.39	110.05
38	11	317	LMG	C1-C2-C3	-3.15	103.43	110.00
45	5	308	KC2	C2A-C1A-NA	3.15	114.46	109.40
31	2	309	CLA	CHB-C4A-NA	3.15	128.87	124.51
31	c	503	CLA	CHC-C1C-NC	3.15	128.99	124.20
31	12	313	CLA	C3B-C4B-NB	-3.15	105.14	109.21
31	12	312	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
43	0	305	A86	O3-C36-C37	-3.15	103.78	109.39
45	7	311	KC2	CBC-CAC-C3C	-3.15	111.95	127.62
31	1	316	CLA	CAA-C2A-C3A	-3.15	106.39	114.26
31	9	307	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
31	C	508	CLA	CHB-C4A-NA	3.15	128.86	124.51
43	2	304	A86	C3-C2-C1	-3.15	122.82	127.31
43	11	302	A86	C40-C32-C33	3.14	123.17	109.05
43	19	304	A86	C12-C11-C13	3.14	121.30	116.02
43	1	305	A86	O1-C15-C20	-3.14	56.33	59.40
31	8	307	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
31	B	604	CLA	CHB-C4A-NA	3.14	128.86	124.51
43	16	302	A86	C19-C18-C17	-3.14	104.71	110.77
31	11	307	CLA	C1D-ND-C4D	3.14	108.57	106.33
31	1	310	CLA	CHB-C4A-NA	3.14	128.85	124.51
43	6	305	A86	O4-C38-O5	-3.14	116.73	122.96
31	17	310	CLA	CHB-C4A-NA	3.14	128.85	124.51
31	13	307	CLA	CAC-C3C-C4C	3.14	128.88	124.81
43	19	305	A86	C14-C15-C16	-3.14	106.74	118.75
43	3	303	A86	C40-C32-C33	3.14	123.13	109.05
38	p	614	LMG	O6-C1-O1	-3.14	102.55	109.97
31	1	308	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
43	10	302	A86	C35-C34-C33	-3.14	104.40	109.88
31	c	508	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
31	B	611	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
31	18	306	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
38	k	101	LMG	O1-C7-C8	-3.13	103.34	110.90
43	14	303	A86	C40-C32-C31	3.13	113.28	110.47
31	Z	101	CLA	CHB-C4A-NA	3.13	128.84	124.51
45	13	309	KC2	C4B-C3B-C2B	-3.13	104.18	106.75
43	p	613	A86	C25-C26-C27	-3.13	122.84	127.31
38	K	101	LMG	O1-C7-C8	-3.13	103.34	110.90
31	8	312	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
43	12	305	A86	C9-C10-C11	-3.13	117.41	126.61
43	13	302	A86	C19-C18-C17	-3.13	104.73	110.77
39	C	520	DGD	O5D-C6D-C5D	-3.13	103.26	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	13	301	A86	C9-C8-C6	-3.13	117.63	126.42
31	c	514	CLA	CHB-C4A-NA	3.13	128.84	124.51
31	A	406	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
38	P	614	LMG	O6-C1-O1	-3.13	102.57	109.97
38	B	620	LMG	O1-C7-C8	-3.13	103.35	110.90
31	p	604	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
31	16	314	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
45	3	311	KC2	C3B-C2B-C1B	-3.13	104.09	107.08
43	9	304	A86	C28-C27-C26	-3.12	118.55	122.92
41	e	101	HEM	CMC-C2C-C3C	3.12	130.52	124.68
45	13	309	KC2	C3B-C2B-C1B	-3.12	104.09	107.08
45	3	309	KC2	C4B-C3B-C2B	-3.12	104.19	106.75
33	C	517	BCR	C15-C16-C17	-3.12	117.07	123.47
31	8	314	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
31	3	307	CLA	O2D-CGD-CBD	3.12	116.81	111.27
43	P	613	A86	C40-C32-C33	-3.12	95.03	109.05
43	0	302	A86	C28-C27-C26	-3.12	118.55	122.92
45	2	310	KC2	C3A-C4A-NA	3.12	113.98	110.57
31	C	514	CLA	CHB-C4A-NA	3.12	128.82	124.51
43	10	318	A86	C19-C18-C17	-3.12	104.75	110.77
31	a	406	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
43	p	613	A86	C40-C32-C33	-3.12	95.05	109.05
31	b	605	CLA	CHB-C4A-NA	3.12	128.82	124.51
42	5	313	KC1	C3B-C2B-C1B	-3.12	104.10	107.08
41	E	101	HEM	CMC-C2C-C3C	3.12	130.51	124.68
39	c	520	DGD	O5D-C6D-C5D	-3.11	103.28	109.05
31	B	605	CLA	CMA-C3A-C4A	3.11	120.14	111.77
43	3	302	A86	C36-C31-C32	3.11	122.78	119.70
35	d	406	PL9	C22-C23-C24	-3.11	120.17	127.66
31	c	504	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
43	4	302	A86	C36-C31-C32	3.11	122.78	119.70
43	19	302	A86	C9-C10-C11	-3.11	117.46	126.61
35	D	406	PL9	C22-C23-C24	-3.11	120.17	127.66
41	V	201	HEM	C4A-C3A-C2A	3.11	109.16	107.00
43	12	304	A86	C28-C27-C26	-3.11	118.57	122.92
38	d	403	LMG	O3-C3-C2	-3.11	103.16	110.35
43	2	302	A86	C41-C32-C31	-3.11	107.69	110.47
43	6	305	A86	C3-C4-C5	-3.11	117.11	123.47
43	6	302	A86	O1-C20-C21	3.11	118.78	115.06
43	12	306	A86	C4-C3-C2	-3.11	117.11	123.47
38	b	621	LMG	O1-C7-C8	-3.11	103.40	110.90
31	c	512	CLA	O2D-CGD-O1D	-3.11	117.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	604	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
43	17	306	A86	C3-C2-C1	-3.11	122.88	127.31
43	11	304	A86	C3-C4-C5	-3.11	117.11	123.47
42	4	313	KC1	O2D-CGD-O1D	-3.11	117.77	123.84
39	11	318	DGD	O6D-C1D-O3G	-3.10	102.62	109.97
42	19	314	KC1	C4C-C3C-C2C	-3.10	102.37	106.90
42	18	313	KC1	O2D-CGD-CBD	3.10	116.78	111.27
43	13	305	A86	O1-C15-C20	-3.10	56.37	59.40
31	7	307	CLA	CMB-C2B-C3B	3.10	130.48	124.68
43	1	319	A86	C12-C11-C13	3.10	121.23	116.02
31	C	503	CLA	CHC-C1C-NC	3.10	128.91	124.20
43	1	302	A86	C4-C3-C2	-3.10	117.12	123.47
31	19	313	CLA	C3C-C4C-NC	-3.10	107.09	110.57
43	10	302	A86	O-C13-C11	-3.10	114.30	121.15
43	11	305	A86	C3-C2-C1	-3.10	122.89	127.31
33	C	515	BCR	C15-C16-C17	-3.10	117.13	123.47
43	2	305	A86	C22-C16-C17	-3.10	103.60	108.98
43	17	316	A86	C10-C9-C8	-3.10	113.55	123.22
42	16	315	KC1	C3A-C4A-NA	3.10	113.95	110.57
43	3	305	A86	C20-C19-C18	-3.10	106.62	112.75
43	15	303	A86	C40-C32-C31	3.10	113.24	110.47
31	p	606	CLA	C3C-C4C-NC	-3.09	107.10	110.57
42	11	314	KC1	O2D-CGD-CBD	3.09	116.77	111.27
38	15	314	LMG	O6-C1-O1	-3.09	102.65	109.97
43	4	303	A86	C12-C11-C13	3.09	121.22	116.02
43	17	301	A86	O-C13-C14	3.09	127.94	121.66
31	15	311	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
43	9	305	A86	C14-C15-C16	-3.09	106.91	118.75
43	17	302	A86	C4-C3-C2	-3.09	117.14	123.47
31	a	404	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
31	12	312	CLA	CMB-C2B-C3B	3.09	130.46	124.68
31	C	512	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
43	0	304	A86	C41-C32-C40	-3.09	99.05	108.53
31	b	616	CLA	CHB-C4A-NA	3.09	128.78	124.51
31	d	405	CLA	CHB-C4A-NA	3.09	128.78	124.51
43	10	305	A86	C22-C16-C17	-3.09	103.62	108.98
31	C	504	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
43	17	306	A86	C23-C16-C22	3.09	111.92	107.37
39	b	622	DGD	C1D-O6D-C5D	-3.09	107.63	113.69
31	6	311	CLA	CHB-C4A-NA	3.09	128.78	124.51
31	P	606	CLA	C3C-C4C-NC	-3.09	107.11	110.57
31	12	313	CLA	C4A-NA-C1A	3.09	108.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	302	A86	C9-C8-C6	-3.08	117.75	126.42
31	8	307	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
31	13	312	CLA	O2A-CGA-O1A	-3.08	115.61	123.30
43	14	302	A86	C40-C32-C31	-3.08	107.71	110.47
43	1	319	A86	C19-C18-C17	-3.08	104.82	110.77
31	8	312	CLA	CMB-C2B-C3B	3.08	130.45	124.68
31	1	308	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
31	5	306	CLA	CMB-C2B-C3B	3.08	130.44	124.68
38	P	614	LMG	O1-C1-C2	-3.08	103.49	108.30
31	B	615	CLA	CHB-C4A-NA	3.08	128.77	124.51
42	11	314	KC1	C4C-C3C-C2C	-3.08	102.41	106.90
31	6	309	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
32	d	402	PHO	O2D-CGD-O1D	-3.08	117.82	123.84
31	4	312	CLA	O2A-C1-C2	3.08	116.73	108.64
45	4	308	KC2	C1A-NA-C4A	-3.08	105.32	106.71
31	16	311	CLA	CHB-C4A-NA	3.08	128.77	124.51
43	1	305	A86	C41-C32-C33	3.08	122.86	109.05
43	11	303	A86	C12-C11-C13	3.08	121.19	116.02
33	c	515	BCR	C15-C16-C17	-3.08	117.17	123.47
31	14	315	CLA	CHD-C1D-ND	-3.07	121.63	124.45
33	b	619	BCR	C11-C10-C9	-3.07	122.92	127.31
31	b	615	CLA	CHB-C4A-NA	3.07	128.76	124.51
31	4	314	CLA	CHB-C4A-NA	3.07	128.76	124.51
45	15	310	KC2	CBD-CHA-C1A	3.07	134.61	128.88
43	0	303	A86	C21-C20-C19	-3.07	110.82	114.28
31	14	314	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	4	311	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
31	0	307	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
43	1	306	A86	C23-C16-C17	-3.07	103.64	108.98
31	0	308	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
32	D	402	PHO	O2D-CGD-O1D	-3.07	117.83	123.84
31	19	313	CLA	C3A-C2A-C1A	3.07	105.94	101.34
43	13	305	A86	O1-C20-C19	-3.07	111.08	113.38
43	16	307	A86	C41-C32-C31	3.07	113.22	110.47
38	p	614	LMG	O1-C1-C2	-3.07	103.51	108.30
31	d	404	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
45	15	308	KC2	C3C-C2C-C1C	3.07	108.76	106.49
43	6	306	A86	C22-C16-C17	-3.07	103.65	108.98
31	b	602	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
31	A	404	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
42	16	315	KC1	C1B-CHB-C4A	-3.07	119.44	126.06
31	17	315	CLA	O2D-CGD-O1D	-3.07	117.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	13	301	A86	C23-C16-C22	-3.07	102.85	107.37
45	6	312	KC2	C2A-C1A-NA	3.07	114.32	109.40
31	D	405	CLA	CHB-C4A-NA	3.07	128.75	124.51
31	c	506	CLA	CHB-C4A-NA	3.07	128.75	124.51
43	3	304	A86	O4-C38-C39	3.07	116.73	111.09
31	c	507	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
43	2	302	A86	C28-C27-C26	-3.06	118.63	122.92
31	2	312	CLA	CHA-C4D-ND	3.06	138.91	132.50
31	13	307	CLA	CHB-C4A-NA	3.06	128.75	124.51
31	4	314	CLA	CMB-C2B-C3B	3.06	130.41	124.68
45	4	310	KC2	CHB-C1B-C2B	-3.06	119.06	125.48
31	B	601	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
33	Y	101	BCR	C27-C26-C25	3.06	127.18	122.73
43	18	304	A86	C4-C3-C2	-3.06	117.20	123.47
31	11	310	CLA	CHB-C4A-NA	3.06	128.75	124.51
31	b	606	CLA	CMA-C3A-C4A	3.06	120.00	111.77
43	13	301	A86	O-C13-C14	-3.06	115.44	121.66
43	10	301	A86	C9-C8-C6	-3.06	117.82	126.42
39	b	622	DGD	O2D-C2D-C1D	-3.06	102.61	110.05
43	12	306	A86	C40-C32-C33	3.06	122.79	109.05
43	5	302	A86	O1-C15-C20	-3.06	56.41	59.40
42	11	314	KC1	C2A-C1A-NA	3.06	114.31	109.40
31	14	314	CLA	CMB-C2B-C3B	3.06	130.40	124.68
43	14	304	A86	C4-C3-C2	-3.06	117.21	123.47
43	18	305	A86	C4-C3-C2	-3.06	117.21	123.47
43	16	307	A86	C22-C16-C17	-3.06	103.67	108.98
43	10	304	A86	O1-C20-C21	-3.06	111.39	115.06
43	13	302	A86	C9-C8-C6	-3.06	117.83	126.42
31	3	308	CLA	CMB-C2B-C3B	3.06	130.40	124.68
31	3	312	CLA	CMB-C2B-C3B	3.06	130.40	124.68
31	13	308	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
42	2	313	KC1	C4C-C3C-C2C	-3.06	102.44	106.90
43	19	301	A86	C3-C2-C1	-3.06	122.95	127.31
31	W	202	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
41	v	201	HEM	C4A-C3A-C2A	3.05	109.12	107.00
43	12	302	A86	C40-C32-C33	3.05	122.76	109.05
45	8	310	KC2	C3B-C2B-C1B	-3.05	104.16	107.08
31	a	404	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
39	w	204	DGD	C1E-O6E-C5E	3.05	119.68	113.69
31	b	605	CLA	CHC-C1C-NC	3.05	128.83	124.20
43	15	305	A86	C36-C31-C32	3.05	122.72	119.70
31	17	312	CLA	CMB-C2B-C3B	3.05	130.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	306	CLA	CAA-C2A-C3A	-3.05	106.64	114.26
33	y	101	BCR	C27-C26-C25	3.05	127.16	122.73
31	w	203	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
43	7	306	A86	O4-C34-C33	3.05	115.19	107.59
31	C	507	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
43	17	303	A86	C20-C19-C18	-3.05	106.72	112.75
43	0	305	A86	C36-C31-C32	-3.05	116.67	119.70
43	6	307	A86	O1-C15-C20	-3.05	56.42	59.40
31	18	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	8	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	B	606	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
31	10	307	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
45	0	310	KC2	CAB-C3B-C4B	-3.04	117.55	124.90
43	1	306	A86	O-C13-C11	-3.04	114.42	121.15
39	C	520	DGD	O6D-C5D-C6D	-3.04	100.52	106.67
42	18	313	KC1	C3B-C2B-C1B	-3.04	104.17	107.08
43	4	305	A86	C41-C32-C40	3.04	117.86	108.53
42	2	313	KC1	C2B-C1B-NB	3.04	112.34	110.10
31	B	614	CLA	CHB-C4A-NA	3.04	128.72	124.51
31	b	602	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
33	B	618	BCR	C11-C10-C9	-3.04	122.97	127.31
39	11	318	DGD	O6E-C5E-C4E	3.04	115.22	109.69
31	12	312	CLA	CHB-C4A-NA	3.04	128.72	124.51
43	19	305	A86	C28-C27-C26	-3.04	118.67	122.92
31	D	404	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
39	W	203	DGD	C1E-O6E-C5E	3.04	119.65	113.69
31	B	601	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	6	308	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
43	6	303	A86	C21-C20-C19	-3.04	110.86	114.28
39	c	520	DGD	O6D-C5D-C6D	-3.04	100.53	106.67
45	12	311	KC2	C2B-C1B-NB	3.04	112.34	110.10
31	p	608	CLA	CHB-C4A-NA	3.04	128.71	124.51
43	10	301	A86	C34-O4-C38	3.03	123.55	117.90
43	11	302	A86	C14-C15-C16	-3.03	107.14	118.75
43	1	320	A86	C12-C11-C13	3.03	121.12	116.02
43	9	302	A86	C9-C10-C11	-3.03	117.69	126.61
31	18	306	CLA	O2D-CGD-CBD	3.03	116.66	111.27
43	1	302	A86	C25-C24-C1	-3.03	117.90	126.42
45	17	311	KC2	C3A-C4A-NA	3.03	113.88	110.57
45	3	311	KC2	CAB-C3B-C4B	-3.03	117.58	124.90
43	9	305	A86	O-C13-C11	-3.03	114.45	121.15
43	8	303	A86	C26-C25-C24	-3.03	113.77	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	13	311	KC2	CMD-C2D-C1D	3.03	133.12	128.46
31	11	313	CLA	C4-C3-C5	-3.03	110.18	115.27
45	17	311	KC2	C2B-C1B-NB	3.03	112.33	110.10
31	14	315	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
31	9	311	CLA	C3A-C2A-C1A	3.03	105.87	101.34
43	0	301	A86	C9-C8-C6	-3.03	117.92	126.42
31	B	604	CLA	CHC-C1C-NC	3.03	128.79	124.20
45	18	308	KC2	C4B-C3B-C2B	-3.02	104.27	106.75
43	10	304	A86	C41-C32-C40	-3.02	99.25	108.53
43	4	301	A86	C4-C3-C2	-3.02	117.29	123.47
31	P	608	CLA	CHB-C4A-NA	3.02	128.69	124.51
31	B	602	CLA	CMC-C2C-C1C	-3.02	120.44	125.04
43	9	303	A86	O3-C36-C37	-3.02	104.02	109.39
43	3	303	A86	O4-C34-C33	-3.02	100.07	107.59
45	2	310	KC2	C4D-C3D-CAD	3.02	112.69	107.81
43	16	302	A86	C22-C16-C17	-3.02	103.74	108.98
31	18	314	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
43	9	302	A86	O4-C38-C39	3.02	116.64	111.09
31	2	311	CLA	CMB-C2B-C3B	3.02	130.32	124.68
43	2	302	A86	C9-C8-C6	-3.02	117.95	126.42
31	6	314	CLA	CAA-C2A-C3A	-3.02	106.73	114.26
31	b	603	CLA	CMC-C2C-C1C	-3.01	120.45	125.04
43	3	302	A86	C34-O4-C38	3.01	123.51	117.90
31	13	312	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
43	4	302	A86	O1-C20-C19	3.01	115.65	113.38
43	3	305	A86	C3-C2-C1	-3.01	123.01	127.31
43	10	304	A86	C3-C2-C1	-3.01	123.01	127.31
42	4	313	KC1	CGD-CBD-CAD	-3.01	100.97	110.73
31	B	609	CLA	CHB-C4A-NA	3.01	128.68	124.51
43	12	303	A86	C4-C5-C6	-3.01	123.01	127.31
43	9	305	A86	C20-C19-C18	-3.01	106.79	112.75
31	16	314	CLA	CHD-C1D-C2D	3.01	131.80	125.48
31	c	505	CLA	CMB-C2B-C3B	3.01	130.31	124.68
43	0	306	A86	O1-C20-C19	3.01	115.64	113.38
43	2	302	A86	C34-O4-C38	3.01	123.51	117.90
43	16	303	A86	O4-C34-C35	3.01	115.09	107.59
43	5	318	A86	C4-C3-C2	-3.01	117.31	123.47
31	4	315	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
43	4	305	A86	C41-C32-C33	3.01	122.56	109.05
43	10	305	A86	O4-C38-O5	-3.01	116.98	122.96
31	17	308	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
31	14	312	CLA	CAA-C2A-C3A	-3.01	104.54	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	301	A86	O4-C34-C35	3.01	115.08	107.59
31	C	502	CLA	CHB-C4A-NA	3.01	128.67	124.51
31	b	611	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
45	0	310	KC2	CGD-CBD-CAD	-3.01	101.00	110.73
43	14	301	A86	C9-C10-C11	-3.01	117.77	126.61
43	14	304	A86	O1-C20-C19	3.01	115.64	113.38
43	6	302	A86	O4-C34-C35	3.00	115.07	107.59
31	b	610	CLA	CHB-C4A-NA	3.00	128.66	124.51
31	C	506	CLA	CHB-C4A-NA	3.00	128.66	124.51
43	6	301	A86	C28-C27-C29	3.00	125.88	118.93
31	b	607	CLA	O2A-CGA-O1A	-3.00	116.02	123.59
45	3	311	KC2	CAB-C3B-C2B	3.00	138.49	128.60
43	17	303	A86	C25-C24-C1	-3.00	117.99	126.42
31	14	314	CLA	CHB-C4A-NA	3.00	128.66	124.51
43	12	304	A86	C3-C2-C1	-3.00	123.03	127.31
45	16	312	KC2	C3B-C2B-C1B	-3.00	104.21	107.08
43	13	306	A86	C9-C10-C11	-3.00	117.79	126.61
33	B	618	BCR	C15-C16-C17	-3.00	117.33	123.47
31	7	310	CLA	CHB-C4A-NA	3.00	128.66	124.51
45	9	309	KC2	C3A-C4A-NA	3.00	113.84	110.57
31	C	505	CLA	CMB-C2B-C3B	3.00	130.28	124.68
31	B	610	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
38	N	101	LMG	O3-C3-C2	-3.00	103.42	110.35
45	6	312	KC2	CAB-C3B-C4B	-3.00	117.66	124.90
45	1	311	KC2	C2B-C1B-NB	2.99	112.31	110.10
31	A	404	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
31	5	309	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
31	0	313	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
31	C	513	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
43	4	301	A86	O1-C15-C20	-2.99	56.47	59.40
31	18	307	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
43	4	302	A86	C28-C27-C26	-2.99	118.73	122.92
31	0	313	CLA	C2A-C1A-CHA	2.99	129.09	123.86
43	16	304	A86	O1-C15-C20	-2.99	56.48	59.40
31	B	615	CLA	CAC-C3C-C4C	2.99	128.69	124.81
45	3	311	KC2	C3C-C2C-C1C	-2.99	104.27	106.49
43	13	302	A86	C25-C24-C1	-2.99	118.01	126.42
43	4	303	A86	O-C13-C14	-2.99	115.58	121.66
31	8	307	CLA	C7-C6-C5	-2.99	105.24	113.36
31	2	306	CLA	CHB-C4A-NA	2.99	128.65	124.51
42	0	315	KC1	C2B-C1B-NB	2.99	112.31	110.10
45	6	312	KC2	C4D-C3D-CAD	2.99	112.64	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	302	A86	C12-C11-C13	2.99	121.04	116.02
31	c	502	CLA	CHB-C4A-NA	2.99	128.65	124.51
45	5	308	KC2	C3C-C2C-C1C	2.99	108.70	106.49
45	1	309	KC2	CAA-C2A-C1A	2.99	138.48	124.75
31	4	314	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	2	307	CLA	CHB-C4A-NA	2.99	128.64	124.51
43	13	302	A86	O-C13-C11	-2.99	114.55	121.15
34	b	601	SQD	C44-O6-C1	2.99	119.58	113.74
31	2	315	CLA	C2D-C1D-ND	2.99	112.30	110.10
45	6	312	KC2	CAB-C3B-C2B	2.98	138.44	128.60
43	12	306	A86	C22-C16-C17	-2.98	103.80	108.98
45	16	312	KC2	C4D-C3D-CAD	2.98	112.63	107.81
43	0	306	A86	C36-C31-C32	-2.98	116.74	119.70
31	13	312	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
31	6	308	CLA	CAC-C3C-C2C	-2.98	122.43	127.53
43	P	613	A86	C41-C32-C40	-2.98	99.38	108.53
31	3	316	CLA	CMB-C2B-C3B	2.98	130.25	124.68
43	p	613	A86	C41-C32-C40	-2.98	99.38	108.53
43	11	304	A86	O1-C15-C20	-2.98	56.49	59.40
43	17	306	A86	C22-C16-C17	-2.98	103.81	108.98
33	c	515	BCR	C24-C23-C22	-2.98	121.73	126.23
33	c	517	BCR	C24-C23-C22	-2.98	121.73	126.23
33	b	619	BCR	C15-C16-C17	-2.98	117.37	123.47
36	P	615	LHG	O8-C23-C24	2.98	119.19	111.38
43	7	306	A86	O4-C38-C39	2.98	116.57	111.09
43	3	304	A86	O1-C15-C20	-2.98	56.49	59.40
31	3	307	CLA	CHB-C4A-NA	2.98	128.63	124.51
31	0	314	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
34	B	623	SQD	C44-O6-C1	2.98	119.56	113.74
43	13	302	A86	C3-C4-C5	-2.98	117.38	123.47
43	16	306	A86	C28-C27-C26	-2.98	118.75	122.92
31	16	309	CLA	CHB-C4A-NA	2.98	128.63	124.51
33	C	517	BCR	C24-C23-C22	-2.98	121.74	126.23
43	4	306	A86	C7-C6-C8	2.97	122.76	118.08
31	C	512	CLA	CMB-C2B-C3B	2.97	130.24	124.68
31	10	317	CLA	O2D-CGD-CBD	2.97	116.55	111.27
31	3	312	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
31	3	310	CLA	CHB-C4A-NA	2.97	128.62	124.51
43	12	303	A86	O-C13-C11	-2.97	114.59	121.15
43	3	301	A86	C4-C3-C2	-2.97	117.39	123.47
45	18	308	KC2	C3B-C2B-C1B	-2.97	104.24	107.08
45	12	309	KC2	C4D-C3D-CAD	2.97	112.61	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	605	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
31	19	313	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
31	7	307	CLA	CAA-C2A-C3A	-2.97	109.17	116.10
31	18	314	CLA	CHB-C4A-NA	2.97	128.62	124.51
42	8	313	KC1	CAA-CBA-CGA	-2.97	112.01	127.26
31	c	512	CLA	CMB-C2B-C3B	2.97	130.23	124.68
43	16	304	A86	C9-C8-C6	-2.97	118.08	126.42
31	15	309	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
31	13	316	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
31	r	101	CLA	CHB-C4A-NA	2.97	128.61	124.51
43	3	303	A86	C9-C8-C6	-2.97	118.08	126.42
31	W	202	CLA	CMB-C2B-C3B	2.97	130.23	124.68
43	9	305	A86	O-C13-C14	2.97	127.69	121.66
31	c	513	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
43	P	611	A86	C19-C18-C17	2.97	116.50	110.77
43	13	301	A86	O1-C15-C20	-2.96	56.50	59.40
43	5	302	A86	C28-C27-C26	-2.96	118.77	122.92
42	10	315	KC1	C4D-C3D-CAD	2.96	112.60	107.81
31	11	310	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
31	3	308	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
31	12	307	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
31	17	307	CLA	CMB-C2B-C3B	2.96	130.22	124.68
43	16	302	A86	C20-C19-C18	2.96	118.61	112.75
33	C	515	BCR	C24-C23-C22	-2.96	121.76	126.23
31	B	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
31	1	310	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
43	3	301	A86	O1-C15-C20	-2.96	56.51	59.40
36	p	615	LHG	O8-C23-C24	2.96	119.14	111.38
42	19	314	KC1	C3B-C2B-C1B	-2.96	104.25	107.08
31	B	606	CLA	CHD-C1D-ND	-2.96	121.73	124.45
43	7	302	A86	C25-C24-C1	-2.96	118.11	126.42
45	18	310	KC2	C4D-C3D-CAD	2.96	112.59	107.81
43	12	304	A86	C34-O4-C38	-2.96	112.39	117.90
31	16	309	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
43	17	301	A86	O1-C15-C20	-2.96	56.51	59.40
31	19	315	CLA	CHB-C4A-NA	2.96	128.60	124.51
31	8	307	CLA	OBD-CAD-C3D	2.96	135.63	128.52
45	8	308	KC2	C3B-C2B-C1B	-2.96	104.25	107.08
43	18	305	A86	C9-C8-C6	-2.96	118.11	126.42
43	p	611	A86	C19-C18-C17	2.96	116.48	110.77
43	7	301	A86	C34-O4-C38	2.96	123.40	117.90
43	14	302	A86	C36-C31-C32	2.95	122.63	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	14	304	A86	O1-C15-C20	-2.95	56.51	59.40
43	15	302	A86	O-C13-C14	2.95	127.66	121.66
43	2	301	A86	C4-C5-C6	-2.95	123.09	127.31
31	B	604	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
45	4	308	KC2	CAA-C2A-C1A	2.95	138.32	124.75
31	12	308	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
43	9	303	A86	O1-C20-C19	2.95	115.60	113.38
43	11	305	A86	C9-C10-C11	-2.95	117.93	126.61
43	14	304	A86	C3-C2-C1	2.95	131.52	127.31
43	6	302	A86	C34-O4-C38	2.95	123.40	117.90
31	b	605	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
42	1	314	KC1	C2A-C3A-C4A	2.95	108.67	106.49
31	p	610	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
43	15	302	A86	C23-C16-C22	2.95	111.72	107.37
31	8	312	CLA	CBA-CAA-C2A	2.95	122.57	113.86
31	14	311	CLA	CBC-CAC-C3C	2.95	120.56	112.43
31	11	313	CLA	CHB-C4A-NA	2.95	128.59	124.51
45	16	312	KC2	C3C-C2C-C1C	-2.95	104.30	106.49
43	8	304	A86	C9-C10-C11	-2.95	117.94	126.61
31	R	101	CLA	CHB-C4A-NA	2.95	128.59	124.51
43	12	305	A86	O-C13-C11	-2.95	114.63	121.15
31	12	310	CLA	CHB-C4A-NA	2.95	128.59	124.51
31	b	609	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
43	16	307	A86	C26-C25-C24	-2.95	114.02	123.22
43	2	304	A86	C4-C3-C2	-2.95	117.44	123.47
45	12	309	KC2	C3B-C2B-C1B	-2.95	104.26	107.08
31	3	316	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
31	C	509	CLA	CHB-C4A-NA	2.95	128.59	124.51
31	r	101	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
43	10	305	A86	C36-C31-C32	-2.95	116.77	119.70
43	9	306	A86	C17-C16-C15	2.95	112.17	109.16
45	6	312	KC2	C3B-C2B-C1B	-2.95	104.26	107.08
31	D	401	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
31	w	203	CLA	CMB-C2B-C3B	2.94	130.19	124.68
31	b	607	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
43	19	305	A86	C20-C19-C18	-2.94	106.92	112.75
42	16	301	KC1	C3B-C2B-C1B	-2.94	104.26	107.08
45	2	310	KC2	C2A-C3A-C4A	2.94	108.67	106.49
31	c	509	CLA	CHB-C4A-NA	2.94	128.58	124.51
31	C	503	CLA	C16-C15-C13	-2.94	106.41	115.92
42	16	315	KC1	CMA-C3A-C4A	-2.94	120.56	125.04
31	11	315	CLA	CMB-C2B-C3B	2.94	130.18	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	503	CLA	C16-C15-C13	-2.94	106.41	115.92
43	0	304	A86	C3-C2-C1	-2.94	123.11	127.31
31	d	401	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	8	306	CLA	C2A-C1A-CHA	2.94	129.00	123.86
31	15	306	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
45	16	312	KC2	CAB-C3B-C2B	2.94	138.29	128.60
42	14	313	KC1	C3D-CAD-CBD	2.94	111.48	107.61
43	8	302	A86	O4-C34-C35	2.94	114.91	107.59
31	P	610	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
43	6	301	A86	O1-C20-C19	-2.94	111.17	113.38
43	5	302	A86	C4-C3-C2	-2.94	117.45	123.47
31	P	603	CLA	CMD-C2D-C1D	-2.94	119.53	124.71
38	J	101	LMG	O1-C7-C8	-2.94	103.81	110.90
43	P	611	A86	O4-C38-C39	2.94	116.50	111.09
43	12	303	A86	C25-C26-C27	-2.94	123.12	127.31
31	14	311	CLA	CHB-C4A-NA	2.94	128.57	124.51
31	18	312	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
43	18	301	A86	C4-C3-C2	-2.94	117.46	123.47
43	3	306	A86	C22-C16-C17	-2.93	103.88	108.98
43	10	306	A86	C40-C32-C31	2.93	113.10	110.47
43	16	306	A86	C40-C32-C31	-2.93	107.85	110.47
31	c	510	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
31	15	312	CLA	OBD-CAD-C3D	2.93	135.58	128.52
39	C	519	DGD	C3G-C2G-C1G	-2.93	104.85	111.79
31	18	306	CLA	C2A-C1A-CHA	2.93	128.99	123.86
31	R	101	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
31	17	307	CLA	CHB-C4A-NA	2.93	128.56	124.51
42	16	301	KC1	C3C-C4C-NC	2.93	112.63	109.88
31	C	514	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
31	1	313	CLA	C1-C2-C3	-2.93	120.98	126.04
43	7	305	A86	C22-C16-C17	-2.93	103.90	108.98
31	9	313	CLA	C3A-C2A-C1A	2.93	105.72	101.34
43	5	304	A86	O-C13-C11	-2.93	114.69	121.15
43	17	301	A86	C3-C4-C5	-2.93	117.48	123.47
31	7	307	CLA	CHB-C4A-NA	2.92	128.56	124.51
38	j	101	LMG	O1-C7-C8	-2.92	103.84	110.90
42	5	313	KC1	C2B-C1B-NB	2.92	112.26	110.10
39	c	519	DGD	C3G-C2G-C1G	-2.92	104.87	111.79
31	1	316	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
43	16	302	A86	O-C13-C14	2.92	127.60	121.66
31	4	311	CLA	CHB-C4A-NA	2.92	128.55	124.51
45	8	310	KC2	CBC-CAC-C3C	-2.92	113.09	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	312	CLA	C4D-C3D-CAD	-2.92	104.65	108.10
43	p	611	A86	O4-C38-C39	2.92	116.46	111.09
45	18	310	KC2	CBC-CAC-C3C	-2.92	113.09	127.62
45	7	309	KC2	C4B-C3B-C2B	-2.92	104.35	106.75
42	17	314	KC1	C2A-C1A-NA	2.92	114.09	109.40
31	12	313	CLA	CMB-C2B-C3B	2.92	130.14	124.68
45	12	311	KC2	C3B-C2B-C1B	-2.92	104.29	107.08
31	15	313	CLA	C2D-C1D-ND	-2.92	107.95	110.10
31	P	607	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
45	17	309	KC2	C4B-C3B-C2B	-2.92	104.36	106.75
43	15	305	A86	O1-C20-C21	-2.92	111.56	115.06
39	b	622	DGD	C2G-O2G-C1B	2.92	124.98	117.79
43	8	303	A86	O4-C34-C33	2.92	114.86	107.59
31	P	607	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
31	6	309	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
34	0	318	SQD	C44-O6-C1	2.92	119.44	113.74
39	b	622	DGD	C1E-C2E-C3E	-2.92	103.92	110.00
31	9	311	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
31	14	311	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
43	10	306	A86	O1-C15-C20	-2.92	56.55	59.40
42	7	314	KC1	C4B-C3B-C2B	-2.92	104.36	106.75
43	19	301	A86	C28-C27-C29	2.92	125.68	118.93
31	C	510	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
45	14	310	KC2	O2D-CGD-O1D	-2.92	118.14	123.84
43	0	302	A86	O1-C15-C20	-2.92	56.55	59.40
43	8	302	A86	C10-C9-C8	-2.92	114.12	123.22
43	15	302	A86	O4-C34-C35	-2.92	100.33	107.59
31	P	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
43	13	304	A86	C20-C19-C18	-2.91	106.98	112.75
43	4	305	A86	O1-C15-C20	-2.91	56.55	59.40
31	16	309	CLA	CMB-C2B-C3B	2.91	130.13	124.68
31	14	312	CLA	C2D-C1D-ND	-2.91	107.96	110.10
43	7	306	A86	C12-C11-C13	2.91	120.91	116.02
43	19	301	A86	C4-C3-C2	-2.91	117.51	123.47
31	13	310	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
43	9	303	A86	C23-C16-C22	-2.91	103.08	107.37
31	p	603	CLA	CMD-C2D-C1D	-2.91	119.58	124.71
43	15	304	A86	O1-C15-C20	-2.91	56.55	59.40
31	10	307	CLA	CHA-C1A-NA	-2.91	119.73	126.40
43	15	304	A86	C4-C3-C2	-2.91	117.51	123.47
31	c	507	CLA	CHB-C4A-NA	2.91	128.54	124.51
31	16	308	CLA	C2A-C1A-CHA	2.91	128.95	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	314	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	18	311	CLA	C2A-C1A-CHA	2.91	128.94	123.86
31	b	602	CLA	CHB-C4A-NA	2.91	128.53	124.51
31	D	401	CLA	CHB-C4A-NA	2.91	128.53	124.51
43	P	613	A86	C35-C34-C33	-2.91	104.80	109.88
31	13	315	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	1	312	CLA	O1D-CGD-CBD	2.91	130.43	124.48
43	2	304	A86	C9-C10-C11	-2.91	118.06	126.61
42	5	313	KC1	C3A-C4A-NA	2.91	113.75	110.57
31	12	307	CLA	O2D-CGD-CBD	2.91	116.43	111.27
43	19	305	A86	O-C13-C11	-2.91	114.73	121.15
31	13	312	CLA	CHB-C4A-NA	2.90	128.53	124.51
31	c	514	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
31	10	308	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
31	2	307	CLA	CMB-C2B-C3B	2.90	130.11	124.68
38	14	316	LMG	C9-C8-C7	-2.90	104.92	111.79
43	9	301	A86	C3-C2-C1	-2.90	123.17	127.31
45	12	311	KC2	O2D-CGD-O1D	-2.90	118.17	123.84
36	b	623	LHG	O8-C23-C24	2.90	121.01	111.91
31	6	309	CLA	CHB-C4A-NA	2.90	128.52	124.51
43	17	316	A86	C3-C2-C1	-2.90	123.17	127.31
31	2	315	CLA	CMC-C2C-C3C	2.90	133.99	126.12
42	13	314	KC1	CGD-CBD-CAD	-2.90	101.35	110.73
45	7	309	KC2	C3B-C2B-C1B	-2.90	104.31	107.08
31	12	316	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
45	16	312	KC2	C2A-C1A-NA	2.90	114.05	109.40
31	16	308	CLA	CHB-C4A-NA	2.90	128.52	124.51
43	0	306	A86	O1-C15-C20	-2.90	56.57	59.40
43	p	613	A86	C21-C20-C19	2.90	117.54	114.28
43	4	306	A86	C41-C32-C33	2.90	122.05	109.05
45	16	312	KC2	CAB-C3B-C4B	-2.90	117.90	124.90
31	p	601	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
43	p	613	A86	C35-C34-C33	-2.90	104.82	109.88
31	12	315	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
43	16	304	A86	C4-C3-C2	-2.89	117.55	123.47
35	D	406	PL9	O1-C4-C3	-2.89	117.53	120.72
31	19	308	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
43	15	305	A86	C7-C6-C8	2.89	122.64	118.08
43	8	303	A86	C10-C9-C8	-2.89	114.19	123.22
31	6	313	CLA	CMB-C2B-C3B	2.89	130.09	124.68
43	1	306	A86	C36-C31-C32	-2.89	116.83	119.70
31	p	607	CLA	CMB-C2B-C1B	-2.89	124.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	0	305	A86	C9-C8-C6	-2.89	118.29	126.42
31	16	308	CLA	CAC-C3C-C2C	-2.89	122.58	127.53
43	19	303	A86	O4-C38-O5	-2.89	117.22	122.96
31	13	307	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
31	14	307	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
31	6	308	CLA	CMB-C2B-C3B	2.89	130.08	124.68
31	d	401	CLA	CHB-C4A-NA	2.89	128.51	124.51
31	p	607	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
43	4	306	A86	C10-C9-C8	-2.89	114.20	123.22
31	2	312	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
45	14	308	KC2	CAB-C3B-C2B	2.89	138.12	128.60
45	14	308	KC2	CAB-C3B-C4B	-2.89	117.92	124.90
45	2	310	KC2	C2B-C1B-NB	2.89	112.23	110.10
31	3	307	CLA	C3A-C2A-C1A	2.89	105.66	101.34
43	7	304	A86	C20-C19-C18	-2.89	107.04	112.75
31	P	610	CLA	CHB-C4A-NA	2.89	128.50	124.51
31	18	307	CLA	CHB-C4A-NA	2.89	128.50	124.51
43	2	303	A86	C23-C16-C17	-2.88	103.97	108.98
31	C	507	CLA	CHB-C4A-NA	2.88	128.50	124.51
31	Z	101	CLA	CMB-C2B-C3B	2.88	130.07	124.68
31	B	604	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
43	13	302	A86	C4-C3-C2	-2.88	117.57	123.47
43	13	305	A86	C28-C27-C26	-2.88	118.89	122.92
31	1	307	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
31	b	603	CLA	CHB-C4A-NA	2.88	128.50	124.51
31	8	314	CLA	CHB-C4A-NA	2.88	128.50	124.51
43	3	301	A86	C41-C32-C40	-2.88	99.69	108.53
41	V	201	HEM	CAD-CBD-CGD	-2.88	107.41	113.60
45	14	310	KC2	C4D-C3D-CAD	2.88	112.46	107.81
31	3	315	CLA	CMB-C2B-C3B	2.88	130.06	124.68
43	7	304	A86	C41-C32-C33	2.88	121.97	109.05
43	4	306	A86	C4-C5-C6	-2.88	123.20	127.31
36	B	622	LHG	O8-C23-C24	2.88	120.94	111.91
31	p	610	CLA	CHB-C4A-NA	2.88	128.49	124.51
31	18	311	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
34	a	408	SQD	O8-S-C6	2.88	110.33	105.74
31	B	616	CLA	CHB-C4A-NA	2.88	128.49	124.51
45	15	310	KC2	C3B-C2B-C1B	-2.88	104.33	107.08
43	5	304	A86	C4-C3-C2	-2.88	117.58	123.47
31	B	602	CLA	CHB-C4A-NA	2.88	128.49	124.51
31	2	312	CLA	C3B-C4B-NB	-2.88	105.49	109.21
43	4	306	A86	C20-C19-C18	2.88	118.44	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	19	307	CLA	CHB-C4A-NA	2.88	128.49	124.51
38	w	201	LMG	O6-C5-C4	2.88	114.92	109.69
31	2	314	CLA	CMB-C2B-C3B	2.88	130.06	124.68
31	14	306	CLA	C2D-C1D-ND	-2.88	107.98	110.10
42	0	315	KC1	O2D-CGD-O1D	-2.87	118.22	123.84
38	K	101	LMG	O6-C1-O1	-2.87	103.17	109.97
41	v	201	HEM	CAD-CBD-CGD	-2.87	107.42	113.60
31	6	308	CLA	O2D-CGD-CBD	2.87	116.38	111.27
31	b	612	CLA	CHB-C4A-NA	2.87	128.49	124.51
42	p	609	KC1	C3C-C4C-NC	2.87	112.58	109.88
43	6	301	A86	C34-O4-C38	-2.87	112.54	117.90
31	4	315	CLA	CHD-C1D-ND	-2.87	121.81	124.45
45	11	311	KC2	CBC-CAC-C3C	-2.87	113.33	127.62
43	19	303	A86	C23-C16-C22	-2.87	103.13	107.37
43	16	302	A86	C34-O4-C38	-2.87	112.54	117.90
42	8	313	KC1	C3D-CAD-CBD	-2.87	103.82	107.61
43	15	305	A86	O4-C38-C39	2.87	116.37	111.09
31	0	308	CLA	CMB-C2B-C3B	2.87	130.05	124.68
45	17	309	KC2	O2D-CGD-O1D	-2.87	118.23	123.84
43	11	303	A86	C40-C32-C33	2.87	121.94	109.05
45	6	312	KC2	C3C-C2C-C1C	-2.87	104.36	106.49
31	B	601	CLA	CHB-C4A-NA	2.87	128.48	124.51
31	15	306	CLA	CHB-C4A-NA	2.87	128.48	124.51
45	11	311	KC2	C2A-C1A-NA	2.87	114.00	109.40
43	13	303	A86	O1-C15-C20	-2.87	56.60	59.40
45	12	311	KC2	C3A-C4A-NA	2.87	113.70	110.57
43	2	303	A86	O2-C18-C17	-2.87	104.10	109.80
43	15	305	A86	C20-C19-C18	2.87	118.42	112.75
42	16	315	KC1	C3B-C2B-C1B	-2.87	104.34	107.08
31	9	313	CLA	CAA-C2A-C1A	-2.87	102.58	111.97
31	10	311	CLA	CHB-C4A-NA	2.87	128.47	124.51
43	P	613	A86	C21-C20-C19	2.86	117.50	114.28
43	1	320	A86	C3-C4-C5	-2.86	117.61	123.47
45	7	309	KC2	O2D-CGD-O1D	-2.86	118.24	123.84
42	18	313	KC1	C2A-C1A-NA	2.86	114.00	109.40
43	2	305	A86	C23-C16-C22	2.86	111.59	107.37
35	d	406	PL9	O1-C4-C3	-2.86	117.57	120.72
43	P	611	A86	C7-C6-C8	2.86	122.59	118.08
31	1	307	CLA	C2A-C1A-CHA	2.86	128.87	123.86
38	4	316	LMG	C8-O7-C10	2.86	124.84	117.79
43	14	303	A86	C22-C16-C17	-2.86	104.01	108.98
31	d	404	CLA	C3B-C4B-NB	-2.86	105.51	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	622	DGD	C4E-C3E-C2E	-2.86	105.83	110.82
31	c	503	CLA	CAC-C3C-C4C	-2.86	121.10	124.81
43	5	305	A86	O1-C15-C20	-2.86	56.60	59.40
39	B	621	DGD	C4E-C3E-C2E	-2.86	105.83	110.82
31	11	315	CLA	CMC-C2C-C3C	2.86	133.88	126.12
43	3	302	A86	C25-C24-C1	-2.86	118.38	126.42
31	b	617	CLA	CHB-C4A-NA	2.86	128.47	124.51
43	13	305	A86	C4-C3-C2	-2.86	117.61	123.47
31	C	503	CLA	CAC-C3C-C4C	-2.86	121.10	124.81
31	2	306	CLA	C2A-C1A-CHA	2.86	128.86	123.86
43	18	301	A86	O4-C38-C39	2.86	116.35	111.09
43	0	305	A86	C35-C34-C33	-2.86	104.89	109.88
31	W	202	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
43	18	304	A86	C9-C10-C11	-2.86	118.20	126.61
38	k	101	LMG	O6-C1-O1	-2.86	103.20	109.97
31	c	504	CLA	CHB-C4A-NA	2.86	128.47	124.51
31	15	311	CLA	O2D-CGD-CBD	2.86	116.35	111.27
31	19	310	CLA	CHB-C4A-NA	2.86	128.47	124.51
43	19	305	A86	O-C13-C14	2.86	127.47	121.66
43	15	301	A86	C28-C27-C26	-2.86	118.92	122.92
43	8	301	A86	C9-C8-C6	-2.86	118.39	126.42
31	6	309	CLA	CMB-C2B-C3B	2.86	130.02	124.68
43	5	304	A86	O1-C15-C20	-2.86	56.61	59.40
31	13	308	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
43	7	304	A86	O4-C38-O5	-2.86	117.29	122.96
45	4	310	KC2	O2D-CGD-O1D	-2.86	118.25	123.84
31	9	310	CLA	CHB-C4A-NA	2.86	128.46	124.51
43	13	306	A86	O4-C38-C39	2.85	116.34	111.09
43	9	306	A86	C3-C4-C5	-2.85	117.63	123.47
31	9	315	CLA	CHB-C4A-NA	2.85	128.46	124.51
31	12	308	CLA	CAA-C2A-C3A	-2.85	104.96	112.78
43	3	305	A86	C7-C6-C8	2.85	122.57	118.08
33	C	517	BCR	C15-C14-C13	-2.85	123.24	127.31
31	B	609	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
45	10	310	KC2	CAB-C3B-C4B	-2.85	118.01	124.90
31	z	101	CLA	CMB-C2B-C3B	2.85	130.01	124.68
31	2	307	CLA	CBC-CAC-C3C	2.85	120.29	112.43
43	8	304	A86	O4-C38-O5	-2.85	117.30	122.96
43	13	305	A86	O4-C38-O5	-2.85	117.30	122.96
38	f	102	LMG	C6-C5-C4	-2.85	106.33	113.00
43	17	302	A86	O1-C15-C20	-2.85	56.61	59.40
43	19	303	A86	O1-C20-C19	2.85	115.52	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	314	KC1	C3B-C2B-C1B	-2.85	104.35	107.08
43	15	302	A86	C41-C32-C40	-2.85	99.78	108.53
38	F	102	LMG	C6-C5-C4	-2.85	106.33	113.00
43	1	304	A86	O1-C15-C20	-2.85	56.62	59.40
31	16	313	CLA	CMB-C2B-C3B	2.85	130.00	124.68
43	3	303	A86	C25-C24-C1	-2.85	118.42	126.42
43	17	303	A86	C9-C8-C6	-2.85	118.42	126.42
43	3	304	A86	O1-C20-C19	2.85	115.52	113.38
43	12	305	A86	C25-C24-C1	-2.85	118.42	126.42
31	c	511	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
31	0	316	CLA	CHB-C4A-NA	2.85	128.45	124.51
43	9	301	A86	C4-C3-C2	-2.85	117.64	123.47
43	10	303	A86	C21-C20-C19	-2.85	111.08	114.28
43	7	301	A86	O1-C15-C20	-2.85	56.62	59.40
34	A	408	SQD	O8-S-C6	2.84	110.27	105.74
43	3	302	A86	C8-C6-C5	2.84	123.31	118.94
45	9	309	KC2	CBD-CHA-C1A	2.84	134.19	128.88
43	0	301	A86	C14-C15-C16	-2.84	107.87	118.75
31	w	203	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
45	17	309	KC2	C3B-C2B-C1B	-2.84	104.36	107.08
31	D	404	CLA	C3B-C4B-NB	-2.84	105.53	109.21
38	f	102	LMG	O6-C1-O1	-2.84	103.24	109.97
43	p	611	A86	C7-C6-C8	2.84	122.56	118.08
38	W	201	LMG	O6-C5-C4	2.84	114.86	109.69
31	2	315	CLA	CBC-CAC-C3C	2.84	120.27	112.43
43	14	305	A86	O1-C15-C20	-2.84	56.62	59.40
31	C	504	CLA	CHB-C4A-NA	2.84	128.44	124.51
45	1	311	KC2	C2A-C1A-NA	2.84	113.96	109.40
31	P	607	CLA	CBA-CAA-C2A	-2.84	108.03	114.02
31	8	311	CLA	CMB-C2B-C3B	2.84	129.99	124.68
31	10	308	CLA	CMB-C2B-C3B	2.84	129.99	124.68
42	9	314	KC1	C3B-C2B-C1B	-2.84	104.36	107.08
43	9	302	A86	C23-C16-C17	-2.84	104.05	108.98
42	4	313	KC1	CAA-CBA-CGA	-2.84	112.68	127.26
43	19	302	A86	C9-C8-C6	-2.84	118.45	126.42
31	0	311	CLA	CHB-C4A-NA	2.84	128.43	124.51
31	b	610	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
43	7	301	A86	O4-C34-C35	2.83	114.65	107.59
39	B	621	DGD	C3G-O3G-C1D	2.83	119.28	113.74
39	b	622	DGD	C3G-O3G-C1D	2.83	119.28	113.74
31	B	611	CLA	CHB-C4A-NA	2.83	128.43	124.51
31	B	602	CLA	CAA-CBA-CGA	-2.83	104.97	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	F	102	LMG	O6-C1-O1	-2.83	103.26	109.97
39	H	102	DGD	C1E-O6E-C5E	2.83	119.25	113.69
31	C	511	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
43	16	302	A86	C3-C4-C5	-2.83	117.68	123.47
31	10	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
43	14	301	A86	C12-C11-C13	2.83	120.77	116.02
31	10	309	CLA	CHB-C4A-NA	2.83	128.42	124.51
31	7	308	CLA	CMB-C2B-C3B	2.83	129.97	124.68
31	b	603	CLA	CAA-CBA-CGA	-2.83	105.00	113.25
43	3	305	A86	O-C13-C11	-2.83	114.91	121.15
31	p	607	CLA	CBA-CAA-C2A	-2.83	108.05	114.02
35	a	409	PL9	C7-C3-C2	-2.83	119.58	123.30
45	17	311	KC2	C3D-CAD-CBD	-2.83	103.89	107.61
45	3	311	KC2	C2A-C3A-C4A	2.83	108.58	106.49
43	5	301	A86	O-C13-C14	-2.82	115.92	121.66
43	7	304	A86	C14-C15-C16	-2.82	107.94	118.75
31	b	612	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
38	D	403	LMG	C4-C3-C2	2.82	115.75	110.82
43	3	305	A86	C25-C24-C1	-2.82	118.49	126.42
31	b	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
43	3	302	A86	O1-C15-C20	-2.82	56.64	59.40
31	b	603	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
31	b	602	CLA	CMB-C2B-C3B	2.82	129.96	124.68
43	13	304	A86	C41-C32-C40	-2.82	99.87	108.53
43	15	304	A86	C34-O4-C38	2.82	123.15	117.90
34	A	408	SQD	O47-C7-C8	2.82	117.58	111.50
45	2	310	KC2	C3C-C2C-C1C	-2.82	104.39	106.49
43	6	301	A86	C28-C27-C26	-2.82	118.97	122.92
45	3	309	KC2	O2D-CGD-O1D	-2.82	118.33	123.84
38	5	315	LMG	O3-C3-C2	-2.82	103.83	110.35
31	B	605	CLA	C1-C2-C3	-2.82	121.17	126.04
31	b	608	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
43	17	301	A86	O4-C38-O5	-2.82	117.36	122.96
45	12	311	KC2	CBC-CAC-C3C	-2.82	113.60	127.62
33	c	517	BCR	C15-C14-C13	-2.82	123.29	127.31
42	P	609	KC1	C3C-C4C-NC	2.82	112.53	109.88
31	14	314	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	C	508	CLA	C2A-C1A-CHA	2.82	128.78	123.86
31	17	315	CLA	CMB-C2B-C3B	2.82	129.94	124.68
31	17	313	CLA	C3D-C2D-C1D	2.81	109.67	105.83
45	11	311	KC2	C2B-C1B-NB	2.81	112.18	110.10
43	19	306	A86	C17-C16-C15	2.81	112.03	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	313	CLA	CHB-C4A-NA	2.81	128.40	124.51
31	c	503	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
43	2	304	A86	C28-C27-C26	-2.81	118.98	122.92
39	h	102	DGD	C1E-O6E-C5E	2.81	119.21	113.69
43	19	302	A86	O4-C38-C39	2.81	116.27	111.09
33	b	618	BCR	C7-C8-C9	-2.81	121.98	126.23
31	13	313	CLA	CMB-C2B-C3B	2.81	129.94	124.68
43	4	301	A86	C25-C24-C1	-2.81	118.52	126.42
45	5	308	KC2	CAB-C3B-C2B	2.81	137.87	128.60
31	15	313	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
34	B	623	SQD	O47-C7-C8	2.81	117.56	111.50
42	12	314	KC1	CMB-C2B-C1B	2.81	129.67	124.71
36	18	315	LHG	O8-C23-C24	2.81	120.73	111.91
43	16	304	A86	C25-C26-C27	-2.81	123.30	127.31
43	13	306	A86	C4-C3-C2	-2.81	117.72	123.47
31	B	609	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
31	B	611	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
43	1	320	A86	O1-C15-C20	-2.81	56.65	59.40
34	b	601	SQD	O47-C7-C8	2.81	117.55	111.50
31	W	202	CLA	C1-C2-C3	-2.81	121.19	126.04
31	7	307	CLA	C2D-C1D-ND	-2.81	108.03	110.10
43	19	306	A86	C3-C4-C5	-2.81	117.72	123.47
43	14	301	A86	O4-C38-O5	-2.81	117.39	122.96
31	D	404	CLA	CMC-C2C-C1C	2.81	129.31	125.04
31	C	503	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
31	C	503	CLA	CMB-C2B-C3B	-2.81	119.43	124.68
35	A	409	PL9	C7-C3-C2	-2.81	119.61	123.30
45	10	310	KC2	C3D-CAD-CBD	-2.81	103.91	107.61
42	4	313	KC1	C1A-NA-C4A	-2.80	105.44	106.71
36	8	315	LHG	O8-C23-C24	2.80	120.71	111.91
43	6	305	A86	O-C13-C11	-2.80	114.95	121.15
43	1	320	A86	O-C13-C14	2.80	127.36	121.66
43	1	320	A86	C25-C24-C1	-2.80	118.54	126.42
31	5	312	CLA	CMB-C2B-C3B	2.80	129.92	124.68
31	b	606	CLA	C1-C2-C3	-2.80	121.20	126.04
45	14	308	KC2	C3B-C2B-C1B	-2.80	104.40	107.08
43	5	318	A86	C26-C25-C24	-2.80	114.48	123.22
43	19	302	A86	C4-C3-C2	-2.80	117.74	123.47
43	10	305	A86	C9-C8-C6	-2.80	118.55	126.42
31	19	308	CLA	C1-C2-C3	2.80	130.88	126.04
43	2	301	A86	C41-C32-C31	2.80	112.98	110.47
43	1	302	A86	C9-C10-C11	-2.80	118.38	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	306	A86	C26-C25-C24	-2.80	114.48	123.22
43	15	301	A86	O-C13-C14	-2.80	115.97	121.66
31	13	313	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
43	5	304	A86	C3-C4-C5	-2.80	117.74	123.47
43	18	303	A86	O1-C20-C21	-2.80	111.70	115.06
31	3	310	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
34	a	408	SQD	O47-C7-C8	2.80	117.53	111.50
43	4	304	A86	C22-C16-C17	-2.80	104.12	108.98
43	7	302	A86	C19-C18-C17	2.80	116.17	110.77
45	1	311	KC2	C3B-C2B-C1B	-2.80	104.41	107.08
31	5	314	CLA	CHB-C4A-NA	2.80	128.38	124.51
38	w	201	LMG	C1-C2-C3	-2.80	104.17	110.00
31	18	306	CLA	C3A-C2A-C1A	2.80	105.53	101.34
31	4	312	CLA	C1-C2-C3	-2.79	121.21	126.04
31	c	508	CLA	C2A-C1A-CHA	2.79	128.75	123.86
31	19	310	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
31	b	613	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
31	c	503	CLA	CMB-C2B-C3B	-2.79	119.45	124.68
45	18	310	KC2	C3A-C4A-NA	2.79	113.62	110.57
42	16	301	KC1	C4D-C3D-CAD	2.79	112.32	107.81
31	B	605	CLA	CMA-C3A-C2A	-2.79	102.56	113.83
43	12	303	A86	C40-C32-C31	2.79	112.97	110.47
31	2	306	CLA	CAC-C3C-C2C	-2.79	122.75	127.53
31	9	312	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
43	0	306	A86	O4-C34-C33	2.79	114.55	107.59
31	B	612	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
31	7	315	CLA	CMB-C2B-C3B	2.79	129.90	124.68
31	18	306	CLA	CMB-C2B-C3B	2.79	129.90	124.68
43	8	303	A86	C3-C4-C5	-2.79	117.76	123.47
31	d	404	CLA	CMC-C2C-C1C	2.79	129.29	125.04
43	7	301	A86	C36-C31-C32	2.79	122.47	119.70
43	14	305	A86	O4-C38-O5	-2.79	117.42	122.96
31	8	312	CLA	CHD-C1D-C2D	2.79	131.33	125.48
43	13	302	A86	C40-C32-C33	2.79	121.57	109.05
43	17	302	A86	C34-O4-C38	2.79	123.09	117.90
31	9	307	CLA	CHB-C4A-NA	2.79	128.37	124.51
31	5	311	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	b	607	CLA	CMD-C2D-C1D	2.79	129.63	124.71
31	6	308	CLA	C2A-C1A-CHA	2.79	128.73	123.86
31	P	608	CLA	CMB-C2B-C3B	2.79	129.89	124.68
43	11	305	A86	C9-C8-C6	-2.79	118.58	126.42
42	P	609	KC1	C2A-C3A-C4A	2.79	108.55	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	5	310	KC2	CHD-C4C-NC	2.79	128.43	124.20
42	1	314	KC1	CMB-C2B-C1B	2.79	129.62	124.71
43	13	305	A86	O-C13-C11	-2.79	114.99	121.15
43	4	305	A86	C25-C24-C1	-2.79	118.59	126.42
31	B	604	CLA	CAA-CBA-CGA	-2.78	105.12	113.25
31	B	604	CLA	CAA-C2A-C3A	-2.78	105.15	112.78
43	19	303	A86	C36-C31-C32	-2.78	116.93	119.70
31	B	602	CLA	CAA-C2A-C3A	-2.78	105.15	112.78
31	10	308	CLA	CAC-C3C-C2C	-2.78	122.77	127.53
45	17	309	KC2	CAC-C3C-C4C	2.78	137.44	124.47
43	17	306	A86	C4-C3-C2	-2.78	117.77	123.47
38	d	403	LMG	C4-C3-C2	2.78	115.68	110.82
43	6	305	A86	C41-C32-C40	-2.78	99.99	108.53
31	16	309	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
31	B	601	CLA	CMB-C2B-C3B	2.78	129.88	124.68
43	0	304	A86	O1-C15-C20	-2.78	56.68	59.40
45	13	309	KC2	C1A-NA-C4A	-2.78	105.45	106.71
38	W	201	LMG	C1-C2-C3	-2.78	104.20	110.00
45	6	310	KC2	O2D-CGD-O1D	-2.78	118.40	123.84
43	15	304	A86	C3-C4-C5	-2.78	117.78	123.47
31	p	603	CLA	O2D-CGD-CBD	2.78	116.21	111.27
31	B	607	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
31	8	312	CLA	CAA-CBA-CGA	2.78	121.38	113.25
31	P	601	CLA	CMB-C2B-C3B	2.78	129.88	124.68
45	6	310	KC2	CBC-CAC-C3C	-2.78	113.79	127.62
31	5	311	CLA	C4D-C3D-CAD	-2.78	104.82	108.10
31	b	605	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
43	11	306	A86	C9-C10-C11	-2.78	118.44	126.61
31	P	603	CLA	O2D-CGD-CBD	2.78	116.20	111.27
31	11	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
43	0	303	A86	C9-C10-C11	-2.78	118.44	126.61
43	1	319	A86	C3-C4-C5	-2.78	117.78	123.47
43	6	301	A86	C4-C3-C2	-2.78	117.78	123.47
31	5	306	CLA	CHB-C4A-NA	2.78	128.35	124.51
43	10	304	A86	O1-C15-C20	-2.78	56.69	59.40
31	4	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
31	b	605	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
43	14	303	A86	O1-C15-C20	-2.78	56.69	59.40
34	l	101	SQD	C4-C3-C2	2.78	115.67	110.82
31	z	103	CLA	O2D-CGD-CBD	2.78	116.20	111.27
31	4	307	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
31	10	316	CLA	CHB-C4A-NA	2.77	128.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	2	308	KC2	CAC-C3C-C4C	2.77	137.40	124.47
31	19	311	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
43	5	305	A86	C7-C6-C8	2.77	122.45	118.08
31	15	313	CLA	CHB-C4A-NA	2.77	128.35	124.51
45	1	309	KC2	C3B-C2B-C1B	-2.77	104.43	107.08
31	17	308	CLA	CMB-C2B-C3B	2.77	129.87	124.68
35	D	406	PL9	C7-C8-C9	-2.77	122.18	126.79
31	10	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
43	3	302	A86	C23-C16-C22	-2.77	103.28	107.37
31	B	616	CLA	CMB-C2B-C3B	2.77	129.86	124.68
42	6	315	KC1	C3B-C2B-C1B	-2.77	104.43	107.08
43	3	302	A86	C33-C32-C31	-2.77	106.52	109.21
31	p	608	CLA	CMB-C2B-C3B	2.77	129.86	124.68
31	p	601	CLA	CMB-C2B-C3B	2.77	129.86	124.68
31	a	404	CLA	CHB-C4A-NA	2.77	128.34	124.51
43	3	305	A86	C9-C10-C11	-2.77	118.47	126.61
31	9	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	6	316	CLA	CHB-C4A-NA	2.77	128.34	124.51
43	17	316	A86	C25-C24-C1	-2.77	118.64	126.42
43	5	302	A86	C25-C26-C27	-2.77	123.36	127.31
35	d	406	PL9	C7-C8-C9	-2.77	122.19	126.79
43	10	303	A86	O4-C34-C35	-2.77	100.70	107.59
43	9	302	A86	C9-C8-C6	-2.76	118.65	126.42
31	15	313	CLA	CMB-C2B-C3B	2.76	129.85	124.68
31	B	604	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
42	8	313	KC1	C1A-C2A-C3A	-2.76	104.92	107.11
31	B	606	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
43	19	304	A86	O1-C15-C20	-2.76	56.70	59.40
31	w	203	CLA	C1-C2-C3	-2.76	121.27	126.04
31	13	307	CLA	O2D-CGD-CBD	2.76	116.18	111.27
31	A	403	CLA	C2D-C1D-ND	-2.76	108.07	110.10
31	0	312	CLA	CAC-C3C-C2C	2.76	132.25	127.53
31	C	503	CLA	CAC-C3C-C2C	2.76	132.25	127.53
42	p	609	KC1	C2A-C3A-C4A	2.76	108.53	106.49
43	12	306	A86	C20-C19-C18	2.76	118.21	112.75
43	6	302	A86	C36-C31-C32	2.76	122.44	119.70
45	4	308	KC2	C3B-C2B-C1B	-2.76	104.44	107.08
31	16	316	CLA	CHB-C4A-NA	2.76	128.33	124.51
42	7	314	KC1	CMB-C2B-C1B	2.76	129.57	124.71
31	b	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
43	5	305	A86	C8-C6-C5	-2.76	114.71	118.94
43	6	301	A86	O1-C20-C21	-2.76	111.75	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	302	A86	C7-C6-C5	-2.76	119.06	122.92
31	13	312	CLA	CMB-C2B-C3B	2.76	129.83	124.68
33	B	619	BCR	C29-C30-C25	2.76	114.72	110.48
43	19	303	A86	C3-C4-C5	-2.75	117.83	123.47
31	7	312	CLA	CMB-C2B-C3B	2.75	129.83	124.68
38	D	403	LMG	O6-C1-O1	-2.75	103.45	109.97
43	4	304	A86	O1-C15-C20	-2.75	56.71	59.40
43	13	305	A86	C9-C10-C11	-2.75	118.51	126.61
45	8	310	KC2	C4D-C3D-CAD	2.75	112.26	107.81
43	1	302	A86	C40-C32-C33	2.75	121.41	109.05
31	p	604	CLA	O2D-CGD-CBD	2.75	116.16	111.27
43	6	305	A86	O4-C34-C33	2.75	114.44	107.59
43	16	302	A86	C25-C24-C1	-2.75	118.69	126.42
43	18	305	A86	O1-C15-C20	-2.75	56.71	59.40
43	0	301	A86	O4-C34-C35	2.75	114.44	107.59
31	P	603	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
43	5	301	A86	O1-C15-C20	-2.75	56.71	59.40
43	2	304	A86	C3-C4-C5	-2.75	117.84	123.47
31	z	103	CLA	CMB-C2B-C3B	2.75	129.82	124.68
33	B	617	BCR	C7-C8-C9	-2.75	122.08	126.23
43	7	301	A86	C28-C27-C26	-2.75	119.08	122.92
31	10	313	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
43	0	301	A86	C8-C6-C5	2.75	123.16	118.94
34	A	408	SQD	O6-C1-C2	2.75	112.59	108.30
43	15	305	A86	C9-C10-C11	-2.75	118.54	126.61
45	0	310	KC2	CAB-C3B-C2B	2.75	137.65	128.60
31	P	604	CLA	O2D-CGD-CBD	2.75	116.15	111.27
43	10	301	A86	C14-C15-C16	-2.74	108.24	118.75
43	6	307	A86	C-C1-C24	2.74	122.40	118.08
31	b	617	CLA	CMB-C2B-C3B	2.74	129.81	124.68
43	2	305	A86	C9-C8-C6	-2.74	118.71	126.42
31	0	309	CLA	CHB-C4A-NA	2.74	128.30	124.51
34	a	408	SQD	O6-C1-C2	2.74	112.58	108.30
43	9	304	A86	O1-C15-C20	-2.74	56.72	59.40
31	C	509	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
34	L	102	SQD	C4-C3-C2	2.74	115.61	110.82
43	10	303	A86	C9-C8-C6	-2.74	118.72	126.42
43	10	301	A86	O4-C34-C35	2.74	114.42	107.59
43	10	301	A86	C36-C31-C32	2.74	122.42	119.70
42	1	314	KC1	C4B-C3B-C2B	-2.74	104.50	106.75
42	19	314	KC1	C4D-C3D-CAD	2.74	112.23	107.81
31	14	309	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	14	301	A86	C41-C32-C31	-2.74	108.02	110.47
31	r	101	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
43	10	303	A86	C9-C10-C11	-2.74	118.56	126.61
31	p	603	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
43	8	301	A86	O4-C38-O5	2.74	128.40	122.96
43	0	306	A86	C20-C19-C18	2.74	118.16	112.75
31	4	309	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
43	5	303	A86	C20-C19-C18	2.73	118.16	112.75
39	C	520	DGD	CDB-CCB-CBB	-2.73	100.55	114.42
43	13	302	A86	O1-C20-C19	2.73	115.44	113.38
43	3	303	A86	C4-C3-C2	-2.73	117.88	123.47
31	c	503	CLA	CAC-C3C-C2C	2.73	132.20	127.53
31	9	312	CLA	CHB-C4A-NA	2.73	128.29	124.51
31	W	202	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
42	7	314	KC1	CHB-C1B-C2B	-2.73	119.75	125.48
34	i	101	SQD	O8-S-C6	2.73	110.09	105.74
43	15	302	A86	C9-C10-C11	-2.73	118.58	126.61
31	10	317	CLA	CMB-C2B-C3B	2.73	129.79	124.68
43	1	302	A86	O-C13-C11	-2.73	115.12	121.15
31	17	307	CLA	O2D-CGD-CBD	2.73	116.12	111.27
39	B	621	DGD	C1E-C2E-C3E	-2.73	104.31	110.00
34	A	411	SQD	O8-S-C6	2.73	110.09	105.74
31	P	604	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
31	14	312	CLA	CHA-C1A-NA	-2.73	120.15	126.40
45	4	310	KC2	C4D-C3D-CAD	2.73	112.22	107.81
31	3	315	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
42	5	313	KC1	OBD-CAD-C3D	-2.73	123.45	127.98
42	p	609	KC1	C3B-C2B-C1B	-2.73	104.47	107.08
43	19	302	A86	C23-C16-C17	-2.73	104.24	108.98
36	C	521	LHG	O8-C23-C24	2.73	120.47	111.91
43	7	302	A86	O4-C34-C33	2.73	114.38	107.59
43	5	305	A86	C9-C8-C6	-2.73	118.76	126.42
31	2	315	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
39	c	520	DGD	CDB-CCB-CBB	-2.73	100.58	114.42
31	11	312	CLA	CHB-C4A-NA	2.73	128.28	124.51
31	A	406	CLA	CHB-C4A-NA	2.73	128.28	124.51
31	a	406	CLA	CHB-C4A-NA	2.73	128.28	124.51
31	6	308	CLA	C3A-C2A-C1A	2.73	105.42	101.34
45	7	309	KC2	CAC-C3C-C4C	2.73	137.17	124.47
31	c	509	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
38	15	314	LMG	O3-C3-C2	-2.72	104.05	110.35
43	17	305	A86	C20-C19-C18	-2.72	107.36	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	16	310	KC2	C3B-C2B-C1B	-2.72	104.47	107.08
31	18	309	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
43	14	305	A86	O1-C20-C19	2.72	115.43	113.38
45	11	311	KC2	C3B-C2B-C1B	-2.72	104.48	107.08
43	12	304	A86	O4-C34-C33	2.72	114.37	107.59
43	15	301	A86	O1-C15-C20	-2.72	56.74	59.40
31	10	316	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
43	5	303	A86	C28-C27-C29	2.72	125.23	118.93
31	R	101	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	C	509	CLA	CMD-C2D-C3D	2.72	133.87	127.61
43	0	301	A86	C28-C27-C26	-2.72	119.11	122.92
43	7	305	A86	C4-C3-C2	-2.72	117.90	123.47
31	1	315	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
43	0	303	A86	C9-C8-C6	-2.72	118.78	126.42
43	6	307	A86	C26-C25-C24	-2.72	114.73	123.22
31	b	616	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
31	B	615	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
42	P	609	KC1	C3B-C2B-C1B	-2.72	104.48	107.08
31	2	307	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	b	606	CLA	CMA-C3A-C2A	-2.72	102.87	113.83
43	13	304	A86	O4-C38-O5	-2.72	117.56	122.96
43	6	305	A86	O4-C34-C35	2.72	114.36	107.59
45	10	310	KC2	O2D-CGD-O1D	-2.72	118.53	123.84
31	10	313	CLA	CAC-C3C-C4C	2.72	128.34	124.81
43	7	304	A86	C3-C4-C5	-2.72	117.91	123.47
33	b	620	BCR	C29-C30-C25	2.72	114.66	110.48
36	w	202	LHG	O8-C23-C24	2.72	120.43	111.91
36	P	615	LHG	C11-C10-C9	-2.72	100.64	114.42
43	8	304	A86	C23-C16-C17	2.72	113.70	108.98
31	5	312	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
31	14	312	CLA	C1D-ND-C4D	2.71	108.26	106.33
31	A	406	CLA	O2D-CGD-CBD	2.71	116.09	111.27
36	L	101	LHG	C11-C10-C9	-2.71	100.65	114.42
43	16	306	A86	C20-C19-C18	-2.71	107.38	112.75
43	9	304	A86	C25-C26-C27	-2.71	123.44	127.31
45	13	311	KC2	C3B-C2B-C1B	-2.71	104.49	107.08
41	v	201	HEM	CHD-C1D-ND	2.71	127.38	124.43
41	V	201	HEM	CAA-C2A-C3A	-2.71	119.46	127.25
31	C	508	CLA	CMB-C2B-C3B	2.71	129.75	124.68
36	l	102	LHG	C11-C10-C9	-2.71	100.67	114.42
31	C	502	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
31	c	502	CLA	O2D-CGD-O1D	-2.71	118.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	p	615	LHG	C11-C10-C9	-2.71	100.67	114.42
43	1	303	A86	C19-C18-C17	-2.71	105.54	110.77
43	17	303	A86	C19-C18-C17	2.71	116.00	110.77
43	2	304	A86	O4-C38-C39	2.71	116.07	111.09
31	0	316	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
43	15	304	A86	O2-C18-C19	-2.71	104.42	109.80
31	10	308	CLA	CHB-C4A-NA	2.71	128.26	124.51
39	h	102	DGD	CDB-CCB-CBB	-2.71	100.68	114.42
31	0	313	CLA	CMB-C2B-C3B	2.71	129.74	124.68
31	4	315	CLA	CMB-C2B-C3B	2.71	129.74	124.68
31	c	509	CLA	CMD-C2D-C3D	2.71	133.84	127.61
31	w	203	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
45	16	310	KC2	O2D-CGD-O1D	-2.71	118.55	123.84
31	8	311	CLA	CMA-C3A-C4A	2.71	119.05	111.77
43	13	303	A86	C25-C24-C1	-2.71	118.81	126.42
31	2	314	CLA	O2D-CGD-CBD	2.71	116.08	111.27
39	H	102	DGD	CDB-CCB-CBB	-2.70	100.70	114.42
41	v	201	HEM	CAA-C2A-C3A	-2.70	119.48	127.25
31	a	406	CLA	O2D-CGD-CBD	2.70	116.07	111.27
44	p	612	DD6	C3-C4-C5	2.70	129.01	123.47
31	A	404	CLA	CHB-C4A-NA	2.70	128.25	124.51
31	p	604	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
31	3	307	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
31	p	605	CLA	CHB-C4A-NA	2.70	128.25	124.51
34	0	318	SQD	O48-C23-O10	-2.70	116.78	123.59
31	13	315	CLA	CMB-C2B-C3B	2.70	129.73	124.68
39	B	621	DGD	C5B-C4B-C3B	-2.70	100.72	114.42
45	8	308	KC2	O2D-CGD-O1D	-2.70	118.56	123.84
31	3	312	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
42	8	313	KC1	C3A-C4A-NA	2.70	113.52	110.57
31	0	313	CLA	CAC-C3C-C4C	2.70	128.31	124.81
43	4	304	A86	C25-C24-C1	-2.70	118.84	126.42
43	2	304	A86	C17-C16-C15	-2.70	106.41	109.16
43	1	303	A86	C9-C8-C6	-2.70	118.84	126.42
31	3	316	CLA	C3A-C2A-C1A	2.70	105.38	101.34
34	10	320	SQD	O48-C23-O10	-2.70	116.78	123.59
35	A	409	PL9	C22-C23-C24	-2.70	121.17	127.66
31	B	606	CLA	C3A-C2A-C1A	2.70	105.38	101.34
43	16	303	A86	O1-C15-C20	-2.69	56.77	59.40
31	a	403	CLA	C2D-C1D-ND	-2.69	108.12	110.10
43	6	305	A86	C28-C27-C26	-2.69	119.15	122.92
43	12	302	A86	C4-C3-C2	-2.69	117.96	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	6	310	KC2	C3B-C2B-C1B	-2.69	104.50	107.08
43	6	302	A86	O1-C15-C20	-2.69	56.77	59.40
31	3	308	CLA	CHB-C4A-NA	2.69	128.23	124.51
31	13	313	CLA	C4A-NA-C1A	2.69	107.92	106.71
44	P	612	DD6	C3-C2-C1	-2.69	123.47	127.31
31	c	508	CLA	CMB-C2B-C3B	2.69	129.71	124.68
43	1	303	A86	C40-C32-C33	2.69	121.13	109.05
43	10	306	A86	C20-C19-C18	2.69	118.07	112.75
45	1	309	KC2	C2A-C1A-CHA	-2.69	118.54	127.44
43	P	611	A86	C4-C5-C6	-2.69	123.47	127.31
43	1	306	A86	O1-C20-C21	-2.69	111.83	115.06
31	18	312	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
43	5	318	A86	O1-C15-C20	-2.69	56.77	59.40
31	5	306	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
31	12	308	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
38	j	101	LMG	O3-C3-C2	-2.69	104.14	110.35
31	0	314	CLA	CHB-C4A-NA	2.69	128.23	124.51
31	3	316	CLA	CAA-C2A-C1A	-2.69	103.17	111.97
38	J	101	LMG	O3-C3-C2	-2.69	104.14	110.35
35	a	409	PL9	C22-C23-C24	-2.69	121.19	127.66
31	9	313	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
31	0	312	CLA	C2D-C1D-ND	-2.69	108.12	110.10
31	B	612	CLA	CMD-C2D-C1D	-2.68	119.98	124.71
31	4	314	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
43	10	306	A86	C9-C8-C6	-2.68	118.88	126.42
31	17	308	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
45	15	310	KC2	CAA-CBA-CGA	-2.68	113.47	127.26
31	3	307	CLA	C2A-C1A-CHA	2.68	128.55	123.86
45	5	308	KC2	O2D-CGD-O1D	-2.68	118.59	123.84
31	8	312	CLA	CMD-C2D-C1D	2.68	129.44	124.71
42	11	314	KC1	CMB-C2B-C1B	2.68	129.44	124.71
45	3	309	KC2	C1A-NA-C4A	2.68	107.91	106.71
43	17	305	A86	C-C1-C2	-2.68	119.17	122.92
45	11	311	KC2	C4D-C3D-CAD	2.68	112.14	107.81
43	0	306	A86	C9-C8-C6	-2.68	118.89	126.42
31	8	307	CLA	CMB-C2B-C3B	2.68	129.69	124.68
31	6	308	CLA	CHB-C4A-NA	2.68	128.22	124.51
43	15	302	A86	C36-C31-C32	2.68	122.35	119.70
45	8	310	KC2	CAB-C3B-C2B	2.68	137.43	128.60
45	12	309	KC2	C3A-C4A-NA	2.68	113.50	110.57
31	P	607	CLA	CHB-C4A-NA	2.68	128.22	124.51
31	2	315	CLA	CHB-C4A-NA	2.68	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	8	308	KC2	CAC-C3C-C2C	-2.68	119.78	128.60
43	8	304	A86	C3-C4-C5	-2.68	117.99	123.47
31	4	312	CLA	C3B-C4B-NB	-2.68	105.75	109.21
31	0	312	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
41	e	101	HEM	CMB-C2B-C1B	-2.67	120.97	125.04
31	5	309	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
31	2	307	CLA	CAC-C3C-C4C	2.67	128.28	124.81
31	c	511	CLA	CHB-C4A-NA	2.67	128.21	124.51
41	E	101	HEM	CMB-C2B-C1B	-2.67	120.97	125.04
45	18	308	KC2	CAB-C3B-C4B	2.67	131.35	124.90
38	d	408	LMG	O1-C7-C8	-2.67	104.45	110.90
31	7	307	CLA	C2A-C1A-CHA	2.67	128.52	123.85
44	P	612	DD6	C32-C31-C36	-2.67	118.86	122.63
43	14	304	A86	O4-C34-C35	2.67	114.25	107.59
43	16	306	A86	O4-C34-C35	2.67	114.25	107.59
31	13	313	CLA	C3B-C4B-NB	-2.67	105.75	109.21
31	12	313	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
43	13	301	A86	C20-C19-C18	2.67	118.04	112.75
31	1	321	CLA	C2D-C1D-ND	-2.67	108.14	110.10
42	19	314	KC1	C2B-C1B-NB	2.67	112.07	110.10
43	11	305	A86	O1-C15-C20	-2.67	56.79	59.40
43	16	304	A86	C41-C32-C31	-2.67	108.08	110.47
42	0	315	KC1	C4C-C3C-C2C	-2.67	103.00	106.90
39	c	519	DGD	CDB-CCB-CBB	-2.67	100.87	114.42
43	16	307	A86	C9-C8-C6	-2.67	118.92	126.42
43	6	305	A86	C20-C19-C18	-2.67	107.47	112.75
45	19	309	KC2	C2A-C3A-C4A	2.67	108.47	106.49
31	2	307	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
43	2	303	A86	O-C13-C11	-2.67	115.25	121.15
43	17	301	A86	C14-C15-C16	2.67	128.97	118.75
43	4	304	A86	C4-C3-C2	-2.67	118.01	123.47
43	17	301	A86	C34-O4-C38	-2.67	112.93	117.90
45	12	311	KC2	C4D-C3D-CAD	2.67	112.12	107.81
31	16	308	CLA	CMB-C2B-C3B	2.67	129.67	124.68
43	6	302	A86	C4-C3-C2	-2.67	118.01	123.47
31	11	308	CLA	CMA-C3A-C4A	2.67	118.94	111.77
31	6	316	CLA	CMB-C2B-C3B	2.67	129.66	124.68
43	13	301	A86	O4-C34-C35	2.67	114.23	107.59
45	16	310	KC2	CAC-C3C-C4C	2.66	136.89	124.47
43	0	304	A86	C4-C5-C6	-2.66	123.51	127.31
41	V	201	HEM	CHD-C1D-ND	2.66	127.33	124.43
45	15	308	KC2	O2D-CGD-O1D	-2.66	118.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	13	310	CLA	CHB-C4A-NA	2.66	128.19	124.51
31	12	313	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
43	7	305	A86	C34-O4-C38	2.66	122.86	117.90
43	p	611	A86	C4-C5-C6	-2.66	123.51	127.31
38	14	316	LMG	O7-C10-O9	-2.66	117.27	123.70
31	b	607	CLA	C3A-C2A-C1A	2.66	105.33	101.34
31	p	607	CLA	CHB-C4A-NA	2.66	128.19	124.51
43	1	303	A86	O3-C36-C37	-2.66	104.66	109.39
43	10	304	A86	C20-C19-C18	2.66	118.01	112.75
42	p	609	KC1	C4D-C3D-CAD	2.66	112.11	107.81
31	c	505	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
42	14	313	KC1	CED-O2D-CGD	2.66	121.95	115.94
32	D	402	PHO	OBD-CAD-CBD	-2.66	121.92	125.82
43	12	306	A86	O1-C20-C21	-2.66	111.87	115.06
45	2	308	KC2	O2D-CGD-O1D	-2.66	118.64	123.84
31	18	309	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
42	5	313	KC1	CGD-CBD-CAD	-2.66	102.13	110.73
43	11	304	A86	O1-C20-C19	2.66	115.38	113.38
39	C	519	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
45	19	309	KC2	CAA-C2A-C1A	2.66	136.95	124.75
31	b	613	CLA	CMD-C2D-C1D	-2.66	120.03	124.71
31	C	511	CLA	CHB-C4A-NA	2.65	128.18	124.51
31	P	605	CLA	CHB-C4A-NA	2.65	128.18	124.51
43	6	307	A86	C12-C11-C10	2.65	129.85	123.42
31	6	309	CLA	CAC-C3C-C4C	2.65	128.25	124.81
43	10	304	A86	C4-C5-C6	-2.65	123.52	127.31
33	b	620	BCR	C37-C22-C21	-2.65	119.20	122.92
42	5	313	KC1	C1C-C2C-C3C	-2.65	104.17	106.96
31	8	311	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
31	9	310	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
43	6	305	A86	C40-C32-C31	-2.65	108.10	110.47
31	B	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
31	10	307	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
45	9	309	KC2	CAA-C2A-C1A	2.65	136.93	124.75
43	11	306	A86	C25-C24-C1	-2.65	118.97	126.42
31	d	401	CLA	O2D-CGD-CBD	2.65	115.98	111.27
31	C	505	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
44	p	612	DD6	C32-C31-C36	-2.65	118.89	122.63
38	4	316	LMG	O7-C10-C11	2.65	117.21	111.50
45	2	308	KC2	C3B-C2B-C1B	-2.65	104.55	107.08
43	12	303	A86	C20-C19-C18	2.65	117.99	112.75
43	16	305	A86	C41-C32-C31	2.65	112.84	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	18	305	A86	C28-C27-C26	-2.65	119.21	122.92
31	b	611	CLA	CHB-C4A-NA	2.65	128.18	124.51
31	3	315	CLA	CHB-C4A-NA	2.65	128.18	124.51
31	C	503	CLA	C11-C12-C13	-2.65	107.36	115.92
45	12	309	KC2	C2B-C1B-NB	2.65	112.06	110.10
38	D	408	LMG	O1-C7-C8	-2.65	104.51	110.90
31	C	509	CLA	CAC-C3C-C4C	2.65	128.25	124.81
43	5	302	A86	C9-C10-C11	-2.65	118.82	126.61
43	17	305	A86	C25-C24-C1	-2.65	118.98	126.42
42	P	609	KC1	C4D-C3D-CAD	2.65	112.09	107.81
43	P	613	A86	O1-C20-C19	-2.65	111.39	113.38
42	17	314	KC1	CMA-C3A-C4A	-2.65	121.01	125.04
43	0	304	A86	C20-C19-C18	2.65	117.98	112.75
43	17	306	A86	C34-O4-C38	2.65	122.83	117.90
45	5	310	KC2	C2A-C1A-NA	2.65	113.64	109.40
34	A	411	SQD	O48-C23-C24	2.65	120.21	111.91
43	15	305	A86	O1-C15-C20	-2.64	56.81	59.40
45	7	311	KC2	C3C-C2C-C1C	-2.64	104.52	106.49
31	B	606	CLA	C3C-C4C-NC	-2.64	107.61	110.57
32	d	402	PHO	OBD-CAD-CBD	-2.64	121.94	125.82
31	0	312	CLA	CHB-C4A-NA	2.64	128.17	124.51
31	P	605	CLA	CAC-C3C-C4C	2.64	128.24	124.81
31	p	605	CLA	CAC-C3C-C4C	2.64	128.24	124.81
34	i	101	SQD	O48-C23-C24	2.64	120.21	111.91
42	9	314	KC1	C4D-C3D-CAD	2.64	112.08	107.81
45	12	311	KC2	CBD-CHA-C1A	2.64	133.81	128.88
31	17	313	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
31	18	311	CLA	CHA-C1A-NA	-2.64	120.34	126.40
31	P	603	CLA	CMD-C2D-C3D	2.64	133.69	127.61
45	2	310	KC2	O2D-CGD-O1D	-2.64	118.67	123.84
31	12	307	CLA	CHB-C4A-NA	2.64	128.17	124.51
31	19	312	CLA	CHB-C4A-NA	2.64	128.17	124.51
31	9	308	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
43	5	302	A86	C26-C25-C24	-2.64	114.97	123.22
31	D	401	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
31	P	605	CLA	CMB-C2B-C3B	2.64	129.62	124.68
33	B	619	BCR	C37-C22-C21	-2.64	119.22	122.92
43	4	301	A86	C20-C19-C18	-2.64	107.52	112.75
43	3	302	A86	O4-C34-C35	2.64	114.17	107.59
39	C	520	DGD	O2D-C2D-C1D	-2.64	103.63	110.05
31	19	313	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
31	16	308	CLA	C3A-C2A-C1A	2.64	105.29	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	621	DGD	C2G-O2G-C1B	2.64	124.29	117.79
31	11	315	CLA	C2D-C1D-ND	-2.64	108.16	110.10
43	1	320	A86	O4-C34-C35	2.64	114.17	107.59
31	b	613	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
43	5	304	A86	C10-C9-C8	-2.64	114.98	123.22
43	8	304	A86	C-C1-C2	-2.64	119.23	122.92
43	14	303	A86	C4-C3-C2	-2.64	118.07	123.47
43	1	302	A86	O1-C15-C20	-2.64	56.82	59.40
43	2	301	A86	C25-C24-C1	-2.64	119.01	126.42
43	1	304	A86	C7-C6-C8	2.64	122.23	118.08
31	14	306	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
31	5	306	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
31	B	606	CLA	O2A-C1-C2	-2.64	101.71	108.64
43	0	303	A86	C28-C27-C26	-2.64	119.23	122.92
43	6	306	A86	C9-C8-C6	-2.63	119.02	126.42
31	0	309	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
31	12	312	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
43	19	301	A86	O4-C34-C35	2.63	114.15	107.59
43	4	301	A86	O3-C36-C37	-2.63	104.70	109.39
43	5	302	A86	O-C13-C14	2.63	127.01	121.66
31	c	503	CLA	C11-C12-C13	-2.63	107.41	115.92
35	A	409	PL9	C7-C8-C9	-2.63	122.41	126.79
31	13	310	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
31	p	603	CLA	CMD-C2D-C3D	2.63	133.67	127.61
31	d	401	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
43	18	301	A86	C19-C18-C17	-2.63	105.69	110.77
31	7	308	CLA	CMA-C3A-C2A	-2.63	109.96	116.10
42	5	313	KC1	C4C-C3C-C2C	-2.63	103.06	106.90
31	12	316	CLA	CMB-C2B-C3B	2.63	129.60	124.68
31	3	316	CLA	C1D-ND-C4D	-2.63	104.47	106.33
34	0	318	SQD	O8-S-C6	2.63	109.93	105.74
31	p	607	CLA	CBC-CAC-C3C	2.63	119.68	112.43
43	6	306	A86	C4-C3-C2	-2.63	118.09	123.47
31	5	312	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
38	K	101	LMG	O3-C3-C2	-2.63	104.27	110.35
38	k	101	LMG	O3-C3-C2	-2.63	104.27	110.35
33	B	617	BCR	C15-C16-C17	-2.63	118.09	123.47
31	7	315	CLA	CHB-C4A-NA	2.63	128.15	124.51
31	B	612	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	11	308	CLA	CBC-CAC-C3C	2.63	119.67	112.43
43	14	301	A86	C14-C15-C16	2.63	128.81	118.75
45	8	310	KC2	C3A-C4A-NA	2.63	113.44	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	520	DGD	O2D-C2D-C1D	-2.63	103.67	110.05
31	p	605	CLA	CMB-C2B-C3B	2.63	129.59	124.68
31	B	603	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	D	401	CLA	O2D-CGD-CBD	2.63	115.93	111.27
33	h	101	BCR	C27-C26-C25	2.62	126.54	122.73
31	11	316	CLA	CMA-C3A-C2A	-2.62	109.97	116.10
45	8	310	KC2	CAB-C3B-C4B	-2.62	118.56	124.90
33	c	515	BCR	C11-C10-C9	-2.62	123.56	127.31
31	11	315	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
31	15	309	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
31	19	312	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
43	14	303	A86	C25-C24-C1	-2.62	119.05	126.42
31	D	404	CLA	CBC-CAC-C3C	2.62	119.66	112.43
43	11	302	A86	C9-C8-C6	-2.62	119.05	126.42
31	c	509	CLA	CAC-C3C-C4C	2.62	128.21	124.81
31	12	308	CLA	C3A-C2A-C1A	2.62	105.27	101.34
31	19	308	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
31	P	607	CLA	CBC-CAC-C3C	2.62	119.66	112.43
33	B	618	BCR	C7-C8-C9	-2.62	122.27	126.23
33	Y	101	BCR	C38-C26-C27	-2.62	108.58	113.62
31	11	313	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
43	0	303	A86	O4-C34-C35	-2.62	101.07	107.59
31	11	307	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
31	12	308	CLA	CBC-CAC-C3C	2.62	119.65	112.43
31	17	308	CLA	CGD-CBD-CAD	-2.62	102.25	110.73
31	12	307	CLA	C2A-C1A-CHA	2.62	128.44	123.86
31	b	604	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
31	c	510	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
31	c	507	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
31	C	505	CLA	CAC-C3C-C2C	-2.62	123.05	127.53
33	y	101	BCR	C38-C26-C27	-2.62	108.59	113.62
45	4	310	KC2	CGD-CBD-CAD	-2.62	102.26	110.73
43	0	302	A86	C20-C19-C18	2.62	117.92	112.75
34	l	101	SQD	O8-S-C6	2.62	109.91	105.74
43	3	305	A86	C35-C34-C33	-2.62	105.31	109.88
31	8	314	CLA	CMB-C2B-C3B	2.61	129.57	124.68
31	5	314	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
43	p	613	A86	O1-C20-C19	-2.61	111.42	113.38
43	15	305	A86	C8-C6-C5	-2.61	114.93	118.94
31	1	310	CLA	C1-C2-C3	-2.61	122.52	126.75
31	10	309	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
33	C	515	BCR	C11-C10-C9	-2.61	123.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	610	CLA	CHB-C4A-NA	2.61	128.13	124.51
43	1	320	A86	C41-C32-C33	-2.61	97.31	109.05
38	n	701	LMG	O7-C10-O9	-2.61	117.39	123.70
31	d	404	CLA	CBC-CAC-C3C	2.61	119.63	112.43
31	C	507	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
31	10	313	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
31	17	315	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	C	510	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
33	H	101	BCR	C27-C26-C25	2.61	126.52	122.73
42	12	314	KC1	C2B-C1B-NB	2.61	112.03	110.10
43	4	305	A86	C21-C20-C19	2.61	117.22	114.28
31	10	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	1	308	CLA	C4-C3-C5	2.61	119.66	115.27
43	0	303	A86	O-C13-C11	-2.61	115.38	121.15
43	11	320	A86	C10-C9-C8	-2.61	115.08	123.22
31	8	309	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
31	1	315	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
35	a	409	PL9	C7-C8-C9	-2.61	122.45	126.79
31	B	602	CLA	CHC-C1C-NC	2.61	128.16	124.20
43	1	305	A86	C34-O4-C38	-2.61	113.04	117.90
43	16	303	A86	C34-O4-C38	2.61	122.76	117.90
43	14	305	A86	C23-C16-C17	-2.61	104.45	108.98
43	16	303	A86	C25-C24-C1	-2.61	119.09	126.42
39	c	518	DGD	CDB-CCB-CBB	-2.61	101.19	114.42
31	0	308	CLA	CAC-C3C-C2C	-2.61	123.07	127.53
31	16	308	CLA	O2D-CGD-CBD	2.61	115.90	111.27
42	16	301	KC1	C3D-CAD-CBD	-2.61	104.17	107.61
31	19	307	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
34	L	102	SQD	O8-S-C6	2.61	109.89	105.74
31	b	615	CLA	O2D-CGD-CBD	2.61	115.90	111.27
43	16	307	A86	C4-C3-C2	-2.60	118.14	123.47
31	0	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
45	11	311	KC2	CAC-C3C-C4C	2.60	136.60	124.47
39	C	518	DGD	CDB-CCB-CBB	-2.60	101.21	114.42
42	12	314	KC1	O2D-CGD-O1D	-2.60	118.75	123.84
31	12	312	CLA	C2A-C1A-CHA	2.60	128.41	123.86
31	B	614	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
43	16	305	A86	C4-C3-C2	-2.60	118.14	123.47
31	8	312	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	c	505	CLA	CAC-C3C-C2C	-2.60	123.08	127.53
33	B	618	BCR	C2-C1-C6	2.60	114.49	110.48
31	b	616	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	10	306	A86	C9-C10-C11	-2.60	118.96	126.61
43	14	301	A86	O1-C20-C21	-2.60	111.94	115.06
43	12	306	A86	O3-C36-C37	-2.60	104.76	109.39
38	B	620	LMG	C38-C37-C36	-2.60	101.22	114.42
43	0	303	A86	C20-C19-C18	2.60	117.89	112.75
31	b	617	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
39	1	318	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
38	d	403	LMG	O8-C28-O10	-2.60	117.03	123.59
43	10	318	A86	C9-C8-C6	-2.60	119.11	126.42
31	3	315	CLA	O2D-CGD-CBD	2.60	115.89	111.27
43	18	301	A86	C9-C8-C6	-2.60	119.12	126.42
31	b	609	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	8	316	LHG	C11-C10-C9	-2.60	101.24	114.42
31	B	603	CLA	CHD-C1D-ND	-2.60	122.07	124.45
45	5	308	KC2	CAB-C3B-C4B	-2.60	118.63	124.90
39	C	519	DGD	O3E-C3E-C2E	-2.60	104.35	110.35
39	c	519	DGD	O3E-C3E-C2E	-2.60	104.35	110.35
45	16	310	KC2	CBC-CAC-C3C	-2.60	114.71	127.62
38	k	101	LMG	O2-C2-C1	-2.60	103.74	110.05
33	b	619	BCR	C7-C8-C9	-2.59	122.31	126.23
31	11	316	CLA	CHB-C4A-NA	2.59	128.10	124.51
42	2	313	KC1	CMA-C3A-C4A	-2.59	121.09	125.04
43	14	302	A86	C41-C32-C31	-2.59	108.15	110.47
31	b	615	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
43	8	301	A86	C20-C19-C18	-2.59	107.62	112.75
42	p	609	KC1	CAC-C3C-C4C	2.59	128.17	124.81
38	K	101	LMG	O2-C2-C1	-2.59	103.75	110.05
31	2	312	CLA	CBA-CAA-C2A	-2.59	106.21	113.86
43	2	302	A86	C14-C15-C16	-2.59	108.83	118.75
33	y	101	BCR	C2-C1-C6	2.59	114.47	110.48
45	10	310	KC2	CAB-C3B-C2B	2.59	137.14	128.60
31	12	307	CLA	C1D-ND-C4D	2.59	108.18	106.33
31	0	309	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
36	5	317	LHG	O8-C23-C24	2.59	120.04	111.91
42	11	314	KC1	C4D-C3D-CAD	2.59	112.00	107.81
31	B	616	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
31	0	313	CLA	C3A-C2A-C1A	2.59	105.22	101.34
43	12	306	A86	C36-C31-C32	-2.59	117.13	119.70
45	7	311	KC2	O2D-CGD-O1D	-2.59	118.78	123.84
38	D	408	LMG	C9-C8-C7	-2.59	105.66	111.79
43	19	302	A86	O4-C34-C33	2.59	114.04	107.59
43	0	306	A86	C9-C10-C11	-2.59	119.00	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	304	A86	C41-C32-C31	2.59	112.79	110.47
43	9	306	A86	C36-C31-C32	-2.59	117.13	119.70
31	4	311	CLA	C2A-C1A-CHA	2.59	128.38	123.86
45	14	310	KC2	CGD-CBD-CAD	-2.59	102.35	110.73
31	8	311	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
31	15	309	CLA	C7-C6-C5	-2.59	106.33	113.36
43	18	304	A86	C3-C4-C5	-2.59	118.17	123.47
31	4	309	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
31	B	615	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
43	10	301	A86	C8-C6-C5	2.59	122.91	118.94
43	3	305	A86	C41-C32-C33	2.59	120.66	109.05
43	10	305	A86	C35-C34-C33	-2.59	105.36	109.88
43	0	301	A86	C34-O4-C38	2.59	122.71	117.90
33	b	618	BCR	C15-C16-C17	-2.58	118.18	123.47
31	17	307	CLA	C2A-C1A-CHA	2.58	128.37	123.85
45	8	310	KC2	O2D-CGD-O1D	-2.58	118.79	123.84
38	f	102	LMG	O3-C3-C2	-2.58	104.38	110.35
43	4	304	A86	C40-C32-C31	2.58	112.78	110.47
43	1	303	A86	C34-O4-C38	-2.58	113.08	117.90
38	F	102	LMG	O3-C3-C2	-2.58	104.38	110.35
31	b	611	CLA	CMB-C2B-C3B	2.58	129.51	124.68
43	7	302	A86	C9-C10-C11	-2.58	119.02	126.61
38	d	408	LMG	C9-C8-C7	-2.58	105.68	111.79
43	16	306	A86	O-C13-C11	-2.58	115.44	121.15
33	h	101	BCR	C15-C16-C17	-2.58	118.18	123.47
31	1	321	CLA	CAA-CBA-CGA	-2.58	105.71	113.25
43	10	306	A86	C25-C24-C1	-2.58	119.16	126.42
31	11	315	CLA	CHB-C4A-NA	2.58	128.08	124.51
31	d	405	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
31	8	309	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
43	4	306	A86	C8-C6-C5	-2.58	114.98	118.94
43	8	301	A86	C3-C4-C5	-2.58	118.19	123.47
38	J	101	LMG	O6-C1-O1	-2.58	103.86	109.97
31	8	306	CLA	C3A-C2A-C1A	2.58	105.20	101.34
33	B	617	BCR	C11-C10-C9	-2.58	123.63	127.31
45	14	310	KC2	C3D-CAD-CBD	-2.58	104.21	107.61
45	15	308	KC2	C3A-C4A-NA	2.58	113.39	110.57
31	c	503	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
43	3	304	A86	C40-C32-C31	-2.58	108.17	110.47
31	B	614	CLA	O2D-CGD-CBD	2.58	115.84	111.27
42	P	609	KC1	CAC-C3C-C4C	2.57	128.15	124.81
43	14	305	A86	C20-C19-C18	2.57	117.84	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	305	A86	C28-C27-C26	-2.57	119.32	122.92
31	2	315	CLA	CHD-C4C-NC	2.57	128.26	124.20
43	8	305	A86	C9-C8-C6	-2.57	119.19	126.42
31	6	314	CLA	C1D-ND-C4D	2.57	108.16	106.33
31	14	311	CLA	C2D-C1D-ND	-2.57	108.21	110.10
43	3	304	A86	C7-C6-C8	2.57	122.13	118.08
31	18	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	12	315	CLA	CMB-C2B-C3B	2.57	129.49	124.68
43	5	302	A86	C3-C4-C5	-2.57	118.21	123.47
31	0	307	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
31	19	308	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
31	B	610	CLA	CMB-C2B-C3B	2.57	129.49	124.68
38	j	101	LMG	O6-C1-O1	-2.57	103.89	109.97
43	1	302	A86	C7-C6-C5	-2.57	119.32	122.92
45	1	309	KC2	CHD-C4C-NC	-2.57	120.31	124.20
43	10	303	A86	C28-C27-C26	-2.57	119.32	122.92
31	b	604	CLA	CHD-C1D-ND	-2.57	122.09	124.45
31	2	306	CLA	C2D-C1D-ND	-2.57	108.21	110.10
31	1	307	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
31	B	606	CLA	CBA-CAA-C2A	2.57	121.44	113.86
33	c	515	BCR	C2-C1-C6	2.57	114.43	110.48
31	10	311	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
43	16	302	A86	O4-C38-O5	-2.57	117.86	122.96
31	0	312	CLA	CAC-C3C-C4C	-2.57	121.48	124.81
31	16	314	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
31	8	311	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
42	9	314	KC1	C2B-C1B-NB	2.57	112.00	110.10
31	14	309	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
43	3	302	A86	C7-C6-C5	-2.57	119.33	122.92
45	1	311	KC2	C4D-C3D-CAD	2.56	111.95	107.81
43	15	303	A86	C33-C32-C31	-2.56	106.72	109.21
31	7	310	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	9	315	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
33	B	619	BCR	C20-C21-C22	-2.56	123.65	127.31
31	17	313	CLA	CHA-C4D-ND	2.56	137.86	132.50
42	13	314	KC1	C4B-C3B-C2B	-2.56	104.65	106.75
31	10	308	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
31	6	309	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
39	c	519	DGD	O3G-C1D-C2D	-2.56	104.30	108.30
31	C	503	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
42	17	314	KC1	CMB-C2B-C1B	2.56	129.23	124.71
43	5	303	A86	C25-C24-C1	-2.56	119.22	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	f	101	BCR	C27-C26-C25	2.56	126.45	122.73
38	w	201	LMG	O2-C2-C1	-2.56	103.83	110.05
31	18	314	CLA	CMB-C2B-C3B	2.56	129.47	124.68
33	b	618	BCR	C11-C10-C9	-2.56	123.66	127.31
43	12	301	A86	C4-C3-C2	-2.56	118.23	123.47
31	D	405	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
45	11	309	KC2	C3B-C2B-C1B	-2.56	104.63	107.08
45	9	309	KC2	C2A-C3A-C4A	2.56	108.38	106.49
34	10	320	SQD	O8-S-C6	2.56	109.82	105.74
31	10	308	CLA	C3C-C4C-NC	-2.56	107.70	110.57
38	n	701	LMG	O6-C1-O1	-2.56	103.92	109.97
33	C	515	BCR	C2-C1-C6	2.56	114.42	110.48
31	0	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
31	p	604	CLA	CHD-C1D-ND	-2.56	122.10	124.45
33	B	619	BCR	C11-C10-C9	-2.56	123.66	127.31
31	16	309	CLA	CAC-C3C-C4C	2.56	128.13	124.81
31	10	309	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
31	16	314	CLA	C3D-C4D-CHA	-2.56	106.88	112.72
31	11	310	CLA	C1-C2-C3	-2.56	122.62	126.75
43	15	303	A86	C20-C19-C18	2.56	117.80	112.75
31	P	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
43	10	303	A86	O2-C18-C17	-2.55	104.73	109.80
45	7	311	KC2	C3D-CAD-CBD	-2.55	104.24	107.61
31	b	603	CLA	CHC-C1C-NC	2.55	128.08	124.20
39	1	318	DGD	O6E-C5E-C4E	2.55	114.33	109.69
31	p	606	CLA	C2C-C1C-NC	-2.55	107.58	109.97
33	b	619	BCR	C2-C1-C6	2.55	114.41	110.48
43	11	320	A86	C17-C16-C15	2.55	111.77	109.16
31	1	312	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
45	14	308	KC2	O2D-CGD-O1D	-2.55	118.85	123.84
31	D	401	CLA	C1-C2-C3	-2.55	121.63	126.04
38	11	317	LMG	O7-C10-O9	-2.55	117.54	123.70
31	8	312	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
35	D	406	PL9	C40-C39-C41	2.55	119.56	115.27
31	16	316	CLA	CMB-C2B-C3B	2.55	129.45	124.68
33	Y	101	BCR	C2-C1-C6	2.55	114.40	110.48
31	C	512	CLA	CHB-C4A-NA	2.55	128.03	124.51
43	0	304	A86	C10-C9-C8	-2.55	115.27	123.22
39	C	519	DGD	O3G-C1D-C2D	-2.55	104.33	108.30
43	16	305	A86	C25-C24-C1	-2.55	119.26	126.42
43	1	304	A86	C9-C10-C11	-2.55	119.12	126.61
31	10	313	CLA	C3A-C2A-C1A	2.55	105.15	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	14	316	LMG	O7-C10-C11	2.55	116.99	111.50
31	a	406	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
43	2	301	A86	C28-C27-C26	-2.54	119.36	122.92
31	17	307	CLA	C3C-C4C-NC	-2.54	107.72	110.57
43	9	302	A86	C3-C4-C5	-2.54	118.26	123.47
31	a	403	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
33	b	620	BCR	C11-C10-C9	-2.54	123.68	127.31
31	2	306	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
31	7	308	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
31	19	315	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
39	C	519	DGD	C3D-C4D-C5D	-2.54	105.70	110.24
31	10	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	2	312	CLA	CHD-C1D-C2D	2.54	130.81	125.48
45	9	309	KC2	C3B-C2B-C1B	-2.54	104.65	107.08
43	14	301	A86	C25-C24-C1	-2.54	119.27	126.42
43	10	304	A86	C10-C9-C8	-2.54	115.28	123.22
31	14	314	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
31	8	312	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
39	B	621	DGD	O3G-C1D-C2D	2.54	112.27	108.30
31	3	316	CLA	C3C-C4C-NC	-2.54	107.72	110.57
43	4	305	A86	O-C13-C11	-2.54	115.53	121.15
31	w	203	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	13	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
31	1	321	CLA	CAA-C2A-C1A	2.54	120.30	111.97
39	c	519	DGD	C3D-C4D-C5D	-2.54	105.71	110.24
31	B	613	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
43	10	303	A86	C20-C19-C18	2.54	117.78	112.75
31	P	605	CLA	CAA-C2A-C3A	-2.54	110.17	116.10
31	13	312	CLA	O1D-CGD-CBD	2.54	129.68	124.48
43	14	303	A86	C33-C32-C31	-2.54	106.74	109.21
31	5	309	CLA	C7-C6-C5	-2.54	106.46	113.36
45	7	311	KC2	C3A-C4A-NA	2.54	113.34	110.57
31	8	306	CLA	C1-O2A-CGA	2.54	123.11	116.44
43	5	304	A86	C12-C11-C13	2.54	120.29	116.02
31	5	306	CLA	C2A-C1A-CHA	2.54	128.30	123.86
43	10	303	A86	O-C13-C11	-2.54	115.54	121.15
38	W	201	LMG	O2-C2-C1	-2.54	103.88	110.05
31	9	308	CLA	CHB-C4A-NA	2.54	128.02	124.51
31	9	307	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
31	A	403	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
31	d	401	CLA	C1-C2-C3	-2.54	121.65	126.04
31	17	307	CLA	C2D-C1D-ND	-2.54	108.23	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	10	320	SQD	C44-O6-C1	2.54	118.70	113.74
31	6	314	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
31	b	607	CLA	C3C-C4C-NC	-2.54	107.73	110.57
31	p	605	CLA	CAA-C2A-C3A	-2.54	110.18	116.10
43	16	305	A86	C40-C32-C31	-2.54	108.20	110.47
43	6	303	A86	C19-C18-C17	2.54	115.67	110.77
43	12	302	A86	O4-C34-C33	-2.54	101.28	107.59
38	p	614	LMG	O3-C3-C2	-2.54	104.49	110.35
35	d	406	PL9	C40-C39-C41	2.54	119.54	115.27
43	5	318	A86	C21-C20-C19	2.54	117.13	114.28
31	P	606	CLA	C2C-C1C-NC	-2.54	107.60	109.97
43	4	305	A86	C3-C4-C5	-2.54	118.28	123.47
43	6	303	A86	C41-C32-C40	-2.54	100.75	108.53
31	w	203	CLA	CAA-C2A-C1A	-2.53	103.67	111.97
33	b	620	BCR	C20-C21-C22	-2.53	123.69	127.31
31	12	308	CLA	CAC-C3C-C4C	2.53	128.10	124.81
31	12	308	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	17	313	CLA	C3B-C4B-NB	-2.53	105.94	109.21
38	J	101	LMG	C38-C37-C36	-2.53	101.57	114.42
33	B	618	BCR	C40-C30-C25	2.53	114.41	110.30
33	H	101	BCR	C15-C16-C17	-2.53	118.29	123.47
31	3	312	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	2	311	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
43	1	320	A86	C20-C19-C18	2.53	117.76	112.75
33	F	101	BCR	C27-C26-C25	2.53	126.41	122.73
43	16	305	A86	O2-C18-C17	-2.53	104.77	109.80
43	12	301	A86	C7-C6-C5	-2.53	119.38	122.92
31	c	512	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	8	306	CLA	CHB-C4A-NA	2.53	128.01	124.51
43	11	303	A86	C19-C18-C17	-2.53	105.89	110.77
31	A	406	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	W	202	CLA	CAA-C2A-C1A	-2.53	103.69	111.97
42	11	314	KC1	C4B-C3B-C2B	-2.53	104.67	106.75
41	e	101	HEM	C1B-NB-C4B	2.53	107.69	105.07
45	12	309	KC2	C3C-C2C-C1C	-2.53	104.61	106.49
43	18	301	A86	C12-C11-C13	2.53	120.27	116.02
31	12	316	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
43	11	320	A86	O1-C15-C20	-2.53	56.93	59.40
31	W	202	CLA	CHB-C4A-NA	2.53	128.01	124.51
45	18	308	KC2	CAC-C3C-C2C	-2.53	120.28	128.60
38	P	614	LMG	O3-C3-C2	-2.53	104.51	110.35
31	C	510	CLA	CHD-C1D-ND	-2.53	122.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	510	CLA	CHD-C1D-ND	-2.53	122.13	124.45
38	j	101	LMG	C38-C37-C36	-2.53	101.60	114.42
31	15	307	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
42	10	315	KC1	O2D-CGD-O1D	-2.53	118.90	123.84
43	11	302	A86	O4-C34-C35	-2.53	101.30	107.59
31	5	314	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	P	603	CLA	CGD-CBD-CAD	-2.53	102.55	110.73
43	13	306	A86	O-C13-C14	2.53	126.79	121.66
31	10	308	CLA	C2D-C1D-ND	-2.53	108.24	110.10
32	a	405	PHO	O2D-CGD-O1D	-2.53	118.90	123.84
38	b	621	LMG	C38-C37-C36	-2.52	101.61	114.42
31	b	607	CLA	CHD-C1D-ND	-2.52	122.14	124.45
31	d	404	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
31	C	503	CLA	CMD-C2D-C3D	2.52	133.42	127.61
31	c	503	CLA	CMD-C2D-C3D	2.52	133.42	127.61
33	C	516	BCR	C29-C30-C25	2.52	114.36	110.48
31	17	307	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
33	B	619	BCR	C30-C25-C26	-2.52	119.06	122.61
45	9	309	KC2	CAA-CBA-CGA	-2.52	114.30	127.26
43	9	302	A86	C4-C3-C2	-2.52	118.31	123.47
45	5	310	KC2	C3B-C2B-C1B	-2.52	104.67	107.08
43	4	302	A86	O1-C15-C20	-2.52	56.93	59.40
42	14	313	KC1	C4B-C3B-C2B	-2.52	104.68	106.75
43	14	302	A86	C4-C3-C2	-2.52	118.31	123.47
43	p	613	A86	C10-C9-C8	-2.52	115.35	123.22
45	15	310	KC2	CAC-C3C-C4C	2.52	136.21	124.47
43	4	301	A86	C9-C8-C6	-2.52	119.34	126.42
43	19	303	A86	O4-C34-C35	2.52	113.87	107.59
43	10	302	A86	C19-C18-C17	-2.52	105.91	110.77
36	8	315	LHG	C11-C10-C9	-2.52	101.64	114.42
31	12	310	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
31	p	603	CLA	CGD-CBD-CAD	-2.52	102.58	110.73
31	17	308	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
43	14	304	A86	C41-C32-C33	-2.52	97.74	109.05
43	13	305	A86	C25-C24-C1	-2.52	119.34	126.42
31	17	308	CLA	CHB-C4A-NA	2.52	127.99	124.51
43	13	301	A86	C4-C3-C2	-2.52	118.32	123.47
31	c	511	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
31	b	614	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
31	P	608	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
43	8	302	A86	C25-C24-C1	-2.52	119.35	126.42
31	p	607	CLA	CMB-C2B-C3B	2.52	129.39	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	404	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
33	c	516	BCR	C29-C30-C25	2.52	114.35	110.48
38	d	403	LMG	O6-C1-O1	-2.52	104.02	109.97
43	3	301	A86	C7-C6-C8	2.52	122.04	118.08
31	p	608	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
43	16	304	A86	C9-C10-C11	-2.51	119.22	126.61
31	1	313	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
33	b	619	BCR	C40-C30-C25	2.51	114.38	110.30
31	12	316	CLA	C3A-C2A-C1A	2.51	105.10	101.34
38	B	620	LMG	O6-C1-C2	-2.51	105.03	110.35
42	16	301	KC1	CHD-C4C-NC	-2.51	120.39	124.20
45	18	308	KC2	O2D-CGD-O1D	-2.51	118.93	123.84
33	B	619	BCR	C38-C26-C27	-2.51	108.79	113.62
43	10	305	A86	C28-C27-C26	-2.51	119.40	122.92
43	8	305	A86	C3-C2-C1	-2.51	123.72	127.31
31	b	617	CLA	CMA-C3A-C2A	-2.51	103.69	113.83
43	15	301	A86	C40-C32-C31	-2.51	108.22	110.47
36	d	407	LHG	O8-C23-C24	2.51	119.79	111.91
43	1	305	A86	C-C1-C2	-2.51	119.41	122.92
43	8	303	A86	C40-C32-C31	-2.51	108.22	110.47
31	P	607	CLA	CMB-C2B-C3B	2.51	129.38	124.68
43	6	304	A86	O2-C18-C17	-2.51	104.81	109.80
43	17	301	A86	C4-C3-C2	-2.51	118.33	123.47
31	0	314	CLA	C2A-C1A-CHA	2.51	128.25	123.86
31	14	306	CLA	CED-O2D-CGD	2.51	121.61	115.94
31	B	606	CLA	CHD-C1D-C2D	2.51	130.74	125.48
43	15	302	A86	C21-C20-C19	2.51	117.10	114.28
31	b	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
33	a	407	BCR	C7-C8-C9	-2.51	122.45	126.23
31	16	309	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
43	11	305	A86	O2-C18-C19	-2.51	104.82	109.80
44	p	612	DD6	C-C1-C2	-2.51	119.41	122.92
31	C	511	CLA	C1B-CHB-C4A	-2.51	125.16	130.12
31	b	616	CLA	C2A-C1A-CHA	2.50	128.24	123.86
31	15	311	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
31	14	312	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
31	14	306	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
38	M	101	LMG	C6-C5-C4	-2.50	107.14	113.00
33	B	617	BCR	C39-C30-C25	2.50	114.36	110.30
31	b	606	CLA	CHD-C1D-ND	-2.50	122.15	124.45
43	14	304	A86	C3-C4-C5	-2.50	118.34	123.47
31	a	403	CLA	C1B-CHB-C4A	-2.50	125.16	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	E	101	HEM	C1B-NB-C4B	2.50	107.66	105.07
43	8	302	A86	C12-C11-C13	2.50	120.23	116.02
43	9	302	A86	C40-C32-C31	2.50	112.71	110.47
31	6	309	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
39	b	622	DGD	C6D-O5D-C1E	2.50	118.63	113.74
43	5	302	A86	C12-C11-C13	2.50	120.23	116.02
43	5	302	A86	C22-C16-C17	-2.50	104.64	108.98
43	11	304	A86	C33-C32-C31	-2.50	106.78	109.21
36	D	407	LHG	O8-C23-C24	2.50	119.76	111.91
43	6	304	A86	C9-C10-C11	-2.50	119.25	126.61
43	2	301	A86	O3-C36-C37	-2.50	104.94	109.39
43	8	303	A86	C14-C15-C16	2.50	128.33	118.75
31	r	101	CLA	CMB-C2B-C3B	2.50	129.36	124.68
33	A	407	BCR	C7-C8-C9	-2.50	122.46	126.23
43	0	305	A86	C28-C27-C26	-2.50	119.42	122.92
38	N	101	LMG	O7-C10-O9	-2.50	117.66	123.70
43	P	613	A86	C10-C9-C8	-2.50	115.41	123.22
32	A	405	PHO	CMC-C2C-C3C	2.50	129.66	124.94
38	5	316	LMG	O3-C3-C2	-2.50	104.57	110.35
39	H	102	DGD	CAB-C9B-C8B	-2.50	101.73	114.42
43	18	303	A86	C40-C32-C31	-2.50	108.23	110.47
43	8	305	A86	C22-C16-C17	-2.50	104.64	108.98
31	B	615	CLA	C2A-C1A-CHA	2.50	128.23	123.86
43	12	302	A86	C3-C4-C5	-2.50	118.36	123.47
43	2	303	A86	C41-C32-C31	2.50	112.71	110.47
43	12	305	A86	C41-C32-C31	2.50	112.71	110.47
31	16	314	CLA	C4D-C3D-CAD	2.50	111.04	108.10
32	a	405	PHO	CMC-C2C-C3C	2.50	129.65	124.94
31	5	314	CLA	CMB-C2B-C3B	2.50	129.35	124.68
43	13	306	A86	O1-C15-C20	-2.50	56.96	59.40
42	4	313	KC1	C4B-C3B-C2B	-2.50	104.70	106.75
45	19	309	KC2	C3B-C2B-C1B	-2.50	104.69	107.08
34	b	601	SQD	O8-S-C6	2.50	109.72	105.74
33	b	618	BCR	C39-C30-C25	2.50	114.35	110.30
43	1	303	A86	C10-C9-C8	-2.50	115.42	123.22
32	A	405	PHO	O2D-CGD-O1D	-2.50	118.96	123.84
43	0	303	A86	O2-C18-C17	-2.50	104.84	109.80
38	b	621	LMG	O6-C1-C2	-2.50	105.07	110.35
43	7	305	A86	C26-C25-C24	-2.49	115.43	123.22
39	h	102	DGD	CAB-C9B-C8B	-2.49	101.76	114.42
43	9	301	A86	C3-C4-C5	-2.49	118.36	123.47
31	14	311	CLA	C2A-C1A-CHA	2.49	128.22	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	1	309	KC2	CMD-C2D-C1D	-2.49	124.63	128.46
31	p	610	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
31	7	307	CLA	O2D-CGD-CBD	2.49	115.70	111.27
43	4	301	A86	O4-C38-C39	2.49	115.68	111.09
43	0	305	A86	O-C13-C14	2.49	126.72	121.66
43	6	307	A86	C24-C1-C2	-2.49	115.12	118.94
45	1	309	KC2	C4D-C3D-CAD	2.49	111.84	107.81
43	12	301	A86	O-C13-C14	-2.49	116.60	121.66
31	b	605	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
45	14	308	KC2	CGD-CBD-CAD	-2.49	102.67	110.73
31	P	610	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
31	b	607	CLA	CBA-CAA-C2A	2.49	121.22	113.86
39	1	318	DGD	O3G-C1D-C2D	-2.49	104.41	108.30
31	18	312	CLA	CAA-CBA-CGA	2.49	120.53	113.25
31	R	101	CLA	CMB-C2B-C3B	2.49	129.34	124.68
31	2	309	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
42	4	313	KC1	O1D-CGD-CBD	-2.49	119.39	124.48
31	7	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
43	11	305	A86	C25-C24-C1	-2.49	119.42	126.42
31	7	307	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
42	16	301	KC1	C1C-C2C-C3C	-2.49	104.34	106.96
43	11	303	A86	C28-C27-C26	-2.49	119.44	122.92
43	1	306	A86	O1-C15-C20	-2.49	56.97	59.40
36	15	316	LHG	O8-C23-C24	2.49	119.72	111.91
33	b	619	BCR	C27-C26-C25	2.49	126.34	122.73
34	B	623	SQD	O8-S-C6	2.49	109.70	105.74
31	B	604	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
43	1	306	A86	O2-C18-C19	2.49	114.75	109.80
43	17	306	A86	C26-C25-C24	-2.49	115.45	123.22
45	4	308	KC2	CGD-CBD-CAD	-2.49	102.68	110.73
43	8	303	A86	O3-C36-C37	-2.49	104.97	109.39
38	B	620	LMG	O6-C1-O1	-2.49	104.08	109.97
34	L	102	SQD	O6-C1-C2	2.49	112.19	108.30
31	16	313	CLA	C2D-C1D-ND	-2.49	108.27	110.10
43	11	304	A86	C9-C10-C11	-2.49	119.30	126.61
31	7	308	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
42	10	315	KC1	CMA-C3A-C4A	-2.49	121.25	125.04
38	B	620	LMG	C40-C39-C38	-2.48	101.81	114.42
39	C	519	DGD	O5D-C6D-C5D	-2.48	104.45	109.05
31	11	316	CLA	CMB-C2B-C3B	2.48	129.33	124.68
31	p	607	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
31	B	616	CLA	CMA-C3A-C2A	-2.48	103.81	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	304	A86	C3-C4-C5	-2.48	118.39	123.47
31	3	315	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
43	11	319	A86	O1-C15-C20	-2.48	56.97	59.40
31	A	403	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
43	10	318	A86	C4-C3-C2	-2.48	118.39	123.47
43	6	303	A86	C4-C3-C2	-2.48	118.39	123.47
45	10	310	KC2	C4D-C3D-CAD	2.48	111.82	107.81
38	15	315	LMG	O3-C3-C2	-2.48	104.61	110.35
31	3	310	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
43	5	305	A86	C25-C24-C1	-2.48	119.45	126.42
41	E	101	HEM	CAD-CBD-CGD	-2.48	108.27	113.60
43	16	305	A86	C9-C10-C11	-2.48	119.31	126.61
43	11	319	A86	O4-C34-C35	2.48	113.77	107.59
43	16	305	A86	C10-C9-C8	-2.48	115.48	123.22
43	16	305	A86	O-C13-C11	-2.48	115.67	121.15
34	l	101	SQD	O6-C1-C2	2.48	112.17	108.30
33	b	620	BCR	C38-C26-C27	-2.48	108.85	113.62
43	9	305	A86	C28-C27-C26	-2.48	119.45	122.92
43	3	301	A86	O4-C38-O5	-2.48	118.04	122.96
31	B	607	CLA	CHB-C4A-NA	2.48	127.94	124.51
31	b	607	CLA	O2D-CGD-CBD	2.48	115.67	111.27
43	2	303	A86	C40-C32-C31	-2.48	108.25	110.47
43	9	301	A86	C-C1-C24	2.48	121.98	118.08
43	5	303	A86	O4-C38-O5	-2.48	118.04	122.96
43	18	303	A86	C3-C4-C5	-2.48	118.40	123.47
31	2	306	CLA	C3C-C4C-NC	-2.48	107.79	110.57
31	15	313	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
31	4	312	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
43	19	301	A86	C-C1-C24	2.48	121.98	118.08
45	7	311	KC2	C2A-C1A-NA	2.48	113.37	109.40
31	B	605	CLA	CHD-C1D-ND	-2.48	122.18	124.45
31	d	401	CLA	CHD-C1D-ND	-2.48	122.18	124.45
31	2	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
31	P	602	CLA	CMD-C2D-C3D	2.48	133.31	127.61
45	5	310	KC2	C2A-C3A-C4A	2.47	108.32	106.49
39	W	203	DGD	O6E-C5E-C4E	2.47	114.19	109.69
31	0	308	CLA	C3C-C4C-NC	-2.47	107.80	110.57
43	19	301	A86	C3-C4-C5	-2.47	118.41	123.47
43	11	302	A86	C25-C24-C1	-2.47	119.47	126.42
31	17	310	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
31	0	313	CLA	O2D-CGD-CBD	2.47	115.66	111.27
31	C	504	CLA	C2A-C1A-CHA	2.47	128.18	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	2	308	KC2	CBC-CAC-C3C	-2.47	115.32	127.62
31	10	312	CLA	C2D-C1D-ND	-2.47	108.28	110.10
38	N	101	LMG	O6-C1-O1	-2.47	104.12	109.97
31	9	308	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
38	m	101	LMG	O2-C2-C1	-2.47	104.04	110.05
31	p	602	CLA	CMD-C2D-C3D	2.47	133.30	127.61
41	e	101	HEM	CAD-CBD-CGD	-2.47	108.28	113.60
43	18	302	A86	C17-C16-C15	2.47	111.68	109.16
39	W	203	DGD	C3G-C2G-C1G	-2.47	105.95	111.79
43	2	305	A86	O4-C34-C33	-2.47	101.44	107.59
31	10	316	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
43	17	316	A86	O2-C18-C17	-2.47	104.90	109.80
31	6	311	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
33	b	620	BCR	C30-C25-C26	-2.47	119.14	122.61
43	18	303	A86	C26-C25-C24	-2.47	115.52	123.22
39	B	621	DGD	O6E-C1E-O5D	-2.47	104.13	109.97
45	18	310	KC2	C2B-C1B-NB	2.47	111.92	110.10
43	0	301	A86	C25-C24-C1	-2.47	119.49	126.42
31	12	315	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	1	321	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
31	10	312	CLA	CAC-C3C-C2C	2.47	131.75	127.53
31	P	607	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
31	16	311	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
33	c	516	BCR	C11-C10-C9	-2.47	123.79	127.31
35	A	409	PL9	O1-C4-C3	-2.47	118.00	120.72
31	b	616	CLA	CHC-C1C-NC	2.46	127.94	124.20
31	5	312	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
45	3	309	KC2	C3C-C2C-C1C	2.46	108.31	106.49
43	9	303	A86	C26-C25-C24	-2.46	115.53	123.22
31	p	602	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
31	10	314	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
43	5	318	A86	C9-C10-C11	-2.46	119.37	126.61
33	C	515	BCR	C31-C1-C6	2.46	114.29	110.30
43	1	303	A86	C3-C4-C5	-2.46	118.43	123.47
43	1	306	A86	C25-C24-C1	-2.46	119.50	126.42
42	7	314	KC1	C2A-C3A-C4A	2.46	108.31	106.49
39	w	204	DGD	C3G-C2G-C1G	-2.46	105.97	111.79
31	B	601	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
43	11	305	A86	C41-C32-C33	2.46	120.09	109.05
31	2	315	CLA	CMB-C2B-C3B	2.46	129.28	124.68
39	C	520	DGD	C3G-C2G-C1G	-2.46	105.97	111.79
31	4	307	CLA	C1B-CHB-C4A	-2.46	125.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	602	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
31	8	306	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
45	3	311	KC2	C3D-CAD-CBD	-2.46	104.37	107.61
31	1	308	CLA	O2D-CGD-CBD	2.46	115.64	111.27
43	6	301	A86	O4-C38-O5	-2.46	118.08	122.96
42	9	314	KC1	CAA-CBA-CGA	-2.46	114.63	127.26
43	10	302	A86	C28-C27-C26	-2.46	119.48	122.92
31	13	316	CLA	CAA-C2A-C1A	-2.46	103.92	111.97
31	11	316	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
43	6	304	A86	C10-C9-C8	-2.46	115.55	123.22
43	9	303	A86	C3-C4-C5	-2.46	118.44	123.47
43	17	302	A86	C23-C16-C22	-2.46	103.75	107.37
32	d	402	PHO	O2D-CGD-CBD	2.46	114.11	111.00
31	P	602	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
31	P	607	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
38	5	316	LMG	C4-C3-C2	2.45	115.11	110.82
43	18	304	A86	C17-C16-C15	-2.45	106.66	109.16
43	P	611	A86	O-C13-C14	2.45	126.65	121.66
33	F	101	BCR	C35-C13-C14	-2.45	119.48	122.92
43	3	306	A86	C4-C3-C2	-2.45	118.45	123.47
33	c	515	BCR	C31-C1-C6	2.45	114.28	110.30
31	b	602	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
31	6	316	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
43	9	305	A86	C40-C32-C31	2.45	112.67	110.47
43	P	611	A86	C40-C32-C33	-2.45	98.03	109.05
42	19	314	KC1	CAA-CBA-CGA	-2.45	114.65	127.26
31	7	307	CLA	C3C-C4C-NC	-2.45	107.82	110.57
43	6	303	A86	O4-C34-C35	2.45	113.70	107.59
33	B	618	BCR	C27-C26-C25	2.45	126.29	122.73
31	14	306	CLA	C3A-C2A-C1A	2.45	105.01	101.34
43	3	304	A86	O1-C20-C21	-2.45	112.12	115.06
38	B	620	LMG	C6-C5-C4	-2.45	107.26	113.00
31	1	316	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
43	19	304	A86	C9-C8-C6	-2.45	119.53	126.42
42	13	314	KC1	O2D-CGD-O1D	-2.45	119.05	123.84
36	l	102	LHG	O8-C23-C24	2.45	119.60	111.91
31	p	607	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
31	6	313	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
31	13	313	CLA	CMC-C2C-C1C	2.45	128.77	125.04
43	13	303	A86	C28-C27-C26	-2.45	119.49	122.92
31	14	306	CLA	CBA-CAA-C2A	2.45	121.09	113.86
43	p	611	A86	C40-C32-C33	-2.45	98.06	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	w	201	LMG	C6-C5-C4	-2.45	107.27	113.00
39	c	519	DGD	O5D-C6D-C5D	-2.45	104.52	109.05
43	2	304	A86	C-C1-C2	-2.45	119.49	122.92
31	6	313	CLA	CHB-C4A-NA	2.45	127.90	124.51
43	14	301	A86	C17-C16-C15	2.45	111.66	109.16
45	6	312	KC2	O2D-CGD-O1D	-2.45	119.05	123.84
45	7	309	KC2	CBC-CAC-C3C	-2.45	115.44	127.62
31	14	315	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
43	P	611	A86	C35-C34-C33	2.45	114.14	109.88
38	11	301	LMG	O7-C10-O9	-2.45	117.79	123.70
43	0	305	A86	C9-C10-C11	-2.45	119.42	126.61
31	5	314	CLA	CMA-C3A-C2A	-2.45	110.39	116.10
31	18	312	CLA	CBA-CAA-C2A	2.45	121.08	113.86
33	A	407	BCR	C15-C16-C17	-2.45	118.47	123.47
43	17	305	A86	C3-C4-C5	-2.45	118.47	123.47
43	2	303	A86	C20-C19-C18	2.44	117.59	112.75
45	3	309	KC2	CBA-CAA-C2A	-2.44	115.95	125.27
43	15	303	A86	C9-C10-C11	-2.44	119.42	126.61
31	P	603	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
38	B	620	LMG	O3-C3-C2	-2.44	104.70	110.35
31	12	316	CLA	CHB-C4A-NA	2.44	127.89	124.51
38	14	316	LMG	C8-O7-C10	2.44	123.81	117.79
31	1	307	CLA	C2D-C1D-ND	-2.44	108.30	110.10
38	1	301	LMG	O7-C10-O9	-2.44	117.80	123.70
44	p	612	DD6	C4-C3-C2	-2.44	118.47	123.47
43	9	305	A86	C12-C11-C13	2.44	120.13	116.02
31	4	312	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
36	d	407	LHG	C5-O7-C7	-2.44	111.78	117.79
43	1	306	A86	O4-C38-O5	-2.44	118.11	122.96
43	12	305	A86	O3-C36-C37	-2.44	105.05	109.39
39	w	204	DGD	O6E-C5E-C4E	2.44	114.13	109.69
44	p	612	DD6	C3-C2-C1	-2.44	123.83	127.31
43	8	302	A86	C20-C19-C18	2.44	117.58	112.75
43	1	303	A86	C26-C25-C24	-2.44	115.60	123.22
43	13	304	A86	C28-C27-C26	-2.44	119.50	122.92
43	10	306	A86	C23-C16-C22	-2.44	103.77	107.37
45	19	309	KC2	O2D-CGD-O1D	-2.44	119.06	123.84
39	C	518	DGD	O4D-C4D-C5D	-2.44	103.24	109.30
43	5	318	A86	O-C13-C11	-2.44	115.76	121.15
31	1	313	CLA	CHB-C4A-NA	2.44	127.89	124.51
31	11	313	CLA	C3B-C4B-NB	-2.44	106.06	109.21
31	0	316	CLA	O2D-CGD-O1D	-2.44	119.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	b	621	LMG	O3-C3-C2	-2.44	104.71	110.35
31	9	308	CLA	C1-C2-C3	2.44	130.26	126.04
39	c	520	DGD	C3G-C2G-C1G	-2.44	106.02	111.79
31	17	310	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
31	9	312	CLA	C20-C18-C17	-2.44	96.47	111.54
34	0	318	SQD	O48-C23-C24	2.44	119.56	111.91
33	C	516	BCR	C11-C10-C9	-2.44	123.83	127.31
43	3	306	A86	C3-C2-C1	-2.44	123.83	127.31
33	a	407	BCR	C15-C16-C17	-2.44	118.48	123.47
36	L	101	LHG	O8-C23-C24	2.44	119.56	111.91
45	19	309	KC2	CAA-CBA-CGA	-2.44	114.74	127.26
31	p	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
31	19	308	CLA	CHB-C4A-NA	2.44	127.88	124.51
38	W	201	LMG	C6-C5-C4	-2.44	107.30	113.00
38	b	621	LMG	C6-C5-C4	-2.44	107.30	113.00
38	b	621	LMG	O6-C1-O1	-2.44	104.20	109.97
31	1	313	CLA	C3B-C4B-NB	-2.44	106.06	109.21
31	15	306	CLA	CAC-C3C-C2C	-2.44	123.36	127.53
31	7	310	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
38	4	316	LMG	O7-C10-O9	-2.44	117.82	123.70
38	11	301	LMG	C4-C3-C2	2.44	115.07	110.82
43	12	301	A86	O1-C15-C20	-2.43	57.02	59.40
43	p	613	A86	O-C13-C14	2.43	126.61	121.66
32	D	402	PHO	O2D-CGD-CBD	2.43	114.08	111.00
45	4	308	KC2	CAB-C3B-C2B	2.43	136.62	128.60
43	p	611	A86	O-C13-C14	2.43	126.61	121.66
33	y	101	BCR	C15-C16-C17	-2.43	118.49	123.47
31	13	313	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	p	607	CLA	CMC-C2C-C1C	2.43	128.75	125.04
31	p	604	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	b	607	CLA	O2A-C1-C2	-2.43	102.24	108.64
31	p	603	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
31	c	504	CLA	C2A-C1A-CHA	2.43	128.11	123.86
42	6	315	KC1	C3A-C4A-NA	2.43	113.23	110.57
38	p	614	LMG	O2-C2-C1	-2.43	104.14	110.05
31	9	307	CLA	CAC-C3C-C2C	-2.43	123.37	127.53
31	8	307	CLA	CAC-C3C-C4C	2.43	127.96	124.81
43	0	301	A86	C7-C6-C5	-2.43	119.52	122.92
31	p	602	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
39	c	518	DGD	O4D-C4D-C5D	-2.43	103.26	109.30
31	z	101	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
43	16	302	A86	O1-C15-C20	-2.43	57.02	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	313	CLA	CMD-C2D-C3D	2.43	133.20	127.61
31	7	313	CLA	C3B-C4B-NB	-2.43	106.07	109.21
31	P	602	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
31	3	307	CLA	CAC-C3C-C2C	-2.43	123.37	127.53
31	P	603	CLA	CHB-C4A-NA	2.43	127.87	124.51
31	7	315	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
31	19	311	CLA	C3A-C2A-C1A	2.43	104.98	101.34
43	p	613	A86	C20-C19-C18	2.43	117.55	112.75
38	C	522	LMG	C38-C37-C36	-2.43	102.10	114.42
35	d	406	PL9	C31-C32-C33	-2.43	103.90	111.88
31	p	606	CLA	CHC-C1C-NC	2.43	127.89	124.20
31	b	611	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
31	4	315	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
35	a	409	PL9	O1-C4-C3	-2.43	118.05	120.72
43	18	302	A86	C20-C19-C18	-2.43	107.95	112.75
43	8	303	A86	C28-C27-C29	2.43	124.55	118.93
38	10	319	LMG	C4-C3-C2	2.43	115.06	110.82
45	11	309	KC2	C2B-C1B-NB	2.43	111.89	110.10
45	4	310	KC2	C3D-CAD-CBD	-2.43	104.41	107.61
33	f	101	BCR	C35-C13-C14	-2.43	119.52	122.92
38	P	614	LMG	O2-C2-C1	-2.43	104.15	110.05
31	19	315	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
43	19	301	A86	C40-C32-C31	2.43	112.64	110.47
43	11	302	A86	C41-C32-C31	-2.43	108.30	110.47
43	6	301	A86	C3-C4-C5	-2.43	118.51	123.47
43	4	306	A86	C28-C27-C26	-2.43	119.53	122.92
43	17	304	A86	C9-C10-C11	-2.43	119.48	126.61
31	5	307	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
31	Z	101	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
31	15	312	CLA	C2D-C1D-ND	-2.42	108.32	110.10
39	B	621	DGD	C7B-C6B-C5B	-2.42	102.12	114.42
31	c	513	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	10	314	CLA	C2A-C1A-CHA	2.42	128.10	123.86
31	0	314	CLA	CHA-C1A-NA	-2.42	120.85	126.40
31	1	321	CLA	C4D-CHA-C1A	2.42	124.20	121.25
31	11	312	CLA	CED-O2D-CGD	-2.42	110.46	115.94
35	D	406	PL9	C31-C32-C33	-2.42	103.92	111.88
43	10	305	A86	C40-C32-C31	2.42	112.64	110.47
43	P	613	A86	O-C13-C14	2.42	126.58	121.66
38	m	101	LMG	O3-C3-C2	-2.42	104.75	110.35
43	12	305	A86	C20-C19-C18	2.42	117.54	112.75
43	9	301	A86	O1-C15-C20	-2.42	57.03	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	302	A86	C4-C3-C2	-2.42	118.51	123.47
31	10	311	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
31	D	401	CLA	CHD-C1D-ND	-2.42	122.23	124.45
31	1	312	CLA	C2A-C1A-CHA	2.42	128.09	123.86
31	B	601	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
31	13	315	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
31	1	316	CLA	CHB-C4A-NA	2.42	127.86	124.51
43	5	302	A86	C33-C32-C31	-2.42	106.86	109.21
31	B	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
38	w	201	LMG	O8-C28-O10	-2.42	117.48	123.59
43	3	304	A86	C36-C31-C32	-2.42	117.30	119.70
31	p	603	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
31	p	605	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
36	D	407	LHG	C5-O7-C7	-2.42	111.83	117.79
31	P	605	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	5	307	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
43	19	301	A86	O1-C15-C20	-2.42	57.04	59.40
31	P	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	P	603	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
38	4	316	LMG	C40-C39-C38	-2.42	102.15	114.42
43	3	302	A86	O2-C18-C19	-2.42	105.00	109.80
31	1	315	CLA	CMB-C2B-C3B	2.42	129.20	124.68
31	13	308	CLA	CHB-C4A-NA	2.42	127.85	124.51
31	17	313	CLA	CHB-C4A-NA	2.42	127.85	124.51
31	5	311	CLA	C3A-C2A-C1A	-2.42	97.72	101.34
31	b	605	CLA	CHD-C4C-NC	2.42	128.01	124.20
31	2	312	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
31	c	511	CLA	C2D-C1D-ND	-2.42	108.32	110.10
43	1	304	A86	O1-C20-C19	2.41	115.20	113.38
31	0	311	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
33	C	516	BCR	C15-C16-C17	-2.41	118.53	123.47
45	17	309	KC2	CBC-CAC-C3C	-2.41	115.61	127.62
43	8	303	A86	C25-C24-C1	-2.41	119.64	126.42
39	11	318	DGD	O3D-C3D-C4D	-2.41	104.77	110.35
31	16	314	CLA	C2A-C3A-C4A	2.41	105.77	101.87
43	8	301	A86	O4-C38-C39	2.41	115.53	111.09
42	19	314	KC1	C2A-C1A-NA	2.41	113.27	109.40
31	2	307	CLA	C3A-C2A-C1A	2.41	104.95	101.34
31	11	312	CLA	O1D-CGD-CBD	2.41	129.42	124.48
31	15	311	CLA	O2A-CGA-O1A	-2.41	117.29	123.30
33	F	101	BCR	C16-C15-C14	-2.41	118.53	123.47
33	f	101	BCR	C16-C15-C14	-2.41	118.53	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	315	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
38	1	301	LMG	C4-C3-C2	2.41	115.03	110.82
43	11	306	A86	C9-C8-C6	-2.41	119.64	126.42
33	c	516	BCR	C15-C16-C17	-2.41	118.54	123.47
43	P	613	A86	C20-C19-C18	2.41	117.52	112.75
43	7	302	A86	C3-C4-C5	-2.41	118.54	123.47
42	P	609	KC1	CGD-CBD-CAD	-2.41	102.93	110.73
43	16	304	A86	C12-C11-C13	2.41	120.07	116.02
31	C	510	CLA	C11-C12-C13	-2.41	108.14	115.92
31	c	510	CLA	C11-C12-C13	-2.41	108.14	115.92
43	15	302	A86	C12-C11-C13	2.41	120.07	116.02
33	Y	101	BCR	C15-C16-C17	-2.41	118.54	123.47
43	1	319	A86	C26-C25-C24	-2.41	115.70	123.22
43	19	301	A86	C14-C15-C16	-2.41	109.54	118.75
42	p	609	KC1	CGD-CBD-CAD	-2.41	102.94	110.73
39	C	519	DGD	O3D-C3D-C4D	-2.41	104.78	110.35
42	2	313	KC1	O2D-CGD-O1D	-2.41	119.13	123.84
42	14	313	KC1	O1D-CGD-CBD	-2.41	119.56	124.48
31	C	511	CLA	C2D-C1D-ND	-2.41	108.33	110.10
38	c	521	LMG	C38-C37-C36	-2.41	102.21	114.42
31	10	314	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
31	5	311	CLA	O2A-CGA-O1A	-2.41	117.30	123.30
38	b	621	LMG	C40-C39-C38	-2.41	102.22	114.42
43	4	303	A86	C-C1-C2	-2.41	119.55	122.92
44	P	612	DD6	C37-C36-C31	-2.40	121.08	124.35
33	c	516	BCR	C20-C21-C22	-2.40	123.88	127.31
43	12	302	A86	C23-C16-C22	2.40	110.92	107.37
31	15	312	CLA	CHA-C1A-NA	-2.40	120.89	126.40
31	1	316	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
31	7	313	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
38	N	101	LMG	O8-C28-O10	-2.40	117.52	123.59
31	14	312	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
31	P	606	CLA	CHC-C1C-NC	2.40	127.85	124.20
43	16	305	A86	C7-C6-C8	2.40	121.86	118.08
43	10	318	A86	C25-C26-C27	-2.40	123.88	127.31
31	14	307	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
31	16	313	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
31	c	505	CLA	CAC-C3C-C4C	2.40	127.93	124.81
41	v	201	HEM	C4B-C3B-C2B	-2.40	105.21	107.11
31	z	103	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
45	18	308	KC2	CBC-CAC-C3C	-2.40	115.67	127.62
31	7	313	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	y	101	BCR	C35-C13-C14	-2.40	119.56	122.92
38	K	101	LMG	C40-C39-C38	-2.40	102.23	114.42
33	B	618	BCR	C31-C1-C6	2.40	114.19	110.30
31	P	607	CLA	CMC-C2C-C1C	2.40	128.70	125.04
43	10	302	A86	O3-C36-C37	-2.40	105.12	109.39
43	p	611	A86	C7-C6-C5	-2.40	119.56	122.92
43	19	305	A86	C12-C11-C13	2.40	120.05	116.02
31	19	308	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
43	8	301	A86	O5-C38-C39	-2.40	116.07	124.81
31	16	316	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
42	16	301	KC1	C4C-C3C-C2C	-2.40	103.40	106.90
43	10	318	A86	C33-C32-C31	-2.40	106.88	109.21
36	B	622	LHG	C11-C10-C9	-2.40	102.25	114.42
36	C	521	LHG	C11-C10-C9	-2.40	102.25	114.42
43	7	304	A86	O4-C34-C33	2.40	113.56	107.59
38	W	201	LMG	O8-C28-O10	-2.40	117.54	123.59
38	k	101	LMG	C40-C39-C38	-2.40	102.25	114.42
45	19	309	KC2	O1D-CGD-CBD	-2.40	119.58	124.48
43	p	611	A86	C-C1-C24	2.40	121.85	118.08
31	C	513	CLA	CHB-C4A-NA	2.40	127.83	124.51
45	16	312	KC2	O2D-CGD-O1D	-2.40	119.16	123.84
43	5	302	A86	O1-C20-C19	2.39	115.18	113.38
38	Z	102	LMG	C1-O6-C5	-2.39	108.99	113.69
43	4	304	A86	C33-C32-C31	-2.39	106.88	109.21
36	b	623	LHG	C11-C10-C9	-2.39	102.27	114.42
43	p	611	A86	C35-C34-C33	2.39	114.05	109.88
31	18	306	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
31	1	307	CLA	C1D-ND-C4D	2.39	108.03	106.33
43	P	611	A86	C7-C6-C5	-2.39	119.57	122.92
31	2	315	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
44	p	612	DD6	C37-C36-C31	-2.39	121.10	124.35
31	5	312	CLA	CBA-CAA-C2A	2.39	120.92	113.86
45	11	309	KC2	CBA-CAA-C2A	2.39	134.39	125.27
43	12	306	A86	O4-C34-C35	2.39	113.55	107.59
31	5	306	CLA	O1D-CGD-CBD	2.39	129.38	124.48
43	9	301	A86	C14-C15-C16	-2.39	109.60	118.75
31	11	310	CLA	C2A-C1A-CHA	2.39	128.04	123.86
39	c	519	DGD	O3D-C3D-C4D	-2.39	104.82	110.35
31	B	604	CLA	CHD-C4C-NC	2.39	127.97	124.20
31	B	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	7	313	CLA	CHA-C4D-ND	2.39	137.50	132.50
36	w	202	LHG	C11-C10-C9	-2.39	102.29	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	13	307	CLA	C2D-C1D-ND	-2.39	108.34	110.10
31	7	312	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
43	14	304	A86	O-C13-C11	-2.39	115.87	121.15
43	10	301	A86	O-C13-C14	-2.39	116.80	121.66
39	1	318	DGD	O5D-C6D-C5D	-2.39	104.63	109.05
43	9	306	A86	C4-C3-C2	-2.39	118.58	123.47
31	11	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
36	14	317	LHG	C20-C19-C18	-2.39	102.30	114.42
31	0	314	CLA	C4D-C3D-CAD	-2.39	105.28	108.10
43	8	303	A86	O4-C38-O5	2.39	127.70	122.96
31	8	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
43	4	303	A86	C20-C19-C18	2.39	117.47	112.75
31	0	307	CLA	CHA-C1A-NA	-2.39	120.93	126.40
38	c	522	LMG	C1-O6-C5	-2.39	109.00	113.69
33	C	516	BCR	C20-C21-C22	-2.39	123.90	127.31
38	C	522	LMG	C40-C39-C38	-2.39	102.31	114.42
31	0	316	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
43	1	305	A86	C7-C6-C5	-2.39	119.58	122.92
45	15	310	KC2	C3A-C4A-NA	2.39	113.18	110.57
43	8	301	A86	C9-C10-C11	-2.39	119.59	126.61
43	0	306	A86	C25-C24-C1	-2.39	119.72	126.42
43	5	303	A86	C9-C10-C11	-2.39	119.59	126.61
39	B	621	DGD	CDB-CCB-CBB	-2.39	102.32	114.42
43	2	304	A86	C40-C32-C33	-2.39	98.34	109.05
31	C	504	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
31	c	504	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
43	18	304	A86	C35-C34-C33	2.38	114.04	109.88
43	3	304	A86	C9-C10-C11	-2.38	119.60	126.61
45	4	310	KC2	C2B-C1B-NB	2.38	111.86	110.10
31	1	312	CLA	CHA-C1A-NA	-2.38	120.94	126.40
45	8	308	KC2	CBC-CAC-C3C	-2.38	115.76	127.62
31	1	313	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
43	P	611	A86	C-C1-C24	2.38	121.83	118.08
43	2	301	A86	C-C1-C24	2.38	121.83	118.08
43	13	306	A86	C3-C4-C5	-2.38	118.59	123.47
43	11	303	A86	C9-C8-C6	-2.38	119.72	126.42
36	D	407	LHG	C11-C10-C9	-2.38	102.33	114.42
31	0	308	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
43	10	305	A86	C9-C10-C11	-2.38	119.60	126.61
31	18	312	CLA	CHB-C4A-NA	2.38	127.81	124.51
39	11	318	DGD	C3G-C2G-C1G	-2.38	106.15	111.79
38	k	101	LMG	C9-C8-C7	-2.38	106.16	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	14	305	A86	O2-C18-C17	-2.38	105.07	109.80
38	f	102	LMG	O2-C2-C1	-2.38	104.26	110.05
43	12	302	A86	C26-C25-C24	-2.38	115.79	123.22
38	d	408	LMG	O3-C3-C2	-2.38	104.84	110.35
31	2	311	CLA	CHB-C4A-NA	2.38	127.80	124.51
31	11	313	CLA	C1-C2-C3	-2.38	121.93	126.04
31	B	606	CLA	O2D-CGD-CBD	2.38	115.50	111.27
31	B	602	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
43	6	307	A86	O4-C38-O5	-2.38	118.24	122.96
36	d	407	LHG	C11-C10-C9	-2.38	102.35	114.42
45	8	308	KC2	C4D-C3D-CAD	2.38	111.65	107.81
33	b	619	BCR	C31-C1-C6	2.38	114.16	110.30
45	7	311	KC2	C2A-C3A-C4A	2.38	108.25	106.49
39	C	520	DGD	O3D-C3D-C4D	-2.38	104.85	110.35
31	1	313	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
31	c	504	CLA	C16-C15-C13	-2.38	108.23	115.92
43	16	306	A86	O4-C38-O5	-2.38	118.24	122.96
43	2	304	A86	O1-C15-C20	-2.38	57.08	59.40
31	17	315	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
43	12	305	A86	C7-C6-C8	2.38	121.82	118.08
43	9	304	A86	C9-C8-C6	-2.38	119.74	126.42
31	C	512	CLA	C1-C2-C3	-2.38	121.93	126.04
31	c	512	CLA	C1-C2-C3	-2.38	121.93	126.04
43	1	304	A86	C36-C31-C32	-2.38	117.34	119.70
38	C	522	LMG	O2-C2-C1	-2.38	104.27	110.05
43	4	302	A86	C41-C32-C31	-2.38	108.35	110.47
31	12	313	CLA	CHB-C4A-NA	2.37	127.80	124.51
38	c	521	LMG	C40-C39-C38	-2.37	102.37	114.42
31	8	307	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
43	15	303	A86	C4-C3-C2	-2.37	118.61	123.47
38	F	102	LMG	O2-C2-C1	-2.37	104.28	110.05
43	17	301	A86	C41-C32-C40	-2.37	101.24	108.53
36	L	101	LHG	C18-C17-C16	-2.37	102.37	114.42
45	0	310	KC2	C4B-C3B-C2B	-2.37	104.80	106.75
43	5	304	A86	C40-C32-C33	-2.37	98.39	109.05
43	7	301	A86	C23-C16-C22	-2.37	103.87	107.37
31	C	504	CLA	C16-C15-C13	-2.37	108.25	115.92
33	f	101	BCR	C24-C23-C22	-2.37	122.65	126.23
38	K	101	LMG	C9-C8-C7	-2.37	106.17	111.79
43	11	303	A86	C10-C9-C8	-2.37	115.81	123.22
31	11	312	CLA	CMB-C2B-C3B	2.37	129.12	124.68
32	A	405	PHO	C1-C2-C3	-2.37	121.94	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Z	102	LMG	O2-C2-C1	-2.37	104.28	110.05
45	18	310	KC2	O2D-CGD-O1D	-2.37	119.20	123.84
31	15	312	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
44	p	612	DD6	C28-C27-C29	2.37	121.53	116.84
36	4	317	LHG	C20-C19-C18	-2.37	102.39	114.42
43	17	302	A86	C40-C32-C33	2.37	119.69	109.05
42	19	314	KC1	CMD-C2D-C1D	-2.37	124.82	128.46
43	10	301	A86	C7-C6-C5	-2.37	119.60	122.92
31	12	308	CLA	C2A-C1A-CHA	2.37	128.00	123.86
38	w	201	LMG	O3-C3-C2	-2.37	104.87	110.35
43	15	303	A86	C34-O4-C38	2.37	122.31	117.90
38	c	521	LMG	O2-C2-C1	-2.37	104.29	110.05
43	2	305	A86	C34-O4-C38	2.37	122.31	117.90
39	H	102	DGD	CBB-CAB-C9B	-2.37	102.40	114.42
36	z	102	LHG	O8-C23-O10	-2.37	117.62	123.59
38	D	408	LMG	O3-C3-C2	-2.37	104.88	110.35
31	b	607	CLA	CHD-C1D-C2D	2.37	130.45	125.48
43	10	306	A86	O4-C34-C33	2.37	113.49	107.59
43	14	302	A86	C10-C9-C8	-2.37	115.83	123.22
36	18	315	LHG	C11-C10-C9	-2.37	102.41	114.42
31	B	602	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	c	506	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
38	M	101	LMG	O2-C2-C1	-2.37	104.30	110.05
36	l	102	LHG	C18-C17-C16	-2.37	102.41	114.42
39	h	102	DGD	CBB-CAB-C9B	-2.37	102.42	114.42
43	4	301	A86	C35-C34-C33	-2.37	105.75	109.88
31	b	603	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	C	505	CLA	CAC-C3C-C4C	2.37	127.88	124.81
39	C	518	DGD	C1D-C2D-C3D	-2.37	105.07	110.00
31	0	308	CLA	C2D-C1D-ND	-2.37	108.36	110.10
38	14	316	LMG	C3-C4-C5	-2.36	106.02	110.24
31	c	510	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
45	12	309	KC2	C2A-C1A-NA	2.36	113.19	109.40
31	2	309	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	13	313	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	10	317	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
38	4	316	LMG	C38-C37-C36	-2.36	102.42	114.42
31	17	312	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
31	17	312	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	3	316	CLA	C4C-C3C-C2C	2.36	110.34	106.90
43	12	301	A86	C14-C15-C16	-2.36	109.71	118.75
31	12	307	CLA	C3C-C4C-NC	-2.36	107.92	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	15	304	A86	O-C13-C11	-2.36	115.93	121.15
31	1	310	CLA	C2A-C1A-CHA	2.36	127.99	123.86
31	B	615	CLA	CMB-C2B-C1B	-2.36	124.83	128.46
31	B	612	CLA	CMD-C2D-C3D	2.36	133.05	127.61
39	c	520	DGD	O3D-C3D-C4D	-2.36	104.89	110.35
43	12	305	A86	C23-C16-C22	-2.36	103.89	107.37
31	p	605	CLA	CHD-C1D-ND	-2.36	122.28	124.45
43	2	301	A86	C3-C4-C5	-2.36	118.64	123.47
31	15	311	CLA	CHA-C1A-NA	-2.36	120.99	126.40
39	C	520	DGD	O6E-C1E-O5D	-2.36	104.38	109.97
31	1	321	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	8	314	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
33	h	101	BCR	C40-C30-C25	2.36	114.13	110.30
31	P	608	CLA	CAC-C3C-C4C	2.36	127.87	124.81
43	18	303	A86	O1-C15-C20	-2.36	57.09	59.40
43	19	305	A86	O4-C38-O5	-2.36	118.27	122.96
38	D	408	LMG	O7-C10-O9	-2.36	118.00	123.70
31	b	606	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
45	18	310	KC2	CAB-C3B-C2B	2.36	136.38	128.60
31	b	603	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
38	c	522	LMG	O2-C2-C1	-2.36	104.32	110.05
31	C	510	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	C	503	CLA	C2A-C1A-CHA	2.36	127.98	123.86
33	B	619	BCR	C27-C26-C25	2.36	126.16	122.73
45	17	309	KC2	C2A-C3A-C4A	2.36	108.23	106.49
31	7	313	CLA	C1-C2-C3	-2.36	122.94	126.75
31	c	508	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
31	10	317	CLA	CHB-C4A-NA	2.36	127.77	124.51
38	W	201	LMG	O3-C3-C2	-2.36	104.90	110.35
31	14	312	CLA	CHA-C4D-ND	2.36	137.43	132.50
31	5	307	CLA	CHB-C4A-NA	2.36	127.77	124.51
43	17	302	A86	O-C13-C11	-2.36	115.94	121.15
31	b	604	CLA	CHB-C4A-NA	2.36	127.77	124.51
31	B	605	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
42	2	313	KC1	C3A-C4A-NA	2.35	113.14	110.57
31	P	605	CLA	CHD-C1D-ND	-2.35	122.29	124.45
43	18	302	A86	C26-C25-C24	2.35	130.56	123.22
43	11	306	A86	O4-C38-O5	-2.35	118.28	122.96
31	16	311	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
33	B	617	BCR	C15-C14-C13	-2.35	123.95	127.31
45	17	311	KC2	C4B-C3B-C2B	-2.35	104.82	106.75
31	15	312	CLA	C3C-C4C-NC	-2.35	107.93	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	318	DGD	C5B-C4B-C3B	-2.35	102.48	114.42
38	d	408	LMG	O7-C10-O9	-2.35	118.02	123.70
42	16	301	KC1	CGD-CBD-CAD	-2.35	103.11	110.73
31	b	603	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
43	6	307	A86	C28-C27-C26	2.35	126.22	122.92
32	a	405	PHO	C1-C2-C3	-2.35	121.97	126.04
43	13	304	A86	C25-C24-C1	-2.35	119.81	126.42
34	L	102	SQD	C45-O47-C7	2.35	123.58	117.79
31	0	314	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
43	11	306	A86	C7-C6-C8	2.35	121.78	118.08
43	14	305	A86	C26-C25-C24	-2.35	115.88	123.22
43	6	304	A86	C7-C6-C8	2.35	121.78	118.08
31	C	508	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
31	3	316	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
45	6	310	KC2	CAC-C3C-C4C	2.35	135.42	124.47
43	2	302	A86	C20-C19-C18	2.35	117.40	112.75
31	1	321	CLA	CAC-C3C-C2C	-2.35	123.51	127.53
43	17	316	A86	C41-C32-C33	2.35	119.60	109.05
33	H	101	BCR	C40-C30-C25	2.35	114.11	110.30
33	F	101	BCR	C24-C23-C22	-2.35	122.69	126.23
31	c	503	CLA	C2A-C1A-CHA	2.35	127.97	123.86
43	10	304	A86	O-C13-C11	-2.35	115.96	121.15
42	P	609	KC1	C2A-C1A-NA	2.35	113.17	109.40
43	7	303	A86	C9-C10-C11	-2.35	119.70	126.61
42	19	314	KC1	O2D-CGD-O1D	-2.35	119.25	123.84
43	18	302	A86	O4-C38-O5	-2.35	118.30	122.96
43	12	302	A86	C41-C32-C40	-2.35	101.32	108.53
31	B	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
43	14	305	A86	C41-C32-C40	-2.35	101.33	108.53
33	b	618	BCR	C15-C14-C13	-2.35	123.96	127.31
39	c	518	DGD	C1D-C2D-C3D	-2.35	105.11	110.00
43	15	304	A86	O4-C34-C35	2.35	113.44	107.59
31	3	313	CLA	CHA-C4D-ND	2.35	137.41	132.50
31	7	307	CLA	CHD-C4C-C3C	2.35	128.29	124.84
31	C	506	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
43	4	302	A86	C26-C25-C24	-2.35	115.90	123.22
45	17	311	KC2	C3C-C2C-C1C	-2.35	104.75	106.49
45	12	309	KC2	C3D-CAD-CBD	-2.35	104.52	107.61
45	3	311	KC2	O2D-CGD-O1D	-2.35	119.25	123.84
43	19	302	A86	C35-C34-C33	-2.34	105.78	109.88
39	B	621	DGD	C6D-O5D-C1E	2.34	118.32	113.74
43	10	305	A86	O-C13-C14	2.34	126.42	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	18	307	CLA	OBD-CAD-C3D	2.34	134.16	128.52
39	c	520	DGD	O6E-C1E-O5D	-2.34	104.42	109.97
31	10	314	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
43	0	302	A86	C40-C32-C31	-2.34	108.38	110.47
43	12	306	A86	O4-C38-O5	-2.34	118.31	122.96
31	11	307	CLA	CBA-CAA-C2A	-2.34	109.07	114.02
31	p	608	CLA	CAC-C3C-C4C	2.34	127.85	124.81
43	2	302	A86	O1-C15-C20	-2.34	57.11	59.40
38	1	317	LMG	C38-C37-C36	-2.34	102.53	114.42
43	3	304	A86	C3-C4-C5	-2.34	118.68	123.47
33	Y	101	BCR	C35-C13-C14	-2.34	119.64	122.92
31	17	307	CLA	CHD-C4C-C3C	2.34	128.28	124.84
43	18	303	A86	O4-C38-O5	-2.34	118.31	122.96
31	b	613	CLA	CMD-C2D-C3D	2.34	133.00	127.61
31	B	604	CLA	C2A-C1A-CHA	2.34	127.95	123.86
43	7	301	A86	O-C13-C11	-2.34	115.98	121.15
42	p	609	KC1	C2A-C1A-NA	2.34	113.16	109.40
31	B	610	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
43	p	613	A86	O4-C38-O5	-2.34	118.31	122.96
32	a	405	PHO	CBA-CAA-C2A	-2.34	106.97	113.81
31	b	605	CLA	C2A-C1A-CHA	2.34	127.95	123.86
38	4	316	LMG	C1-C2-C3	-2.34	105.12	110.00
43	1	305	A86	C4-C3-C2	-2.34	118.68	123.47
43	15	303	A86	O-C13-C11	-2.34	115.98	121.15
42	7	314	KC1	CED-O2D-CGD	2.34	121.22	115.94
43	5	305	A86	O1-C20-C19	2.34	115.14	113.38
45	18	308	KC2	CBA-CAA-C2A	-2.34	116.36	125.27
43	18	305	A86	O4-C38-O5	-2.34	118.32	122.96
43	11	320	A86	C41-C32-C40	-2.34	101.36	108.53
43	5	302	A86	C9-C8-C6	-2.34	119.85	126.42
31	17	313	CLA	C4D-CHA-C1A	-2.34	118.41	121.25
31	11	307	CLA	C2A-C1A-CHA	2.34	127.94	123.86
31	3	307	CLA	C3C-C4C-NC	-2.34	107.95	110.57
31	14	307	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
36	Z	103	LHG	O8-C23-O10	-2.34	117.70	123.59
31	17	313	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
43	5	303	A86	C22-C16-C17	2.34	113.04	108.98
43	15	305	A86	C41-C32-C40	-2.34	101.36	108.53
43	5	303	A86	O3-C36-C37	-2.34	105.24	109.39
31	5	309	CLA	C2A-C1A-CHA	2.34	127.94	123.86
31	1	310	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
43	17	302	A86	C20-C19-C18	2.34	117.37	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	303	A86	C4-C3-C2	-2.33	118.69	123.47
43	P	613	A86	O4-C38-O5	-2.33	118.32	122.96
43	6	304	A86	C4-C3-C2	-2.33	118.69	123.47
31	c	514	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
39	b	622	DGD	O3G-C1D-C2D	2.33	111.95	108.30
31	B	614	CLA	C2D-C1D-ND	-2.33	108.38	110.10
31	7	307	CLA	C1D-ND-C4D	2.33	107.99	106.33
35	D	406	PL9	C8-C7-C3	2.33	118.58	111.98
35	d	406	PL9	C8-C7-C3	2.33	118.58	111.98
31	c	509	CLA	CMD-C2D-C1D	-2.33	120.60	124.71
43	12	304	A86	O1-C15-C20	-2.33	57.12	59.40
43	13	304	A86	C41-C32-C33	2.33	119.52	109.05
43	2	304	A86	C9-C8-C6	-2.33	119.86	126.42
45	3	311	KC2	C2B-C1B-NB	2.33	111.82	110.10
31	15	313	CLA	CMD-C2D-C1D	2.33	128.82	124.71
43	6	301	A86	C19-C18-C17	-2.33	106.27	110.77
31	C	509	CLA	CMD-C2D-C1D	-2.33	120.60	124.71
43	1	319	A86	C9-C8-C6	-2.33	119.86	126.42
31	0	312	CLA	CMC-C2C-C1C	-2.33	121.49	125.04
31	8	311	CLA	CHB-C4A-NA	2.33	127.73	124.51
43	17	304	A86	C14-C15-C16	2.33	127.67	118.75
43	16	305	A86	O4-C38-O5	-2.33	118.34	122.96
35	a	409	PL9	C12-C13-C14	-2.33	122.06	127.66
43	6	303	A86	C9-C8-C6	-2.33	119.88	126.42
43	8	302	A86	C19-C18-C17	-2.33	106.28	110.77
38	14	316	LMG	C40-C39-C38	-2.33	102.61	114.42
45	15	308	KC2	CHD-C4C-NC	-2.33	120.67	124.20
31	b	611	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
32	A	405	PHO	CBA-CAA-C2A	-2.33	107.01	113.81
45	11	309	KC2	O2D-CGD-O1D	-2.33	119.29	123.84
31	r	101	CLA	C2A-C1A-CHA	2.33	127.93	123.86
43	12	303	A86	O3-C36-C37	-2.33	105.25	109.39
31	P	605	CLA	CMA-C3A-C2A	-2.33	110.67	116.10
43	7	306	A86	O4-C34-C35	-2.33	101.80	107.59
31	C	509	CLA	CHC-C1C-NC	2.33	127.73	124.20
31	c	509	CLA	CHC-C1C-NC	2.33	127.73	124.20
41	V	201	HEM	CAA-CBA-CGA	-2.32	107.24	113.76
31	6	311	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
45	11	309	KC2	C4D-C3D-CAD	2.32	111.56	107.81
31	13	308	CLA	C3A-C2A-C1A	2.32	104.82	101.34
38	k	101	LMG	C38-C37-C36	-2.32	102.63	114.42
31	16	313	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	304	A86	C8-C6-C5	2.32	122.51	118.94
43	6	304	A86	O4-C38-O5	-2.32	118.35	122.96
31	C	514	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
43	15	302	A86	C9-C8-C6	-2.32	119.89	126.42
43	15	302	A86	C25-C24-C1	-2.32	119.89	126.42
43	7	304	A86	C40-C32-C31	-2.32	108.39	110.47
39	c	518	DGD	CBB-CAB-C9B	-2.32	102.64	114.42
43	13	305	A86	C19-C18-C17	-2.32	106.29	110.77
42	13	314	KC1	CBD-CHA-C1A	2.32	133.21	128.88
38	K	101	LMG	C38-C37-C36	-2.32	102.64	114.42
31	p	605	CLA	CMA-C3A-C2A	-2.32	110.68	116.10
45	10	310	KC2	C4B-C3B-C2B	-2.32	104.85	106.75
43	6	304	A86	O-C13-C11	-2.32	116.02	121.15
42	4	313	KC1	CED-O2D-CGD	2.32	121.19	115.94
43	9	305	A86	O4-C38-O5	-2.32	118.35	122.96
43	8	305	A86	C4-C3-C2	-2.32	118.72	123.47
38	11	317	LMG	C38-C37-C36	-2.32	102.65	114.42
43	8	303	A86	C23-C16-C22	-2.32	103.95	107.37
45	3	311	KC2	C2A-C1A-NA	2.32	113.12	109.40
31	14	306	CLA	CHD-C1D-ND	-2.32	122.32	124.45
41	V	201	HEM	C4B-C3B-C2B	-2.32	105.27	107.11
31	13	307	CLA	C2A-C1A-CHA	2.32	127.91	123.86
31	0	309	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
31	b	612	CLA	C1-C2-C3	-2.32	122.03	126.04
43	9	306	A86	O4-C38-O5	-2.32	118.36	122.96
31	C	502	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
31	1	307	CLA	CAC-C3C-C2C	-2.32	123.56	127.53
31	W	202	CLA	O2D-CGD-CBD	2.32	115.39	111.27
31	w	203	CLA	O2D-CGD-CBD	2.32	115.39	111.27
39	C	518	DGD	CBB-CAB-C9B	-2.32	102.66	114.42
45	11	311	KC2	O2D-CGD-O1D	-2.32	119.31	123.84
33	b	620	BCR	C27-C26-C25	2.32	126.09	122.73
31	b	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
43	13	303	A86	O1-C20-C19	2.32	115.12	113.38
31	1	312	CLA	CAA-C2A-C1A	2.32	119.56	111.97
31	9	308	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
43	13	305	A86	C3-C4-C5	-2.32	118.73	123.47
43	17	305	A86	C14-C15-C16	-2.32	109.89	118.75
31	B	611	CLA	C1-C2-C3	-2.32	122.04	126.04
31	C	504	CLA	CAA-CBA-CGA	-2.32	106.49	113.25
42	9	314	KC1	C2A-C1A-NA	2.31	113.11	109.40
43	12	303	A86	C28-C27-C29	2.31	124.29	118.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	l	101	SQD	C45-O47-C7	2.31	123.49	117.79
31	R	101	CLA	C2A-C1A-CHA	2.31	127.91	123.86
31	C	505	CLA	CHC-C1C-NC	2.31	127.71	124.20
31	10	316	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
45	15	308	KC2	C4D-C3D-CAD	2.31	111.55	107.81
39	c	520	DGD	O3E-C3E-C2E	-2.31	105.00	110.35
39	c	518	DGD	C3G-C2G-C1G	-2.31	106.32	111.79
42	1	314	KC1	C2B-C1B-NB	2.31	111.81	110.10
33	A	407	BCR	C27-C26-C25	2.31	126.09	122.73
43	5	302	A86	C25-C24-C1	-2.31	119.92	126.42
45	5	308	KC2	C2A-C1A-CHA	-2.31	119.80	127.44
31	18	312	CLA	C4D-CHA-C1A	2.31	124.06	121.25
31	3	313	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
35	A	409	PL9	C12-C13-C14	-2.31	122.10	127.66
43	6	303	A86	C3-C4-C5	-2.31	118.74	123.47
43	4	303	A86	O4-C38-O5	-2.31	118.37	122.96
41	v	201	HEM	CAA-CBA-CGA	-2.31	107.28	113.76
31	9	307	CLA	C2D-C1D-ND	-2.31	108.40	110.10
31	3	307	CLA	CAA-C2A-C3A	-2.31	108.49	114.26
31	2	314	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
38	m	101	LMG	O6-C1-O1	-2.31	104.51	109.97
45	14	310	KC2	C2B-C1B-NB	2.31	111.81	110.10
31	8	311	CLA	C2A-C1A-CHA	2.31	127.89	123.86
43	0	305	A86	C33-C32-C31	-2.31	106.97	109.21
31	D	405	CLA	O2D-CGD-CBD	2.31	115.37	111.27
36	a	410	LHG	C11-C10-C9	-2.31	102.71	114.42
43	11	304	A86	C23-C16-C17	-2.31	104.97	108.98
43	P	613	A86	C14-C15-C16	2.31	127.59	118.75
43	3	301	A86	C28-C27-C29	2.31	124.27	118.93
43	19	304	A86	C28-C27-C29	2.31	124.27	118.93
31	7	307	CLA	C3A-C2A-C1A	2.31	105.55	101.64
31	5	311	CLA	C2D-C1D-ND	-2.31	108.40	110.10
31	c	504	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
33	a	407	BCR	C11-C10-C9	-2.31	124.02	127.31
43	1	319	A86	C4-C3-C2	-2.31	118.75	123.47
42	16	315	KC1	CAA-C2A-C1A	2.31	135.35	124.75
31	1	313	CLA	CHA-C1A-NA	-2.31	121.12	126.40
43	10	302	A86	C25-C24-C1	-2.31	119.94	126.42
43	16	304	A86	C17-C16-C15	2.30	111.51	109.16
43	19	303	A86	C25-C24-C1	-2.30	119.94	126.42
43	19	303	A86	C9-C10-C11	-2.30	119.83	126.61
39	11	318	DGD	C5B-C4B-C3B	-2.30	102.73	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	18	314	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
33	c	517	BCR	C27-C26-C25	2.30	126.07	122.73
43	17	301	A86	C21-C20-C19	2.30	116.87	114.28
39	C	518	DGD	C3G-C2G-C1G	-2.30	106.34	111.79
43	6	305	A86	C41-C32-C33	2.30	119.38	109.05
31	b	616	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
43	p	613	A86	C14-C15-C16	2.30	127.56	118.75
36	A	410	LHG	C11-C10-C9	-2.30	102.75	114.42
45	13	311	KC2	O2D-CGD-O1D	-2.30	119.34	123.84
31	p	606	CLA	O2D-CGD-CBD	2.30	115.36	111.27
36	l	102	LHG	C27-C26-C25	-2.30	102.75	114.42
31	2	312	CLA	CMD-C2D-C1D	2.30	128.77	124.71
31	b	616	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
31	2	311	CLA	C2A-C1A-CHA	2.30	127.88	123.86
43	0	306	A86	C23-C16-C22	-2.30	103.98	107.37
43	11	320	A86	C12-C11-C13	2.30	119.88	116.02
31	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
31	10	309	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
36	a	410	LHG	O8-C23-C24	2.30	119.12	111.91
38	W	201	LMG	C38-C37-C36	-2.30	102.76	114.42
45	16	312	KC2	C2B-C1B-NB	2.30	111.80	110.10
31	6	308	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
36	L	101	LHG	C27-C26-C25	-2.30	102.76	114.42
31	15	312	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
45	5	308	KC2	C4D-C3D-CAD	2.30	111.52	107.81
31	b	607	CLA	CAC-C3C-C4C	2.30	127.79	124.81
43	0	302	A86	C25-C24-C1	-2.30	119.97	126.42
43	5	304	A86	O2-C18-C19	-2.30	105.24	109.80
31	C	510	CLA	C1-C2-C3	-2.30	122.07	126.04
31	3	308	CLA	C3A-C2A-C1A	2.30	104.78	101.34
31	c	505	CLA	CHC-C1C-NC	2.30	127.69	124.20
31	b	614	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
33	C	517	BCR	C27-C26-C25	2.30	126.06	122.73
45	13	309	KC2	C2A-C3A-C4A	2.30	108.19	106.49
31	18	314	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
38	15	315	LMG	C4-C3-C2	2.30	114.83	110.82
31	2	315	CLA	C2A-C1A-CHA	2.30	127.87	123.86
43	12	302	A86	C10-C9-C8	-2.29	116.06	123.22
31	B	612	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
43	19	301	A86	C36-C31-C32	2.29	121.97	119.70
38	w	201	LMG	C38-C37-C36	-2.29	102.78	114.42
33	C	515	BCR	C27-C26-C25	2.29	126.06	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	302	A86	C12-C11-C10	-2.29	117.87	123.42
31	4	307	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
33	B	617	BCR	C29-C30-C25	2.29	114.01	110.48
31	B	608	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
43	6	301	A86	O-C13-C11	-2.29	116.08	121.15
31	0	307	CLA	O2D-CGD-CBD	2.29	115.34	111.27
43	1	305	A86	C25-C24-C1	-2.29	119.97	126.42
43	18	304	A86	C-C1-C2	-2.29	119.71	122.92
33	y	101	BCR	C1-C6-C5	-2.29	119.38	122.61
42	0	315	KC1	C3A-C4A-NA	2.29	113.08	110.57
31	9	312	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
31	13	308	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
33	c	515	BCR	C27-C26-C25	2.29	126.06	122.73
42	p	609	KC1	O2D-CGD-O1D	-2.29	119.36	123.84
43	1	320	A86	C22-C16-C17	-2.29	105.00	108.98
33	a	407	BCR	C27-C26-C25	2.29	126.06	122.73
31	5	306	CLA	C2D-C1D-ND	-2.29	108.42	110.10
45	7	311	KC2	C2B-C1B-NB	2.29	111.79	110.10
43	3	304	A86	C33-C32-C31	2.29	111.44	109.21
31	c	502	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
33	C	516	BCR	C30-C25-C26	-2.29	119.39	122.61
31	D	404	CLA	CMD-C2D-C3D	2.29	132.88	127.61
31	b	613	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
31	12	315	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
31	w	203	CLA	CAC-C3C-C2C	-2.29	123.61	127.53
43	8	304	A86	C21-C20-C19	-2.29	111.70	114.28
31	P	606	CLA	O2D-CGD-CBD	2.29	115.33	111.27
31	c	510	CLA	C1-C2-C3	-2.29	122.08	126.04
34	a	408	SQD	O48-C23-O10	-2.29	117.82	123.59
31	12	307	CLA	C3A-C2A-C1A	2.29	104.77	101.34
43	5	303	A86	C4-C3-C2	-2.29	118.79	123.47
31	18	307	CLA	CMD-C2D-C1D	-2.29	120.68	124.71
31	B	613	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
45	12	309	KC2	CAB-C3B-C2B	2.29	136.13	128.60
43	p	611	A86	C20-C19-C18	-2.29	108.23	112.75
33	c	516	BCR	C30-C25-C26	-2.29	119.39	122.61
43	0	304	A86	O-C13-C11	-2.29	116.10	121.15
43	7	301	A86	C20-C19-C18	2.28	117.27	112.75
45	5	310	KC2	CAA-CBA-CGA	-2.28	115.52	127.26
43	11	305	A86	C7-C6-C8	-2.28	114.48	118.08
36	18	316	LHG	C11-C10-C9	-2.28	102.83	114.42
43	10	302	A86	C21-C20-C19	-2.28	111.71	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	17	307	CLA	C3A-C2A-C1A	2.28	105.51	101.64
39	C	520	DGD	O3E-C3E-C2E	-2.28	105.07	110.35
42	17	314	KC1	CED-O2D-CGD	2.28	121.10	115.94
45	3	309	KC2	CBC-CAC-C3C	-2.28	116.27	127.62
31	14	312	CLA	C3B-C4B-NB	-2.28	106.26	109.21
45	6	310	KC2	CAA-CBA-CGA	-2.28	115.54	127.26
43	3	306	A86	C9-C8-C6	-2.28	120.01	126.42
36	18	315	LHG	C27-C26-C25	-2.28	102.84	114.42
31	17	312	CLA	CHB-C4A-NA	2.28	127.67	124.51
43	16	307	A86	C9-C10-C11	-2.28	119.90	126.61
31	B	613	CLA	CHB-C4A-NA	2.28	127.67	124.51
34	a	408	SQD	C1-C2-C3	-2.28	105.25	110.00
43	18	302	A86	C-C1-C24	2.28	121.67	118.08
31	b	617	CLA	C2D-C1D-ND	-2.28	108.42	110.10
35	D	406	PL9	C36-C37-C38	-2.28	104.39	111.88
43	4	303	A86	C33-C32-C31	-2.28	107.00	109.21
31	d	405	CLA	O2D-CGD-CBD	2.28	115.32	111.27
36	A	410	LHG	O8-C23-C24	2.28	119.06	111.91
31	11	312	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
38	5	316	LMG	O8-C28-O10	-2.28	117.84	123.59
45	5	310	KC2	O2D-CGD-O1D	-2.28	119.38	123.84
45	8	308	KC2	C3C-C2C-C1C	2.28	108.18	106.49
43	10	301	A86	O1-C20-C21	-2.28	112.33	115.06
43	7	302	A86	C-C1-C24	2.28	121.67	118.08
43	18	302	A86	C19-C18-C17	-2.28	106.38	110.77
45	8	310	KC2	C3C-C2C-C1C	-2.28	104.80	106.49
43	11	306	A86	C28-C27-C26	-2.28	119.73	122.92
34	A	408	SQD	C1-C2-C3	-2.28	105.25	110.00
32	d	402	PHO	C4A-C3A-C2A	-2.28	100.67	102.84
31	15	307	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
43	11	306	A86	C23-C16-C17	-2.28	105.03	108.98
39	11	318	DGD	C1E-O6E-C5E	2.28	118.15	113.69
38	F	102	LMG	O6-C1-C2	-2.28	105.53	110.35
31	18	306	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
34	L	102	SQD	O49-C7-C8	-2.27	114.86	123.73
33	b	620	BCR	C28-C27-C26	-2.27	110.02	114.08
31	4	311	CLA	C2D-C1D-ND	-2.27	108.43	110.10
31	13	312	CLA	C2D-C1D-ND	-2.27	108.43	110.10
31	11	307	CLA	C3C-C4C-NC	-2.27	108.02	110.57
31	B	603	CLA	O1D-CGD-CBD	2.27	129.13	124.48
31	10	312	CLA	CMC-C2C-C1C	-2.27	121.58	125.04
31	5	306	CLA	CGD-CBD-CAD	2.27	118.09	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	18	311	CLA	CHB-C4A-NA	2.27	127.65	124.51
31	W	202	CLA	CAC-C3C-C2C	-2.27	123.64	127.53
31	11	310	CLA	C3A-C2A-C1A	2.27	104.74	101.34
34	L	102	SQD	O48-C23-O10	-2.27	117.86	123.59
43	19	305	A86	C10-C9-C8	-2.27	116.13	123.22
31	B	612	CLA	C11-C12-C13	-2.27	108.58	115.92
42	P	609	KC1	O2D-CGD-O1D	-2.27	119.40	123.84
39	C	519	DGD	O2D-C2D-C1D	-2.27	104.53	110.05
42	4	313	KC1	C2B-C1B-NB	2.27	111.78	110.10
31	1	313	CLA	C2A-C1A-CHA	2.27	127.83	123.86
43	2	302	A86	C8-C6-C5	2.27	122.42	118.94
43	13	301	A86	C33-C32-C31	-2.27	107.01	109.21
34	A	411	SQD	O6-C1-C2	2.27	111.84	108.30
45	7	311	KC2	C4B-C3B-C2B	-2.27	104.89	106.75
35	d	406	PL9	C36-C37-C38	-2.27	104.43	111.88
32	D	402	PHO	CMC-C2C-C3C	2.27	129.22	124.94
38	N	101	LMG	C6-C5-C4	-2.27	107.69	113.00
44	p	612	DD6	C12-C11-C13	-2.27	114.50	118.08
31	b	604	CLA	O1D-CGD-CBD	2.27	129.12	124.48
34	A	408	SQD	O48-C23-O10	-2.27	117.87	123.59
43	13	305	A86	C7-C6-C8	2.27	121.65	118.08
43	16	303	A86	C33-C32-C31	-2.27	107.01	109.21
31	12	307	CLA	CAC-C3C-C2C	-2.27	123.65	127.53
43	8	301	A86	C41-C32-C40	-2.27	101.57	108.53
31	z	103	CLA	CHB-C4A-NA	2.27	127.65	124.51
38	14	316	LMG	C1-C2-C3	-2.27	105.28	110.00
31	A	404	CLA	C2D-C1D-ND	-2.27	108.43	110.10
43	0	303	A86	C25-C24-C1	-2.27	120.05	126.42
43	17	316	A86	C28-C27-C26	-2.27	119.75	122.92
43	4	304	A86	C3-C4-C5	-2.27	118.83	123.47
31	z	101	CLA	C2A-C1A-CHA	2.26	127.82	123.86
31	b	615	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
38	f	102	LMG	O6-C1-C2	-2.26	105.56	110.35
43	13	303	A86	C23-C16-C17	-2.26	105.05	108.98
31	9	312	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
31	B	615	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
43	9	306	A86	C9-C10-C11	-2.26	119.95	126.61
36	l	102	LHG	C20-C19-C18	-2.26	102.93	114.42
31	d	404	CLA	CMD-C2D-C3D	2.26	132.82	127.61
31	5	306	CLA	C3C-C4C-NC	-2.26	108.03	110.57
36	B	622	LHG	C27-C26-C25	-2.26	102.94	114.42
43	0	301	A86	C33-C32-C31	-2.26	107.01	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	302	A86	C25-C24-C1	-2.26	120.06	126.42
31	b	613	CLA	C11-C12-C13	-2.26	108.61	115.92
31	12	312	CLA	CAA-C2A-C1A	2.26	119.39	111.97
43	17	305	A86	C28-C27-C26	-2.26	119.75	122.92
43	5	304	A86	C41-C32-C33	2.26	119.20	109.05
45	12	309	KC2	O2D-CGD-O1D	-2.26	119.42	123.84
33	H	101	BCR	C30-C25-C26	-2.26	119.43	122.61
31	18	307	CLA	CAC-C3C-C4C	2.26	127.74	124.81
38	14	316	LMG	O2-C2-C1	-2.26	104.55	110.05
43	0	302	A86	C3-C4-C5	-2.26	118.84	123.47
31	6	308	CLA	C2D-C1D-ND	-2.26	108.44	110.10
31	10	307	CLA	C2D-C1D-ND	-2.26	108.44	110.10
31	1	312	CLA	CHB-C4A-NA	2.26	127.64	124.51
42	9	314	KC1	O2D-CGD-O1D	-2.26	119.42	123.84
31	8	312	CLA	CHD-C1D-ND	-2.26	122.38	124.45
31	c	514	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
33	A	407	BCR	C11-C10-C9	-2.26	124.08	127.31
43	P	611	A86	C20-C19-C18	-2.26	108.28	112.75
42	2	313	KC1	C1C-C2C-C3C	-2.26	104.58	106.96
44	P	612	DD6	C26-C25-C24	-2.26	116.17	123.22
31	17	312	CLA	C2A-C1A-CHA	2.26	127.81	123.86
36	d	407	LHG	C27-C26-C25	-2.26	102.96	114.42
42	9	314	KC1	CMD-C2D-C1D	-2.26	124.99	128.46
31	3	310	CLA	CMA-C3A-C2A	-2.26	110.83	116.10
33	B	619	BCR	C28-C27-C26	-2.26	110.04	114.08
43	14	305	A86	C12-C11-C13	-2.26	112.23	116.02
31	B	615	CLA	CHC-C1C-NC	2.26	127.63	124.20
36	b	623	LHG	C27-C26-C25	-2.26	102.96	114.42
38	M	101	LMG	O3-C3-C2	-2.26	105.13	110.35
43	19	306	A86	C9-C10-C11	-2.26	119.97	126.61
31	P	607	CLA	C3A-C2A-C1A	2.26	104.72	101.34
31	C	503	CLA	C2A-C3A-C4A	2.26	105.52	101.87
34	a	408	SQD	O48-C23-C24	2.26	118.99	111.91
43	16	302	A86	C4-C3-C2	-2.26	118.85	123.47
31	19	312	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
31	9	313	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
33	h	101	BCR	C30-C25-C26	-2.26	119.44	122.61
39	c	519	DGD	O2D-C2D-C1D	-2.26	104.57	110.05
34	i	101	SQD	O6-C1-C2	2.26	111.83	108.30
41	E	101	HEM	CMA-C3A-C4A	-2.26	125.00	128.46
43	9	305	A86	C10-C9-C8	-2.26	116.18	123.22
38	4	316	LMG	O2-C2-C1	-2.26	104.57	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	15	315	LMG	C1-O6-C5	2.26	118.11	113.69
31	7	312	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
31	11	316	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
36	L	101	LHG	C20-C19-C18	-2.25	102.98	114.42
32	d	402	PHO	CMC-C2C-C3C	2.25	129.19	124.94
45	17	309	KC2	C2A-C1A-CHA	-2.25	119.99	127.44
33	B	617	BCR	C33-C5-C6	-2.25	122.00	124.53
38	C	522	LMG	O6-C1-O1	-2.25	104.64	109.97
42	0	315	KC1	C1C-C2C-C3C	-2.25	104.59	106.96
36	D	407	LHG	C27-C26-C25	-2.25	102.98	114.42
43	11	304	A86	C21-C20-C19	-2.25	111.75	114.28
42	13	314	KC1	C3A-C4A-NA	2.25	113.03	110.57
31	C	514	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
34	A	408	SQD	O48-C23-C24	2.25	118.98	111.91
31	p	607	CLA	C3A-C2A-C1A	2.25	104.71	101.34
45	7	309	KC2	C2A-C3A-C4A	2.25	108.16	106.49
43	3	306	A86	C25-C26-C27	-2.25	124.10	127.31
45	2	308	KC2	CAB-C3B-C4B	2.25	130.34	124.90
43	2	305	A86	C12-C11-C13	2.25	119.81	116.02
33	Y	101	BCR	C1-C6-C5	-2.25	119.44	122.61
39	b	622	DGD	CDB-CCB-CBB	-2.25	102.99	114.42
43	11	319	A86	C4-C3-C2	-2.25	118.86	123.47
31	11	308	CLA	C3A-C2A-C1A	2.25	104.71	101.34
43	13	303	A86	C7-C6-C8	2.25	121.62	118.08
43	14	302	A86	O4-C38-O5	-2.25	118.49	122.96
31	12	310	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
43	3	305	A86	C8-C6-C5	-2.25	115.49	118.94
38	B	620	LMG	O6-C5-C4	2.25	113.78	109.69
43	8	305	A86	C25-C26-C27	-2.25	124.10	127.31
42	9	314	KC1	C2A-C3A-C4A	2.25	108.16	106.49
43	15	305	A86	C26-C25-C24	-2.25	116.20	123.22
34	l	101	SQD	O49-C7-C8	-2.25	114.96	123.73
31	c	511	CLA	CHD-C1D-ND	-2.25	122.39	124.45
31	z	101	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
42	7	314	KC1	C1A-NA-C4A	-2.25	105.69	106.71
39	b	622	DGD	C5B-C4B-C3B	-2.25	103.01	114.42
31	b	602	CLA	C2A-C1A-CHA	2.25	127.79	123.86
43	6	307	A86	C40-C32-C33	2.25	119.14	109.05
34	0	318	SQD	C45-O47-C7	2.25	123.32	117.79
43	0	301	A86	O-C13-C14	-2.25	117.09	121.66
31	14	312	CLA	C1-O2A-CGA	2.25	122.34	116.44
34	b	601	SQD	O48-C23-C24	2.25	118.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	309	CLA	C2A-C1A-CHA	2.25	127.78	123.86
31	6	314	CLA	C3D-C2D-C1D	2.25	108.89	105.83
43	14	303	A86	C9-C10-C11	-2.25	120.01	126.61
38	14	316	LMG	C38-C37-C36	-2.24	103.03	114.42
31	7	312	CLA	C2A-C1A-CHA	2.24	127.78	123.86
41	e	101	HEM	CMA-C3A-C4A	-2.24	125.01	128.46
36	8	315	LHG	C27-C26-C25	-2.24	103.03	114.42
31	B	601	CLA	C2A-C1A-CHA	2.24	127.78	123.86
39	1	318	DGD	O3D-C3D-C4D	-2.24	105.16	110.35
44	p	612	DD6	C34-C35-C36	-2.24	107.38	111.85
45	7	309	KC2	C2A-C1A-CHA	-2.24	120.02	127.44
43	16	306	A86	C4-C3-C2	-2.24	118.88	123.47
43	1	320	A86	C4-C3-C2	-2.24	118.88	123.47
43	7	304	A86	C4-C3-C2	-2.24	118.88	123.47
32	A	405	PHO	O2D-CGD-CBD	2.24	113.84	111.00
45	3	309	KC2	CAB-C3B-C4B	2.24	130.31	124.90
31	5	309	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
43	16	304	A86	C26-C25-C24	-2.24	116.22	123.22
33	b	618	BCR	C29-C30-C25	2.24	113.93	110.48
31	p	606	CLA	CMC-C2C-C3C	2.24	132.20	126.12
31	a	403	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
31	z	103	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
43	17	301	A86	C19-C18-C17	-2.24	106.45	110.77
31	c	504	CLA	O2D-CGD-CBD	2.24	115.25	111.27
31	C	503	CLA	C2C-C1C-NC	2.24	112.07	109.97
34	B	623	SQD	O48-C23-C24	2.24	118.94	111.91
45	5	310	KC2	C3A-C4A-NA	2.24	113.02	110.57
31	16	316	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
32	D	402	PHO	C4A-C3A-C2A	-2.24	100.71	102.84
31	0	307	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
31	11	307	CLA	CHD-C4C-C3C	2.24	128.13	124.84
43	17	303	A86	C9-C10-C11	-2.24	120.03	126.61
31	15	313	CLA	CHD-C1D-ND	-2.24	122.40	124.45
31	10	312	CLA	O2D-CGD-CBD	2.24	115.24	111.27
31	2	307	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
31	1	308	CLA	C4-C3-C2	-2.24	117.94	123.68
43	18	302	A86	C9-C8-C6	-2.24	120.14	126.42
32	a	405	PHO	O2D-CGD-CBD	2.24	113.83	111.00
38	d	408	LMG	C3-C4-C5	-2.24	106.25	110.24
43	12	301	A86	C9-C8-C6	-2.23	120.14	126.42
43	19	301	A86	C25-C24-C1	-2.23	120.14	126.42
33	b	618	BCR	C33-C5-C6	-2.23	122.02	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	604	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
43	5	303	A86	C24-C1-C2	2.23	122.37	118.94
31	Z	101	CLA	C2A-C1A-CHA	2.23	127.76	123.86
43	4	304	A86	C9-C10-C11	-2.23	120.04	126.61
45	9	309	KC2	O2D-CGD-O1D	-2.23	119.47	123.84
43	18	301	A86	O4-C34-C33	2.23	113.15	107.59
31	3	312	CLA	C2A-C1A-CHA	2.23	127.76	123.86
31	15	313	CLA	CMA-C3A-C2A	-2.23	110.89	116.10
45	0	310	KC2	CMD-C2D-C1D	-2.23	125.03	128.46
31	10	313	CLA	CMB-C2B-C3B	2.23	128.85	124.68
31	B	614	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
43	7	302	A86	C24-C1-C2	-2.23	115.52	118.94
43	10	318	A86	O1-C20-C21	-2.23	112.38	115.06
43	11	305	A86	O-C13-C14	-2.23	117.13	121.66
31	1	307	CLA	C3A-C2A-C1A	2.23	104.68	101.34
31	A	403	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
43	14	301	A86	O4-C34-C35	2.23	113.14	107.59
31	13	316	CLA	C3A-C2A-C1A	2.23	104.68	101.34
31	C	504	CLA	O2D-CGD-CBD	2.23	115.23	111.27
43	10	318	A86	C34-O4-C38	2.23	122.05	117.90
43	1	305	A86	C28-C27-C26	-2.23	119.80	122.92
43	11	304	A86	C9-C8-C6	-2.23	120.16	126.42
31	P	606	CLA	CMC-C2C-C3C	2.23	132.17	126.12
31	3	310	CLA	CHD-C1D-ND	-2.23	122.41	124.45
45	4	308	KC2	CAB-C3B-C4B	-2.23	119.51	124.90
31	13	313	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
43	11	304	A86	C25-C24-C1	-2.23	120.16	126.42
31	B	610	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
38	k	101	LMG	O1-C1-C2	-2.23	104.83	108.30
45	0	310	KC2	C2A-C1A-NA	2.23	112.97	109.40
31	10	307	CLA	C1D-ND-C4D	2.23	107.92	106.33
31	Z	101	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
38	0	317	LMG	O3-C3-C2	-2.23	105.20	110.35
42	14	313	KC1	C3A-C4A-NA	2.22	113.00	110.57
43	10	304	A86	O4-C34-C35	2.22	113.13	107.59
31	13	308	CLA	C2A-C1A-CHA	2.22	127.75	123.86
45	13	311	KC2	O1D-CGD-CBD	-2.22	119.93	124.48
43	7	303	A86	C14-C15-C16	2.22	127.27	118.75
31	B	609	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
31	b	610	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
44	p	612	DD6	O1-C20-C19	2.22	115.05	113.38
31	9	310	CLA	C1B-CHB-C4A	-2.22	125.71	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	16	310	KC2	CAA-CBA-CGA	-2.22	115.84	127.26
31	8	307	CLA	C4-C3-C5	2.22	119.01	115.27
34	0	318	SQD	C13-C12-C11	-2.22	103.15	114.42
43	12	301	A86	C25-C24-C1	-2.22	120.17	126.42
31	p	604	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
42	19	314	KC1	C3A-C4A-NA	2.22	113.00	110.57
31	5	306	CLA	CHA-C1A-NA	-2.22	121.31	126.40
31	C	512	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
43	17	306	A86	C9-C8-C6	-2.22	120.18	126.42
36	C	521	LHG	C27-C26-C25	-2.22	103.15	114.42
43	16	306	A86	O4-C34-C33	2.22	113.12	107.59
31	7	312	CLA	CHA-C1A-NA	-2.22	121.31	126.40
31	11	315	CLA	C2C-C1C-NC	2.22	112.05	109.97
36	D	407	LHG	C20-C19-C18	-2.22	103.16	114.42
31	14	311	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
43	8	305	A86	C26-C25-C24	-2.22	116.29	123.22
31	c	508	CLA	O1D-CGD-CBD	2.22	129.02	124.48
43	8	301	A86	C-C1-C24	2.22	121.57	118.08
43	10	301	A86	C25-C24-C1	-2.22	120.19	126.42
43	18	301	A86	C25-C24-C1	-2.22	120.19	126.42
31	11	315	CLA	O2D-CGD-CBD	2.22	115.21	111.27
31	b	604	CLA	CHD-C4C-NC	2.22	127.70	124.20
35	D	406	PL9	C7-C3-C4	2.22	118.68	116.88
45	8	308	KC2	C2A-C1A-CHA	-2.22	120.11	127.44
31	19	310	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
31	Z	101	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	1	321	CLA	O2D-CGD-CBD	2.22	115.21	111.27
43	1	320	A86	O1-C20-C21	-2.22	112.40	115.06
31	b	615	CLA	C2D-C1D-ND	-2.22	108.47	110.10
43	6	305	A86	C7-C6-C8	2.22	121.57	118.08
31	5	311	CLA	O2D-CGD-CBD	2.22	115.20	111.27
43	10	303	A86	C14-C15-C16	2.22	127.24	118.75
43	5	303	A86	C-C1-C2	-2.22	119.82	122.92
31	8	311	CLA	CHA-C1A-NA	-2.22	121.33	126.40
45	10	310	KC2	C2A-C1A-NA	2.22	112.95	109.40
31	14	315	CLA	C2A-C3A-C4A	2.22	105.45	101.87
31	7	312	CLA	CHB-C4A-NA	2.22	127.58	124.51
38	D	408	LMG	C3-C4-C5	-2.21	106.29	110.24
43	p	611	A86	C14-C15-C16	-2.21	110.27	118.75
43	12	302	A86	C9-C8-C6	-2.21	120.19	126.42
39	11	318	DGD	O3G-C1D-C2D	-2.21	104.85	108.30
31	0	309	CLA	CMC-C2C-C1C	2.21	128.41	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	515	BCR	C15-C14-C13	-2.21	124.15	127.31
36	d	407	LHG	C20-C19-C18	-2.21	103.19	114.42
43	4	304	A86	O-C13-C14	2.21	126.16	121.66
43	P	611	A86	C14-C15-C16	-2.21	110.28	118.75
43	6	306	A86	C9-C10-C11	-2.21	120.10	126.61
43	5	302	A86	C28-C27-C29	2.21	124.05	118.93
31	b	611	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
31	C	508	CLA	O1D-CGD-CBD	2.21	129.01	124.48
31	a	404	CLA	C2D-C1D-ND	-2.21	108.47	110.10
31	3	312	CLA	O2D-CGD-CBD	2.21	115.20	111.27
38	4	316	LMG	C3-C4-C5	-2.21	106.30	110.24
31	c	503	CLA	C2A-C3A-C4A	2.21	105.44	101.87
38	W	201	LMG	C40-C39-C38	-2.21	103.21	114.42
43	16	305	A86	C20-C19-C18	2.21	117.12	112.75
36	A	410	LHG	C27-C26-C25	-2.21	103.21	114.42
36	a	410	LHG	C27-C26-C25	-2.21	103.22	114.42
31	14	312	CLA	C2A-C1A-CHA	2.21	127.72	123.86
43	2	302	A86	C7-C6-C5	-2.21	119.83	122.92
36	w	202	LHG	C27-C26-C25	-2.21	103.22	114.42
31	15	312	CLA	CHD-C1D-C2D	2.21	130.11	125.48
38	w	201	LMG	C40-C39-C38	-2.21	103.23	114.42
31	z	103	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
45	4	308	KC2	CAA-CBA-CGA	-2.20	115.93	127.26
45	9	309	KC2	O1D-CGD-CBD	-2.20	119.97	124.48
43	6	301	A86	C21-C20-C19	2.20	116.76	114.28
31	10	314	CLA	CHA-C4D-ND	2.20	137.11	132.50
43	11	305	A86	C34-O4-C38	-2.20	113.79	117.90
43	7	305	A86	C9-C8-C6	-2.20	120.23	126.42
38	n	701	LMG	O8-C28-O10	-2.20	118.03	123.59
31	17	312	CLA	CHA-C1A-NA	-2.20	121.35	126.40
31	17	308	CLA	CAC-C3C-C4C	2.20	127.67	124.81
45	18	310	KC2	CAB-C3B-C4B	-2.20	119.58	124.90
31	13	316	CLA	C1-C2-C3	-2.20	122.23	126.04
42	p	609	KC1	C4C-C3C-C2C	-2.20	103.69	106.90
31	19	307	CLA	C2D-C1D-ND	-2.20	108.48	110.10
43	14	305	A86	C4-C5-C6	-2.20	124.17	127.31
38	14	316	LMG	O1-C1-C2	-2.20	104.87	108.30
31	c	512	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
31	13	316	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
38	4	316	LMG	C42-C41-C40	-2.20	103.25	114.42
43	P	611	A86	C41-C32-C33	2.20	118.93	109.05
44	P	612	DD6	C7-C6-C5	-2.20	119.84	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	19	312	CLA	C20-C18-C17	-2.20	97.95	111.54
31	15	311	CLA	CAA-C2A-C1A	2.20	119.18	111.97
38	11	317	LMG	O2-C2-C1	-2.20	104.70	110.05
43	8	303	A86	O-C13-C11	-2.20	116.29	121.15
31	2	312	CLA	CAC-C3C-C4C	2.20	127.66	124.81
43	p	611	A86	C41-C32-C33	2.20	118.92	109.05
38	c	521	LMG	O6-C1-O1	-2.20	104.77	109.97
31	p	606	CLA	C2D-C1D-ND	2.20	111.72	110.10
43	11	305	A86	C-C1-C2	-2.20	119.84	122.92
43	12	303	A86	C34-O4-C38	2.20	121.99	117.90
43	11	302	A86	C20-C19-C18	2.20	117.10	112.75
43	11	306	A86	C36-C31-C32	-2.20	117.52	119.70
43	16	305	A86	C28-C27-C29	2.20	124.02	118.93
43	17	316	A86	C3-C4-C5	-2.20	118.97	123.47
43	5	302	A86	C14-C15-C16	2.20	127.16	118.75
43	8	304	A86	C22-C16-C17	-2.20	105.17	108.98
43	6	304	A86	C25-C24-C1	-2.20	120.25	126.42
43	17	316	A86	C36-C31-C32	-2.20	117.52	119.70
31	16	316	CLA	O2D-CGD-CBD	2.20	115.17	111.27
43	15	303	A86	C25-C24-C1	-2.20	120.25	126.42
33	C	516	BCR	C15-C14-C13	-2.20	124.18	127.31
33	c	516	BCR	C15-C14-C13	-2.20	124.18	127.31
38	K	101	LMG	O1-C1-C2	-2.20	104.88	108.30
45	1	311	KC2	CAA-CBA-CGA	-2.19	115.98	127.26
45	13	311	KC2	CBA-CAA-C2A	-2.19	116.90	125.27
33	c	515	BCR	C15-C14-C13	-2.19	124.18	127.31
31	2	315	CLA	C3A-C2A-C1A	2.19	104.63	101.34
31	C	511	CLA	CHD-C1D-ND	-2.19	122.44	124.45
31	w	203	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
31	2	311	CLA	CHA-C1A-NA	-2.19	121.38	126.40
45	15	310	KC2	C2B-C1B-NB	2.19	111.72	110.10
38	1	317	LMG	O2-C2-C1	-2.19	104.72	110.05
43	4	306	A86	C9-C10-C11	-2.19	120.16	126.61
45	7	311	KC2	CBB-CAB-C3B	-2.19	116.72	127.62
31	W	202	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
43	3	301	A86	O3-C36-C37	-2.19	105.49	109.39
34	l	101	SQD	O48-C23-O10	-2.19	118.06	123.59
43	5	301	A86	C28-C27-C29	2.19	124.00	118.93
43	18	302	A86	C25-C24-C1	2.19	132.57	126.42
43	6	303	A86	C26-C25-C24	-2.19	116.38	123.22
31	12	313	CLA	CBC-CAC-C3C	2.19	118.47	112.43
31	15	311	CLA	C1D-ND-C4D	2.19	107.89	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	301	A86	C20-C19-C18	2.19	117.08	112.75
43	9	306	A86	C7-C6-C8	2.19	121.53	118.08
31	5	311	CLA	CHD-C1D-ND	-2.19	122.44	124.45
31	10	317	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
31	15	309	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
43	1	320	A86	C10-C9-C8	-2.19	116.39	123.22
43	11	302	A86	C8-C6-C5	2.19	122.30	118.94
31	2	315	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
43	6	307	A86	C28-C27-C29	2.19	124.00	118.93
33	c	516	BCR	C7-C8-C9	-2.19	122.93	126.23
31	5	306	CLA	CHD-C1D-ND	-2.19	122.44	124.45
43	19	305	A86	C7-C6-C8	2.19	121.52	118.08
31	15	307	CLA	CHB-C4A-NA	2.19	127.53	124.51
31	c	502	CLA	C2D-C1D-ND	-2.19	108.49	110.10
31	18	307	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
38	1	301	LMG	O3-C3-C2	-2.19	105.30	110.35
31	B	606	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
43	8	303	A86	C41-C32-C40	-2.18	101.82	108.53
43	8	302	A86	O-C13-C11	-2.18	116.32	121.15
31	10	308	CLA	CHD-C4C-C3C	2.18	128.05	124.84
31	2	314	CLA	CMA-C3A-C2A	-2.18	111.00	116.10
43	17	302	A86	C-C1-C24	2.18	121.52	118.08
31	16	308	CLA	C2D-C1D-ND	-2.18	108.50	110.10
31	B	603	CLA	CHD-C4C-NC	2.18	127.64	124.20
31	14	315	CLA	C2A-C1A-CHA	2.18	127.68	123.86
31	p	601	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
31	B	615	CLA	C3C-C4C-NC	-2.18	108.12	110.57
32	d	402	PHO	C1B-NB-C4B	2.18	111.57	107.09
38	0	317	LMG	O8-C28-O10	-2.18	118.08	123.59
43	14	304	A86	C21-C20-C19	2.18	116.73	114.28
33	Y	101	BCR	C11-C10-C9	-2.18	124.20	127.31
33	y	101	BCR	C11-C10-C9	-2.18	124.20	127.31
38	n	701	LMG	C6-C5-C4	-2.18	107.89	113.00
31	c	503	CLA	C2C-C1C-NC	2.18	112.02	109.97
38	14	316	LMG	C42-C41-C40	-2.18	103.35	114.42
43	10	303	A86	C25-C24-C1	-2.18	120.29	126.42
31	8	314	CLA	O2D-CGD-CBD	2.18	115.14	111.27
42	3	314	KC1	C3A-C4A-NA	2.18	112.95	110.57
31	4	312	CLA	CHA-C1A-NA	-2.18	121.41	126.40
38	15	315	LMG	C3-C4-C5	2.18	114.13	110.24
31	13	307	CLA	CAC-C3C-C2C	-2.18	123.80	127.53
43	18	305	A86	C7-C6-C5	-2.18	119.87	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	319	A86	C9-C10-C11	-2.18	120.20	126.61
45	6	312	KC2	C2B-C1B-NB	2.18	111.71	110.10
43	14	303	A86	O-C13-C14	2.18	126.08	121.66
31	A	404	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
33	b	618	BCR	C24-C23-C22	-2.18	122.94	126.23
31	1	307	CLA	CHA-C1A-NA	-2.18	121.41	126.40
43	11	303	A86	C25-C24-C1	-2.18	120.30	126.42
31	4	309	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
43	10	318	A86	C3-C2-C1	-2.18	124.20	127.31
43	15	305	A86	C4-C5-C6	-2.18	124.20	127.31
39	C	519	DGD	C2G-O2G-C1B	2.18	123.15	117.79
32	D	402	PHO	C1B-NB-C4B	2.18	111.56	107.09
33	F	101	BCR	C11-C10-C9	-2.18	124.20	127.31
38	N	101	LMG	O6-C1-C2	-2.18	105.74	110.35
31	19	313	CLA	C1-C2-C3	-2.18	122.28	126.04
31	19	308	CLA	C3A-C2A-C1A	2.18	104.60	101.34
43	16	303	A86	C19-C18-C17	-2.17	106.58	110.77
31	4	312	CLA	CAD-C3D-C2D	2.17	151.29	140.80
33	C	516	BCR	C7-C8-C9	-2.17	122.95	126.23
43	19	302	A86	C3-C4-C5	-2.17	119.02	123.47
31	12	313	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
39	w	204	DGD	C5B-C4B-C3B	-2.17	103.39	114.42
31	1	312	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
31	12	310	CLA	C2A-C1A-CHA	2.17	127.66	123.86
43	6	303	A86	C23-C16-C17	2.17	112.76	108.98
43	19	306	A86	O4-C38-O5	-2.17	118.65	122.96
31	a	404	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
36	14	317	LHG	C11-C10-C9	-2.17	103.40	114.42
42	P	609	KC1	C4C-C3C-C2C	-2.17	103.73	106.90
31	6	313	CLA	C2A-C1A-CHA	2.17	127.66	123.86
43	2	304	A86	C35-C34-C33	2.17	113.67	109.88
34	L	102	SQD	O47-C7-C8	2.17	116.18	111.50
42	6	315	KC1	CAA-C2A-C1A	2.17	134.72	124.75
31	P	606	CLA	C2D-C1D-ND	2.17	111.70	110.10
43	0	305	A86	C12-C11-C13	2.17	119.67	116.02
43	2	303	A86	C21-C20-C19	-2.17	111.84	114.28
31	19	307	CLA	CAC-C3C-C2C	-2.17	123.82	127.53
31	C	504	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	P	601	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
43	3	303	A86	O1-C20-C19	2.17	115.01	113.38
45	18	308	KC2	C4D-C3D-CAD	2.17	111.31	107.81
31	10	311	CLA	O2A-CGA-O1A	-2.17	118.12	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	314	CLA	CHB-C4A-NA	2.17	127.51	124.51
43	5	318	A86	C28-C27-C29	2.17	123.95	118.93
31	18	307	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
43	12	305	A86	C9-C8-C6	-2.17	120.33	126.42
31	14	309	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	11	307	CLA	CHA-C1A-NA	-2.17	121.44	126.40
31	b	617	CLA	C3C-C4C-NC	-2.17	108.14	110.57
31	19	313	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	10	312	CLA	CAC-C3C-C4C	-2.17	122.00	124.81
45	3	309	KC2	CAA-CBA-CGA	-2.17	116.13	127.26
32	A	405	PHO	C1B-NB-C4B	2.17	111.54	107.09
33	h	101	BCR	C15-C14-C13	-2.17	124.22	127.31
31	12	316	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
31	c	504	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	5	312	CLA	CHB-C4A-NA	2.16	127.50	124.51
34	l	101	SQD	O47-C7-C8	2.16	116.17	111.50
43	8	302	A86	C41-C32-C33	2.16	118.77	109.05
39	W	203	DGD	C5B-C4B-C3B	-2.16	103.44	114.42
31	13	310	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
31	11	308	CLA	C4-C3-C2	-2.16	118.13	123.68
38	d	403	LMG	O7-C10-O9	-2.16	118.47	123.70
38	11	301	LMG	O3-C3-C2	-2.16	105.35	110.35
32	a	405	PHO	C1B-NB-C4B	2.16	111.53	107.09
42	14	313	KC1	CAA-CBA-CGA	-2.16	116.14	127.26
43	2	303	A86	O2-C18-C19	-2.16	105.50	109.80
31	15	307	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
43	5	301	A86	O1-C20-C19	2.16	115.01	113.38
31	C	502	CLA	C2D-C1D-ND	-2.16	108.51	110.10
34	10	320	SQD	C9-C8-C7	-2.16	105.76	113.62
43	8	305	A86	C9-C10-C11	-2.16	120.25	126.61
31	19	310	CLA	C1-C2-C3	-2.16	122.31	126.04
31	0	311	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
45	2	310	KC2	C3D-CAD-CBD	-2.16	104.76	107.61
31	14	307	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
43	4	303	A86	C7-C6-C5	-2.16	119.90	122.92
31	0	314	CLA	O2D-CGD-CBD	2.16	115.10	111.27
31	11	308	CLA	O2D-CGD-CBD	2.16	115.10	111.27
43	16	303	A86	C28-C27-C26	-2.16	119.90	122.92
43	1	319	A86	C10-C9-C8	-2.16	116.48	123.22
31	8	312	CLA	C3B-C4B-NB	-2.16	106.42	109.21
43	6	305	A86	C10-C9-C8	-2.16	116.48	123.22
43	17	305	A86	C4-C3-C2	-2.16	119.06	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	17	311	KC2	O2D-CGD-O1D	-2.16	119.62	123.84
42	0	315	KC1	CAA-CBA-CGA	-2.16	116.18	127.26
31	B	616	CLA	C11-C12-C13	-2.16	108.95	115.92
31	19	312	CLA	C20-C18-C19	-2.16	100.57	110.51
43	2	303	A86	O4-C38-O5	-2.16	118.68	122.96
38	P	614	LMG	C3-C4-C5	-2.15	106.39	110.24
31	10	314	CLA	CHA-C1A-NA	-2.15	121.46	126.40
31	B	601	CLA	CBA-CAA-C2A	2.15	120.22	113.86
31	4	315	CLA	C2A-C1A-CHA	2.15	127.62	123.86
43	15	303	A86	C-C1-C2	-2.15	119.91	122.92
38	0	317	LMG	C4-C3-C2	2.15	114.58	110.82
42	14	313	KC1	C2B-C1B-NB	2.15	111.69	110.10
45	7	311	KC2	CAB-C3B-C4B	-2.15	119.70	124.90
43	15	305	A86	O2-C18-C17	-2.15	105.53	109.80
31	A	403	CLA	CHB-C4A-NA	2.15	127.49	124.51
31	11	316	CLA	CHD-C1D-ND	-2.15	122.48	124.45
43	11	303	A86	C34-O4-C38	-2.15	113.89	117.90
43	16	307	A86	O-C13-C14	2.15	126.03	121.66
31	3	316	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
31	8	311	CLA	CMD-C2D-C1D	-2.15	120.92	124.71
31	12	313	CLA	C2C-C1C-NC	-2.15	107.96	109.97
31	15	306	CLA	O1D-CGD-CBD	2.15	128.88	124.48
34	l	101	SQD	O48-C23-C24	2.15	118.66	111.91
35	d	406	PL9	C7-C3-C4	2.15	118.62	116.88
43	13	302	A86	C9-C10-C11	-2.15	120.28	126.61
38	b	621	LMG	O6-C5-C4	2.15	113.60	109.69
31	17	307	CLA	CMA-C3A-C2A	-2.15	111.08	116.10
43	18	302	A86	C12-C11-C10	-2.15	118.22	123.42
43	14	305	A86	C35-C34-C33	-2.15	106.12	109.88
43	p	613	A86	C3-C4-C5	-2.15	119.07	123.47
31	z	101	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
43	15	305	A86	C17-C16-C15	2.15	111.36	109.16
43	1	306	A86	C21-C20-C19	2.15	116.70	114.28
43	7	304	A86	C3-C2-C1	-2.15	124.24	127.31
31	P	606	CLA	C1C-C2C-C3C	2.15	109.22	106.96
31	b	602	CLA	CBA-CAA-C2A	2.15	120.21	113.86
31	16	314	CLA	C4A-NA-C1A	2.15	107.67	106.71
43	15	302	A86	C3-C4-C5	-2.15	119.07	123.47
38	p	614	LMG	C3-C4-C5	-2.15	106.41	110.24
43	18	303	A86	C25-C24-C1	-2.15	120.38	126.42
31	13	316	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
31	13	312	CLA	C2A-C1A-CHA	2.15	127.61	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	408	SQD	O9-S-C6	2.15	109.49	106.94
42	3	314	KC1	C2A-C1A-NA	2.15	112.84	109.40
43	19	306	A86	C21-C20-C19	2.15	116.69	114.28
31	4	307	CLA	CHB-C4A-NA	2.15	127.48	124.51
35	d	406	PL9	C20-C19-C21	2.15	118.88	115.27
43	9	305	A86	C7-C6-C8	2.15	121.46	118.08
31	B	610	CLA	C3A-C2A-C1A	2.15	104.55	101.34
43	6	305	A86	C25-C24-C1	-2.15	120.39	126.42
33	A	407	BCR	C15-C14-C13	-2.14	124.25	127.31
31	1	312	CLA	CGD-CBD-CAD	2.14	117.68	110.73
31	c	512	CLA	C2A-C1A-CHA	2.14	127.61	123.86
31	8	307	CLA	O2A-C1-C2	-2.14	103.00	108.64
31	C	511	CLA	O1D-CGD-CBD	2.14	128.87	124.48
31	c	511	CLA	O1D-CGD-CBD	2.14	128.87	124.48
39	C	519	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
39	c	519	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
34	a	408	SQD	O9-S-C6	2.14	109.49	106.94
33	H	101	BCR	C15-C14-C13	-2.14	124.25	127.31
31	4	312	CLA	CAA-CBA-CGA	2.14	119.51	113.25
43	9	306	A86	C25-C24-C1	-2.14	120.40	126.42
43	10	302	A86	C3-C4-C5	-2.14	119.09	123.47
42	8	313	KC1	O2D-CGD-O1D	-2.14	119.65	123.84
31	13	316	CLA	O2D-CGD-CBD	2.14	115.07	111.27
31	16	308	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
39	c	519	DGD	C2G-O2G-C1B	2.14	123.06	117.79
31	9	308	CLA	C3A-C2A-C1A	2.14	104.55	101.34
43	10	301	A86	C4-C3-C2	-2.14	119.09	123.47
43	10	318	A86	C9-C10-C11	-2.14	120.32	126.61
34	10	320	SQD	O48-C23-C24	2.14	118.62	111.91
43	14	303	A86	C3-C4-C5	-2.14	119.09	123.47
38	0	317	LMG	O2-C2-C1	-2.14	104.85	110.05
42	6	315	KC1	CMA-C3A-C4A	-2.14	121.78	125.04
31	B	616	CLA	C2D-C1D-ND	-2.14	108.53	110.10
33	C	517	BCR	C11-C10-C9	-2.14	124.26	127.31
31	18	314	CLA	O2D-CGD-CBD	2.14	115.07	111.27
43	P	613	A86	C3-C4-C5	-2.14	119.09	123.47
43	18	303	A86	C-C1-C2	-2.14	119.93	122.92
43	17	306	A86	C12-C11-C13	2.14	119.61	116.02
31	16	311	CLA	C2A-C1A-CHA	2.14	127.58	123.85
43	0	303	A86	O4-C34-C33	2.14	112.92	107.59
31	12	316	CLA	CHD-C1D-ND	-2.14	122.49	124.45
43	17	316	A86	C14-C15-C16	-2.14	110.57	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	17	310	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
39	C	519	DGD	O6E-C1E-O5D	-2.14	104.91	109.97
45	18	310	KC2	C3D-CAD-CBD	-2.14	104.79	107.61
31	b	616	CLA	C3C-C4C-NC	-2.14	108.17	110.57
34	10	320	SQD	C13-C12-C11	-2.14	103.58	114.42
31	2	312	CLA	C3A-C2A-C1A	2.14	104.54	101.34
45	10	310	KC2	CMB-C2B-C1B	2.14	128.48	124.71
43	6	304	A86	C20-C19-C18	2.14	116.97	112.75
38	1	317	LMG	O7-C10-O9	-2.14	118.54	123.70
31	a	403	CLA	CHB-C4A-NA	2.14	127.47	124.51
43	4	305	A86	C19-C18-C17	-2.14	106.65	110.77
39	C	519	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
33	a	407	BCR	C15-C14-C13	-2.13	124.26	127.31
31	2	309	CLA	C2A-C1A-CHA	2.13	127.59	123.86
43	9	301	A86	C10-C9-C8	-2.13	116.56	123.22
31	3	316	CLA	C2D-C1D-ND	2.13	111.68	110.10
43	18	301	A86	C21-C20-C19	2.13	116.68	114.28
43	7	302	A86	C26-C25-C24	-2.13	116.56	123.22
43	11	302	A86	O1-C15-C20	-2.13	57.31	59.40
43	7	304	A86	C9-C8-C6	-2.13	120.42	126.42
43	9	301	A86	C20-C19-C18	2.13	116.97	112.75
33	c	517	BCR	C11-C10-C9	-2.13	124.27	127.31
44	P	612	DD6	C28-C27-C29	2.13	121.06	116.84
43	18	303	A86	C12-C11-C13	2.13	119.60	116.02
42	14	313	KC1	CBD-CHA-C1A	2.13	132.86	128.88
44	P	612	DD6	C34-C35-C36	-2.13	107.61	111.85
43	2	303	A86	C28-C27-C29	2.13	123.86	118.93
33	c	517	BCR	C40-C30-C25	2.13	113.75	110.30
31	7	315	CLA	O2D-CGD-CBD	2.13	115.05	111.27
39	c	519	DGD	CAB-C9B-C8B	-2.13	103.61	114.42
31	B	613	CLA	O1D-CGD-CBD	2.13	128.84	124.48
38	11	317	LMG	O3-C3-C2	-2.13	105.43	110.35
43	19	301	A86	C20-C19-C18	2.13	116.96	112.75
39	C	520	DGD	CBB-CAB-C9B	-2.13	103.62	114.42
39	c	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.42
43	10	304	A86	C25-C24-C1	-2.13	120.44	126.42
43	2	303	A86	C9-C10-C11	-2.13	120.35	126.61
31	6	316	CLA	O2D-CGD-CBD	2.13	115.05	111.27
43	0	303	A86	C7-C6-C8	2.13	121.43	118.08
31	2	306	CLA	CAA-C2A-C3A	-2.13	108.94	114.26
31	5	307	CLA	C2A-C1A-CHA	2.13	127.58	123.86
35	D	406	PL9	C20-C19-C21	2.13	118.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	h	102	DGD	O3E-C3E-C2E	-2.13	105.43	110.35
31	p	606	CLA	C1C-C2C-C3C	2.13	109.19	106.96
31	4	309	CLA	C2A-C1A-CHA	2.13	127.58	123.86
31	p	601	CLA	CHB-C4A-NA	2.13	127.45	124.51
43	6	305	A86	C3-C2-C1	-2.13	124.28	127.31
31	11	313	CLA	C6-C5-C3	-2.13	107.88	113.45
39	c	519	DGD	O6E-C1E-O5D	-2.13	104.94	109.97
43	14	305	A86	C14-C15-C16	-2.13	110.62	118.75
31	18	312	CLA	CHA-C1A-NA	-2.13	121.53	126.40
43	5	301	A86	O5-C38-C39	-2.13	117.07	124.81
31	1	307	CLA	CHB-C4A-NA	2.12	127.45	124.51
31	C	512	CLA	C2A-C1A-CHA	2.12	127.57	123.86
45	5	310	KC2	CAC-C3C-C4C	2.12	134.36	124.47
33	C	517	BCR	C40-C30-C25	2.12	113.74	110.30
43	P	613	A86	C40-C32-C31	2.12	112.37	110.47
31	18	309	CLA	C2A-C1A-CHA	2.12	127.57	123.86
31	c	502	CLA	C7-C6-C5	-2.12	107.60	113.36
31	15	311	CLA	CMC-C2C-C3C	2.12	131.88	126.12
31	15	311	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
38	4	316	LMG	O8-C28-O10	-2.12	118.24	123.59
39	C	518	DGD	C5B-C4B-C3B	-2.12	103.66	114.42
31	C	502	CLA	C7-C6-C5	-2.12	107.60	113.36
43	4	306	A86	C36-C31-C32	2.12	121.80	119.70
43	11	319	A86	C25-C24-C1	-2.12	120.46	126.42
31	d	404	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
43	9	306	A86	C-C1-C24	2.12	121.42	118.08
31	5	307	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
38	10	319	LMG	O3-C3-C2	-2.12	105.45	110.35
43	13	303	A86	C33-C32-C31	-2.12	107.15	109.21
31	6	316	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
31	C	508	CLA	C4-C3-C5	2.12	118.83	115.27
43	2	301	A86	C7-C6-C8	2.12	121.41	118.08
31	14	306	CLA	C3B-C4B-NB	-2.12	106.47	109.21
43	8	304	A86	O2-C18-C19	2.12	114.01	109.80
31	10	314	CLA	CHD-C1D-C2D	2.12	129.92	125.48
33	y	101	BCR	C37-C22-C21	-2.12	119.96	122.92
43	p	613	A86	C40-C32-C31	2.12	112.37	110.47
43	16	306	A86	C9-C10-C11	-2.12	120.39	126.61
31	b	611	CLA	C3A-C2A-C1A	2.12	104.51	101.34
39	H	102	DGD	O3E-C3E-C2E	-2.12	105.46	110.35
43	9	303	A86	C9-C10-C11	-2.12	120.39	126.61
31	8	314	CLA	CAA-C2A-C3A	-2.12	106.99	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	14	308	KC2	C3C-C2C-C1C	-2.11	104.92	106.49
39	c	518	DGD	C7B-C6B-C5B	-2.11	103.69	114.42
43	P	613	A86	C22-C16-C17	-2.11	105.31	108.98
43	6	306	A86	O-C13-C14	2.11	125.95	121.66
31	7	307	CLA	CMA-C3A-C2A	-2.11	111.16	116.10
42	13	314	KC1	C2B-C1B-NB	2.11	111.66	110.10
45	8	310	KC2	C2B-C1B-NB	2.11	111.66	110.10
31	C	505	CLA	C2D-C1D-ND	-2.11	108.55	110.10
39	c	520	DGD	CBB-CAB-C9B	-2.11	103.69	114.42
39	C	518	DGD	C7B-C6B-C5B	-2.11	103.70	114.42
42	13	314	KC1	CMB-C2B-C1B	2.11	128.44	124.71
31	0	314	CLA	CAA-C2A-C1A	2.11	118.90	111.97
31	c	513	CLA	C4-C3-C5	2.11	118.83	115.27
43	9	303	A86	C28-C27-C29	2.11	123.82	118.93
43	2	305	A86	C25-C26-C27	-2.11	124.30	127.31
38	1	317	LMG	O3-C3-C2	-2.11	105.47	110.35
31	D	404	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
42	18	313	KC1	CAA-CBA-CGA	-2.11	116.41	127.26
43	15	302	A86	C40-C32-C31	-2.11	108.58	110.47
31	1	307	CLA	O2D-CGD-CBD	2.11	115.02	111.27
43	10	305	A86	C12-C11-C13	2.11	119.57	116.02
43	16	306	A86	C4-C5-C6	-2.11	124.30	127.31
43	8	304	A86	C17-C16-C15	-2.11	107.01	109.16
31	6	311	CLA	C2A-C1A-CHA	2.11	127.54	123.85
43	3	304	A86	C25-C24-C1	-2.11	120.49	126.42
31	b	604	CLA	C4C-C3C-C2C	2.11	109.97	106.90
33	h	101	BCR	C38-C26-C27	-2.11	109.56	113.62
31	11	307	CLA	CHD-C1D-C2D	2.11	129.90	125.48
31	B	616	CLA	CHC-C1C-NC	2.11	127.40	124.20
43	10	302	A86	C9-C8-C6	-2.11	120.49	126.42
31	16	313	CLA	C2A-C1A-CHA	2.11	127.55	123.86
39	C	519	DGD	O5E-C6E-C5E	-2.11	104.06	111.29
43	10	303	A86	C7-C6-C8	2.11	121.40	118.08
31	17	308	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
31	11	313	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	11	313	CLA	C5-C3-C2	2.11	125.38	121.12
31	9	310	CLA	C1-C2-C3	-2.11	122.40	126.04
43	1	306	A86	C3-C4-C5	-2.11	119.16	123.47
42	11	314	KC1	C1C-C2C-C3C	-2.11	104.74	106.96
31	P	601	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
31	10	309	CLA	CHD-C1D-ND	-2.11	122.52	124.45
31	p	601	CLA	CAA-C2A-C3A	-2.11	107.01	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Y	101	BCR	C37-C22-C21	-2.11	119.97	122.92
31	11	312	CLA	C2A-C1A-CHA	2.11	127.54	123.86
43	12	306	A86	C19-C18-C17	-2.11	106.71	110.77
43	0	301	A86	O1-C15-C20	-2.11	57.34	59.40
43	4	303	A86	C10-C9-C8	-2.11	116.65	123.22
43	14	304	A86	O4-C38-C39	2.11	114.96	111.09
35	D	406	PL9	C50-C49-C48	-2.11	116.56	122.65
33	f	101	BCR	C11-C10-C9	-2.10	124.31	127.31
43	10	301	A86	O1-C15-C20	-2.10	57.34	59.40
43	18	304	A86	O1-C15-C20	-2.10	57.34	59.40
43	5	304	A86	O4-C38-O5	-2.10	118.78	122.96
43	0	302	A86	C9-C10-C11	-2.10	120.42	126.61
31	c	502	CLA	C11-C12-C13	-2.10	109.12	115.92
38	P	614	LMG	C6-C5-C4	-2.10	108.08	113.00
43	14	305	A86	C-C1-C24	2.10	121.39	118.08
31	14	312	CLA	C4D-C3D-CAD	-2.10	105.62	108.10
45	15	310	KC2	O2D-CGD-O1D	-2.10	119.73	123.84
31	6	313	CLA	CHA-C1A-NA	-2.10	121.58	126.40
44	P	612	DD6	C33-C34-C35	2.10	113.18	110.30
31	7	308	CLA	CBC-CAC-C3C	2.10	118.23	112.43
31	2	309	CLA	CHD-C1D-ND	-2.10	122.52	124.45
31	B	604	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
43	17	304	A86	C36-C31-C32	-2.10	117.61	119.70
31	C	513	CLA	C4-C3-C5	2.10	118.81	115.27
43	p	613	A86	C22-C16-C17	-2.10	105.33	108.98
43	15	304	A86	C23-C16-C17	-2.10	105.33	108.98
43	17	303	A86	C3-C4-C5	-2.10	119.17	123.47
31	14	315	CLA	CAC-C3C-C4C	2.10	127.54	124.81
43	7	304	A86	C9-C10-C11	-2.10	120.43	126.61
43	14	302	A86	C25-C26-C27	-2.10	124.31	127.31
45	1	311	KC2	O2D-CGD-O1D	-2.10	119.73	123.84
31	14	309	CLA	C2A-C1A-CHA	2.10	127.53	123.86
43	5	305	A86	C10-C9-C8	-2.10	116.67	123.22
35	d	406	PL9	C50-C49-C48	-2.10	116.58	122.65
43	19	305	A86	C36-C31-C32	-2.10	117.61	119.70
43	1	304	A86	O1-C20-C21	-2.10	112.54	115.06
31	B	603	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
31	C	503	CLA	CMB-C2B-C1B	2.10	131.69	128.46
43	18	305	A86	C10-C9-C8	-2.10	116.67	123.22
31	b	604	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
43	19	303	A86	C26-C25-C24	-2.10	116.67	123.22
31	c	503	CLA	CMB-C2B-C1B	2.10	131.69	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	307	A86	O4-C34-C33	-2.10	102.37	107.59
43	6	307	A86	O2-C18-C19	-2.10	105.64	109.80
31	11	307	CLA	CHA-C4D-ND	2.10	136.89	132.50
31	10	314	CLA	C3C-C4C-NC	-2.10	108.22	110.57
43	6	302	A86	C19-C18-C17	-2.10	106.72	110.77
31	12	312	CLA	C2D-C1D-ND	-2.10	108.56	110.10
45	13	309	KC2	CBA-CAA-C2A	-2.10	117.28	125.27
38	p	614	LMG	C6-C5-C4	-2.10	108.09	113.00
31	4	311	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
39	c	519	DGD	O5E-C6E-C5E	-2.10	104.10	111.29
43	9	302	A86	C28-C27-C26	-2.10	119.99	122.92
31	b	614	CLA	O1D-CGD-CBD	2.10	128.77	124.48
31	C	502	CLA	C11-C12-C13	-2.10	109.15	115.92
31	c	508	CLA	C4-C3-C5	2.09	118.80	115.27
31	10	307	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
31	a	404	CLA	C2A-C1A-CHA	2.09	127.52	123.86
31	1	313	CLA	CHA-C4D-ND	2.09	136.88	132.50
33	H	101	BCR	C38-C26-C27	-2.09	109.59	113.62
31	18	312	CLA	C3C-C4C-NC	-2.09	108.22	110.57
43	1	306	A86	C10-C9-C8	-2.09	116.68	123.22
34	A	408	SQD	C44-O6-C1	2.09	117.83	113.74
31	10	309	CLA	CMC-C2C-C1C	2.09	128.23	125.04
43	4	306	A86	C35-C34-C33	-2.09	106.22	109.88
43	16	304	A86	O4-C38-C39	2.09	114.94	111.09
31	B	603	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
43	1	305	A86	C4-C5-C6	-2.09	124.32	127.31
39	c	518	DGD	CAB-C9B-C8B	-2.09	103.80	114.42
31	15	311	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
43	3	303	A86	C9-C10-C11	-2.09	120.45	126.61
42	1	314	KC1	CAA-CBA-CGA	-2.09	116.51	127.26
31	15	306	CLA	C2A-C1A-CHA	2.09	127.52	123.86
43	9	304	A86	O4-C34-C35	-2.09	102.38	107.59
33	B	617	BCR	C24-C23-C22	-2.09	123.07	126.23
45	1	309	KC2	CBC-CAC-C3C	-2.09	117.21	127.62
31	C	509	CLA	CHD-C4C-NC	2.09	127.50	124.20
39	C	520	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
43	16	303	A86	O-C13-C11	-2.09	116.53	121.15
43	19	304	A86	C36-C31-C32	-2.09	117.62	119.70
42	13	314	KC1	C3D-CAD-CBD	-2.09	104.85	107.61
31	b	604	CLA	CAC-C3C-C2C	-2.09	123.95	127.53
31	c	509	CLA	CHD-C4C-NC	2.09	127.50	124.20
31	B	603	CLA	C4C-C3C-C2C	2.09	109.94	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	314	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
39	w	204	DGD	O2D-C2D-C3D	-2.09	105.52	110.35
31	A	404	CLA	C2A-C1A-CHA	2.09	127.51	123.86
31	16	313	CLA	CHA-C1A-NA	-2.09	121.61	126.40
31	b	604	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
45	1	309	KC2	C2B-C1B-NB	2.09	111.64	110.10
43	0	304	A86	O4-C34-C35	2.09	112.79	107.59
43	5	301	A86	C7-C6-C5	-2.09	120.00	122.92
43	3	306	A86	C41-C32-C33	-2.09	99.67	109.05
42	P	609	KC1	CAB-C3B-C2B	2.09	135.48	128.60
38	5	316	LMG	C1-O6-C5	2.09	117.78	113.69
31	10	307	CLA	O2D-CGD-CBD	2.09	114.98	111.27
42	16	301	KC1	O1D-CGD-CBD	-2.09	120.21	124.48
31	8	309	CLA	C2A-C1A-CHA	2.09	127.51	123.86
43	16	304	A86	C14-C15-C16	2.09	126.74	118.75
38	0	317	LMG	O6-C1-O1	-2.09	105.03	109.97
31	17	313	CLA	O1D-CGD-CBD	2.09	128.75	124.48
31	4	315	CLA	CAC-C3C-C4C	2.09	127.52	124.81
32	A	405	PHO	CMA-C3A-C4A	-2.09	109.81	114.38
43	7	306	A86	C4-C3-C2	-2.09	119.20	123.47
31	c	505	CLA	C2D-C1D-ND	-2.09	108.57	110.10
43	6	302	A86	O-C13-C11	-2.09	116.54	121.15
39	b	622	DGD	O6E-C1E-O5D	-2.09	105.04	109.97
43	19	301	A86	C10-C9-C8	-2.09	116.71	123.22
33	a	407	BCR	C39-C30-C25	2.09	113.68	110.30
36	D	407	LHG	C18-C17-C16	-2.09	103.84	114.42
31	b	617	CLA	CHC-C1C-NC	2.08	127.37	124.20
43	14	301	A86	O1-C20-C19	-2.08	111.82	113.38
31	14	312	CLA	C1-C2-C3	-2.08	122.44	126.04
32	a	405	PHO	CMA-C3A-C4A	-2.08	109.81	114.38
39	C	518	DGD	CAB-C9B-C8B	-2.08	103.85	114.42
43	18	305	A86	C34-O4-C38	-2.08	114.01	117.90
43	18	304	A86	C21-C20-C19	-2.08	111.94	114.28
31	B	615	CLA	C11-C10-C8	-2.08	109.19	115.92
36	d	407	LHG	C18-C17-C16	-2.08	103.85	114.42
31	0	314	CLA	C2D-C1D-ND	-2.08	108.57	110.10
34	a	408	SQD	C44-O6-C1	2.08	117.81	113.74
31	14	307	CLA	CHB-C4A-NA	2.08	127.39	124.51
43	5	318	A86	C33-C32-C31	-2.08	107.19	109.21
31	P	606	CLA	CAC-C3C-C4C	2.08	127.51	124.81
39	C	518	DGD	O6E-C5E-C6E	-2.08	101.26	106.44
45	13	309	KC2	O2D-CGD-O1D	-2.08	119.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	303	A86	C36-C31-C32	-2.08	117.63	119.70
31	1	321	CLA	C4A-NA-C1A	2.08	107.64	106.71
45	12	311	KC2	C3D-CAD-CBD	-2.08	104.86	107.61
31	0	308	CLA	CHD-C4C-C3C	2.08	127.90	124.84
31	10	317	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
43	1	303	A86	C-C1-C24	2.08	121.36	118.08
43	15	304	A86	C25-C26-C27	-2.08	124.34	127.31
31	p	606	CLA	CAC-C3C-C4C	2.08	127.51	124.81
31	7	308	CLA	CAC-C3C-C4C	2.08	127.51	124.81
31	p	608	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
31	12	313	CLA	CAC-C3C-C4C	2.08	127.51	124.81
43	0	304	A86	C25-C24-C1	-2.08	120.57	126.42
39	w	204	DGD	C8B-C7B-C6B	-2.08	103.86	114.42
39	c	520	DGD	CAB-C9B-C8B	-2.08	103.86	114.42
42	8	313	KC1	CMA-C3A-C4A	-2.08	121.87	125.04
42	4	313	KC1	C3A-C4A-NA	2.08	112.84	110.57
31	5	307	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	1	310	CLA	C3A-C2A-C1A	2.08	104.45	101.34
39	11	318	DGD	CDB-CCB-CBB	-2.08	103.87	114.42
31	9	312	CLA	CAC-C3C-C4C	2.08	127.51	124.81
33	A	407	BCR	C39-C30-C25	2.08	113.67	110.30
43	p	611	A86	C23-C16-C17	-2.08	105.37	108.98
31	P	608	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
45	0	310	KC2	CMB-C2B-C1B	2.08	128.37	124.71
39	W	203	DGD	C7B-C6B-C5B	-2.08	103.88	114.42
39	w	204	DGD	C7B-C6B-C5B	-2.08	103.88	114.42
45	4	310	KC2	CAA-CBA-CGA	-2.08	116.59	127.26
45	16	312	KC2	O1D-CGD-CBD	-2.08	120.23	124.48
43	12	305	A86	O4-C38-O5	-2.08	118.84	122.96
38	F	102	LMG	O5-C6-C5	-2.08	104.17	111.29
34	B	623	SQD	O47-C7-O49	-2.08	118.69	123.70
43	12	302	A86	O3-C36-C37	-2.08	105.70	109.39
38	b	621	LMG	O2-C2-C1	-2.08	105.00	110.05
31	11	307	CLA	CHB-C4A-NA	2.08	127.38	124.51
31	2	315	CLA	C2C-C1C-NC	-2.08	108.03	109.97
39	W	203	DGD	O2D-C2D-C3D	-2.07	105.55	110.35
31	A	403	CLA	C7-C6-C5	-2.07	107.72	113.36
43	1	320	A86	C17-C16-C15	2.07	111.28	109.16
43	5	303	A86	O4-C34-C35	2.07	112.76	107.59
43	11	303	A86	C28-C27-C29	2.07	123.73	118.93
31	b	605	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
43	9	305	A86	C3-C4-C5	-2.07	119.23	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	510	CLA	C3C-C4C-NC	-2.07	108.25	110.57
31	16	308	CLA	C3C-C4C-NC	-2.07	108.25	110.57
43	7	305	A86	C12-C11-C13	2.07	119.50	116.02
42	5	313	KC1	O2D-CGD-O1D	-2.07	119.78	123.84
31	11	308	CLA	CHD-C1D-ND	-2.07	122.55	124.45
39	W	203	DGD	C8B-C7B-C6B	-2.07	103.90	114.42
31	b	617	CLA	C11-C12-C13	-2.07	109.22	115.92
42	p	609	KC1	CAB-C3B-C2B	2.07	135.43	128.60
31	r	101	CLA	CHA-C1A-NA	-2.07	121.65	126.40
43	17	305	A86	C36-C31-C32	-2.07	117.64	119.70
31	18	307	CLA	CMD-C2D-C3D	2.07	132.38	127.61
43	9	302	A86	C41-C32-C31	-2.07	108.62	110.47
31	a	403	CLA	C7-C6-C5	-2.07	107.73	113.36
43	2	305	A86	C26-C25-C24	-2.07	116.75	123.22
34	b	601	SQD	O47-C7-O49	-2.07	118.70	123.70
38	b	621	LMG	C33-C32-C31	-2.07	103.92	114.42
42	12	314	KC1	CBA-CAA-C2A	-2.07	117.38	125.27
33	B	618	BCR	C38-C26-C27	-2.07	109.64	113.62
43	4	301	A86	O4-C34-C33	2.07	112.74	107.59
31	2	315	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
43	7	302	A86	C23-C16-C17	2.07	112.58	108.98
31	5	311	CLA	O1D-CGD-CBD	2.07	128.72	124.48
31	A	404	CLA	C3A-C2A-C1A	2.07	104.44	101.34
31	14	306	CLA	O1D-CGD-CBD	2.07	128.71	124.48
44	p	612	DD6	C33-C34-C35	2.07	113.13	110.30
31	11	308	CLA	C4-C3-C5	2.07	118.75	115.27
31	A	403	CLA	CAA-CBA-CGA	-2.07	107.22	113.25
31	p	606	CLA	CHD-C4C-C3C	2.07	127.88	124.84
33	y	101	BCR	C2-C3-C4	-2.07	106.76	111.38
31	B	616	CLA	CHA-C1A-NA	-2.06	121.67	126.40
38	f	102	LMG	O5-C6-C5	-2.06	104.21	111.29
31	P	610	CLA	C2A-C1A-CHA	2.06	127.46	123.85
31	p	610	CLA	C2A-C1A-CHA	2.06	127.46	123.85
31	12	312	CLA	C3A-C2A-C1A	2.06	104.43	101.34
42	19	314	KC1	C3D-CAD-CBD	-2.06	104.89	107.61
31	p	605	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
33	c	517	BCR	C30-C25-C26	-2.06	119.71	122.61
38	D	403	LMG	O8-C28-O10	-2.06	118.39	123.59
43	10	318	A86	C7-C6-C5	-2.06	120.03	122.92
31	c	503	CLA	C1-C2-C3	-2.06	122.47	126.04
38	B	620	LMG	C33-C32-C31	-2.06	103.95	114.42
38	B	620	LMG	O2-C2-C1	-2.06	105.03	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	4	316	LMG	O3-C3-C2	-2.06	105.58	110.35
43	2	301	A86	C23-C16-C22	-2.06	104.33	107.37
39	c	518	DGD	O6E-C5E-C6E	-2.06	101.31	106.44
45	7	311	KC2	CAB-C3B-C2B	2.06	135.40	128.60
43	15	304	A86	C40-C32-C33	-2.06	99.79	109.05
33	Y	101	BCR	C2-C3-C4	-2.06	106.77	111.38
45	8	308	KC2	CBA-CAA-C2A	-2.06	117.41	125.27
45	7	309	KC2	CHC-C1C-C2C	2.06	128.20	124.98
31	b	615	CLA	O2A-C1-C2	-2.06	103.22	108.64
31	0	312	CLA	CMC-C2C-C3C	2.06	131.71	126.12
43	13	302	A86	C14-C15-C16	-2.06	110.86	118.75
31	16	309	CLA	C4-C3-C5	2.06	118.74	115.27
31	c	510	CLA	C3C-C4C-NC	-2.06	108.26	110.57
31	5	306	CLA	C3A-C2A-C1A	2.06	104.42	101.34
38	15	315	LMG	O8-C28-O10	-2.06	118.39	123.59
41	E	101	HEM	C4B-CHC-C1C	2.06	125.28	122.56
31	0	307	CLA	C2A-C1A-CHA	2.06	127.46	123.86
31	16	316	CLA	C2A-C1A-CHA	2.06	127.46	123.86
43	5	305	A86	C20-C19-C18	2.06	116.82	112.75
31	B	603	CLA	CAC-C3C-C2C	-2.06	124.01	127.53
31	p	605	CLA	O2D-CGD-CBD	2.06	114.93	111.27
43	16	307	A86	C34-O4-C38	2.06	121.73	117.90
38	4	316	LMG	O6-C1-O1	-2.06	105.10	109.97
31	p	602	CLA	CHB-C4A-NA	2.06	127.36	124.51
39	11	318	DGD	CFB-CEB-CDB	-2.06	103.97	114.42
31	15	307	CLA	C2A-C1A-CHA	2.06	127.46	123.86
31	17	307	CLA	C1D-ND-C4D	2.06	107.80	106.33
34	L	102	SQD	O48-C23-C24	2.06	118.36	111.91
39	H	102	DGD	C5B-C4B-C3B	-2.06	103.98	114.42
43	4	305	A86	C40-C32-C33	-2.06	99.81	109.05
31	D	401	CLA	CMC-C2C-C3C	2.06	131.70	126.12
43	7	305	A86	O4-C34-C33	-2.06	102.47	107.59
43	8	302	A86	C21-C20-C19	-2.06	111.97	114.28
31	8	307	CLA	C5-C3-C2	-2.06	116.96	121.12
31	B	607	CLA	O2D-CGD-CBD	2.06	114.92	111.27
31	R	101	CLA	CHA-C1A-NA	-2.06	121.69	126.40
42	9	314	KC1	O1D-CGD-CBD	-2.06	120.28	124.48
31	B	612	CLA	C2A-C1A-CHA	2.06	127.45	123.86
33	b	619	BCR	C3-C4-C5	-2.06	110.41	114.08
39	h	102	DGD	C5B-C4B-C3B	-2.05	103.99	114.42
43	10	301	A86	C20-C19-C18	2.05	116.81	112.75
43	19	304	A86	C20-C19-C18	2.05	116.81	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	619	BCR	C38-C26-C27	-2.05	109.67	113.62
45	19	309	KC2	CBD-CHA-C1A	2.05	132.71	128.88
43	3	305	A86	C4-C5-C6	-2.05	124.38	127.31
31	13	315	CLA	CAA-C2A-C3A	-2.05	107.15	112.78
43	3	305	A86	O4-C38-O5	-2.05	118.88	122.96
31	z	103	CLA	CED-O2D-CGD	-2.05	111.29	115.94
43	9	303	A86	C23-C16-C17	-2.05	105.42	108.98
45	5	310	KC2	O1D-CGD-CBD	-2.05	120.28	124.48
31	B	606	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
31	19	312	CLA	O1D-CGD-CBD	2.05	128.68	124.48
31	P	605	CLA	C3C-C4C-NC	-2.05	108.27	110.57
43	p	613	A86	C7-C6-C8	2.05	121.31	118.08
43	17	316	A86	C-C1-C24	2.05	121.31	118.08
43	12	306	A86	C21-C20-C19	2.05	116.59	114.28
31	a	403	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
31	5	311	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
31	11	308	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
31	C	503	CLA	C1-C2-C3	-2.05	122.49	126.04
43	14	302	A86	C-C1-C2	-2.05	120.05	122.92
36	4	317	LHG	C18-C17-C16	-2.05	104.01	114.42
31	B	616	CLA	C2A-C1A-CHA	2.05	127.45	123.86
31	B	602	CLA	C3A-C2A-C1A	2.05	104.41	101.34
31	8	306	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	p	605	CLA	C3C-C4C-NC	-2.05	108.27	110.57
43	P	611	A86	C23-C16-C17	-2.05	105.42	108.98
31	18	306	CLA	C2D-C1D-ND	-2.05	108.59	110.10
42	19	314	KC1	C2A-C3A-C4A	2.05	108.01	106.49
42	1	314	KC1	C1C-C2C-C3C	-2.05	104.80	106.96
43	p	611	A86	C4-C3-C2	-2.05	119.28	123.47
38	M	101	LMG	O8-C28-O10	-2.05	118.42	123.59
31	15	306	CLA	C3A-C2A-C1A	2.05	104.41	101.34
31	0	308	CLA	O2D-CGD-CBD	2.05	114.91	111.27
43	10	306	A86	C26-C25-C24	-2.05	116.82	123.22
43	3	306	A86	C9-C10-C11	-2.05	120.58	126.61
43	11	304	A86	O2-C18-C19	-2.05	105.73	109.80
33	C	517	BCR	C30-C25-C26	-2.05	119.73	122.61
43	0	301	A86	C4-C3-C2	-2.05	119.28	123.47
31	a	404	CLA	C3A-C2A-C1A	2.05	104.41	101.34
43	9	303	A86	O4-C34-C35	2.05	112.69	107.59
43	7	301	A86	C25-C24-C1	-2.05	120.66	126.42
31	p	602	CLA	C11-C10-C8	-2.05	109.30	115.92
42	P	609	KC1	C2B-C1B-NB	2.05	111.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	18	302	A86	C33-C32-C31	-2.05	107.22	109.21
45	5	308	KC2	CGD-CBD-CAD	-2.05	104.10	110.73
43	18	304	A86	C22-C16-C17	-2.05	105.43	108.98
43	8	302	A86	C3-C4-C5	-2.05	119.28	123.47
43	P	613	A86	C7-C6-C8	2.05	121.30	118.08
31	P	602	CLA	C11-C10-C8	-2.05	109.30	115.92
45	6	310	KC2	CED-O2D-CGD	2.05	120.57	115.94
31	12	307	CLA	CHA-C1A-NA	-2.05	121.71	126.40
45	2	308	KC2	CHC-C1C-C2C	2.05	128.18	124.98
43	18	304	A86	O1-C20-C21	-2.05	112.60	115.06
31	P	604	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
31	b	604	CLA	CHC-C1C-NC	2.05	127.31	124.20
31	b	613	CLA	C2A-C1A-CHA	2.05	127.44	123.86
43	6	301	A86	C14-C15-C16	2.05	126.59	118.75
31	4	307	CLA	CAA-C2A-C3A	-2.05	107.18	112.78
43	13	301	A86	C40-C32-C33	2.05	118.23	109.05
45	17	311	KC2	CBB-CAB-C3B	-2.04	117.45	127.62
39	c	518	DGD	O3G-C1D-C2D	-2.04	105.11	108.30
42	3	314	KC1	CED-O2D-CGD	2.04	120.56	115.94
43	17	316	A86	C9-C10-C11	-2.04	120.60	126.61
31	17	313	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
43	18	304	A86	C24-C1-C2	2.04	122.08	118.94
43	3	303	A86	C23-C16-C22	2.04	110.38	107.37
43	11	305	A86	O4-C38-O5	-2.04	118.90	122.96
31	B	616	CLA	C3C-C4C-NC	-2.04	108.28	110.57
31	5	309	CLA	C2D-C1D-ND	-2.04	108.60	110.10
31	B	608	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
31	c	504	CLA	CHA-C4D-ND	2.04	136.77	132.50
31	17	315	CLA	O2D-CGD-CBD	2.04	114.90	111.27
43	5	304	A86	C25-C26-C27	-2.04	124.40	127.31
43	5	301	A86	C8-C6-C5	2.04	122.07	118.94
34	0	318	SQD	O47-C7-C8	2.04	115.90	111.50
31	4	311	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	18	306	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	p	608	CLA	C2D-C1D-ND	-2.04	108.60	110.10
42	17	314	KC1	C2B-C1B-NB	2.04	111.61	110.10
45	6	312	KC2	O1D-CGD-CBD	-2.04	120.31	124.48
43	8	302	A86	C14-C15-C16	-2.04	110.94	118.75
31	P	608	CLA	CHC-C1C-NC	2.04	127.30	124.20
31	0	311	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
42	10	315	KC1	C1C-C2C-C3C	-2.04	104.81	106.96
43	19	303	A86	C23-C16-C17	-2.04	105.44	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	605	CLA	O2D-CGD-CBD	2.04	114.89	111.27
31	P	606	CLA	CHD-C4C-C3C	2.04	127.84	124.84
31	10	311	CLA	C2A-C1A-CHA	2.04	127.42	123.86
31	13	315	CLA	C2D-C1D-ND	-2.04	108.60	110.10
31	15	307	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	6	313	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
31	11	312	CLA	C2D-C1D-ND	-2.04	108.60	110.10
45	0	310	KC2	C2B-C1B-NB	2.04	111.61	110.10
43	17	303	A86	C10-C9-C8	-2.04	116.86	123.22
31	5	312	CLA	CGD-CBD-CAD	2.04	117.33	110.73
31	17	313	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
38	F	102	LMG	O1-C7-C8	-2.04	105.98	110.90
31	d	404	CLA	CHB-C4A-NA	2.04	127.33	124.51
45	16	312	KC2	C3D-CAD-CBD	-2.04	104.92	107.61
45	18	308	KC2	C2A-C1A-CHA	-2.04	120.71	127.44
45	12	309	KC2	CAB-C3B-C4B	-2.04	119.98	124.90
31	17	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
36	l	102	LHG	O8-C23-O10	-2.04	118.45	123.59
38	10	319	LMG	O6-C1-O1	-2.04	105.15	109.97
31	C	504	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	d	401	CLA	CMC-C2C-C3C	2.04	131.64	126.12
31	3	307	CLA	CHD-C1D-ND	-2.03	122.58	124.45
31	13	307	CLA	C3C-C4C-NC	-2.03	108.29	110.57
31	b	609	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
31	P	610	CLA	O2D-CGD-CBD	2.03	114.88	111.27
39	C	518	DGD	O3G-C1D-C2D	-2.03	105.13	108.30
45	1	311	KC2	C3C-C2C-C1C	-2.03	104.98	106.49
31	13	313	CLA	CAC-C3C-C4C	2.03	127.45	124.81
45	12	309	KC2	CBA-CAA-C2A	-2.03	117.52	125.27
43	4	302	A86	C-C1-C24	2.03	121.28	118.08
34	0	318	SQD	C1-C2-C3	2.03	114.23	110.00
33	B	617	BCR	C38-C26-C27	-2.03	109.71	113.62
43	6	305	A86	C9-C10-C11	-2.03	120.63	126.61
31	P	605	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
31	18	307	CLA	C5-C3-C2	-2.03	117.00	121.12
33	b	618	BCR	C28-C27-C26	-2.03	110.45	114.08
31	2	311	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
31	19	312	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
31	3	308	CLA	CAC-C3C-C4C	2.03	127.45	124.81
31	7	313	CLA	CGD-CBD-CAD	2.03	117.32	110.73
33	b	618	BCR	C38-C26-C27	-2.03	109.71	113.62
31	D	404	CLA	CHB-C4A-NA	2.03	127.32	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	602	CLA	CHB-C4A-NA	2.03	127.32	124.51
43	13	303	A86	C9-C10-C11	-2.03	120.63	126.61
45	16	310	KC2	CED-O2D-CGD	2.03	120.53	115.94
31	c	508	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
43	9	302	A86	C36-C31-C32	-2.03	117.68	119.70
31	C	508	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
31	c	514	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
31	P	601	CLA	CHB-C4A-NA	2.03	127.32	124.51
31	6	314	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
31	0	311	CLA	C2A-C1A-CHA	2.03	127.41	123.86
31	5	309	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	19	313	CLA	O1D-CGD-CBD	2.03	128.64	124.48
31	C	513	CLA	O2D-CGD-CBD	2.03	114.87	111.27
39	C	520	DGD	C5B-C4B-C3B	-2.03	104.12	114.42
31	p	610	CLA	O2D-CGD-CBD	2.03	114.87	111.27
36	L	101	LHG	O8-C23-O10	-2.03	118.47	123.59
45	14	310	KC2	CAA-CBA-CGA	-2.03	116.84	127.26
43	3	302	A86	C40-C32-C33	2.03	118.16	109.05
43	3	306	A86	C12-C11-C13	2.03	119.43	116.02
38	M	101	LMG	C9-C8-C7	-2.03	106.99	111.79
39	c	520	DGD	C5B-C4B-C3B	-2.03	104.13	114.42
31	b	616	CLA	C11-C10-C8	-2.03	109.36	115.92
31	B	611	CLA	O2D-CGD-CBD	2.03	114.87	111.27
31	b	608	CLA	O2D-CGD-CBD	2.03	114.87	111.27
31	4	314	CLA	C2D-C1D-ND	-2.03	108.61	110.10
43	8	303	A86	O5-C38-C39	-2.03	117.42	124.81
31	12	313	CLA	CHA-C4D-ND	2.03	136.74	132.50
43	8	304	A86	O2-C18-C17	2.03	113.83	109.80
31	b	603	CLA	C3A-C2A-C1A	2.03	104.37	101.34
31	0	314	CLA	CHA-C4D-ND	2.03	136.74	132.50
43	18	303	A86	C34-O4-C38	-2.03	114.12	117.90
43	2	302	A86	C4-C3-C2	-2.03	119.33	123.47
31	B	602	CLA	CMC-C2C-C3C	2.03	131.62	126.12
31	b	608	CLA	CHD-C1D-ND	-2.03	122.59	124.45
31	C	504	CLA	CHA-C4D-ND	2.03	136.74	132.50
31	0	312	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
43	P	611	A86	C4-C3-C2	-2.02	119.33	123.47
42	17	314	KC1	C2A-C3A-C4A	2.02	107.99	106.49
43	7	306	A86	C9-C8-C6	-2.02	120.73	126.42
31	6	316	CLA	C2A-C1A-CHA	2.02	127.40	123.86
31	8	312	CLA	C3D-C2D-C1D	2.02	108.59	105.83
43	6	307	A86	C10-C9-C8	-2.02	116.90	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	19	304	A86	C25-C24-C1	-2.02	120.73	126.42
45	17	311	KC2	CAB-C3B-C4B	-2.02	120.01	124.90
43	8	304	A86	C25-C24-C1	-2.02	120.73	126.42
33	b	620	BCR	C1-C6-C5	-2.02	119.77	122.61
31	12	307	CLA	CHD-C1D-C2D	2.02	129.72	125.48
38	D	403	LMG	C8-O7-C10	2.02	122.77	117.79
31	3	307	CLA	C2D-C1D-ND	-2.02	108.61	110.10
43	5	304	A86	C23-C16-C17	-2.02	105.47	108.98
43	14	304	A86	C40-C32-C33	2.02	118.13	109.05
33	B	617	BCR	C28-C27-C26	-2.02	110.47	114.08
31	B	603	CLA	CHC-C1C-NC	2.02	127.27	124.20
38	w	201	LMG	O1-C7-C8	2.02	115.78	110.90
43	18	301	A86	C36-C31-C32	-2.02	117.69	119.70
31	C	514	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
36	Z	103	LHG	O10-C23-C24	-2.02	115.85	123.73
45	11	309	KC2	CBD-CHA-C1A	2.02	132.65	128.88
42	4	313	KC1	C2A-C1A-CHA	-2.02	120.76	127.44
31	18	306	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
34	A	408	SQD	O47-C7-O49	-2.02	118.82	123.70
31	B	605	CLA	CHD-C4C-NC	2.02	127.39	124.20
43	2	304	A86	O3-C36-C37	-2.02	105.80	109.39
39	h	102	DGD	O5E-C6E-C5E	-2.02	104.36	111.29
35	d	406	PL9	C11-C12-C13	-2.02	105.24	111.88
43	11	320	A86	C20-C19-C18	2.02	116.74	112.75
31	p	608	CLA	CHC-C1C-NC	2.02	127.27	124.20
33	b	619	BCR	C30-C25-C26	-2.02	119.77	122.61
45	6	312	KC2	C3D-CAD-CBD	-2.02	104.95	107.61
38	5	315	LMG	O2-C2-C3	-2.02	105.68	110.35
31	3	312	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
31	4	312	CLA	CGD-CBD-CAD	-2.02	104.20	110.73
43	8	303	A86	C9-C10-C11	-2.02	120.67	126.61
45	15	308	KC2	CGD-CBD-CAD	-2.02	104.20	110.73
31	2	315	CLA	CHD-C1D-ND	-2.02	122.60	124.45
43	3	302	A86	C20-C19-C18	2.02	116.74	112.75
31	c	504	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
31	p	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
33	Y	101	BCR	C30-C25-C26	-2.02	119.77	122.61
31	b	607	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
31	B	610	CLA	O2D-CGD-CBD	2.02	114.85	111.27
31	2	314	CLA	C2A-C1A-CHA	2.02	127.37	123.85
31	C	507	CLA	O1D-CGD-CBD	2.02	128.61	124.48
31	7	310	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Z	102	LMG	O3-C3-C2	-2.02	105.69	110.35
43	18	301	A86	C35-C34-C33	-2.01	106.36	109.88
43	4	301	A86	C12-C11-C13	2.01	119.41	116.02
31	b	617	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
31	b	606	CLA	CHB-C4A-NA	2.01	127.30	124.51
31	15	312	CLA	C4D-CHA-C1A	2.01	123.70	121.25
31	1	312	CLA	CMD-C2D-C3D	2.01	132.25	127.61
31	B	609	CLA	C2A-C1A-CHA	2.01	127.38	123.86
43	16	306	A86	C41-C32-C33	2.01	118.09	109.05
43	7	302	A86	C28-C27-C29	2.01	123.59	118.93
45	16	310	KC2	CHC-C1C-C2C	2.01	128.12	124.98
31	15	313	CLA	CHA-C4D-ND	2.01	136.71	132.50
31	7	310	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
35	D	406	PL9	C11-C12-C13	-2.01	105.27	111.88
31	r	101	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
44	P	612	DD6	C3-C4-C5	-2.01	119.35	123.47
39	H	102	DGD	O5E-C6E-C5E	-2.01	104.39	111.29
43	2	303	A86	O3-C36-C37	-2.01	105.81	109.39
43	11	303	A86	O3-C36-C37	-2.01	105.81	109.39
39	C	518	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
39	c	518	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
31	b	617	CLA	CHA-C1A-NA	-2.01	121.79	126.40
41	e	101	HEM	C4B-CHC-C1C	2.01	125.21	122.56
31	b	612	CLA	O2D-CGD-CBD	2.01	114.84	111.27
31	B	603	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
38	f	102	LMG	O1-C7-C8	-2.01	106.05	110.90
31	b	603	CLA	CMC-C2C-C3C	2.01	131.57	126.12
43	3	305	A86	C9-C8-C6	-2.01	120.77	126.42
38	W	201	LMG	O1-C7-C8	2.01	115.75	110.90
31	0	316	CLA	C3A-C2A-C1A	2.01	104.35	101.34
31	b	606	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
43	19	306	A86	C7-C6-C8	2.01	121.24	118.08
42	9	314	KC1	C3A-C4A-NA	2.01	112.77	110.57
36	14	317	LHG	O8-C6-C5	-2.01	102.59	108.43
31	c	506	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
41	e	101	HEM	C3B-C2B-C1B	2.01	107.98	106.49
31	14	311	CLA	CHA-C1A-NA	-2.01	121.80	126.40
39	C	518	DGD	O2E-C2E-C1E	-2.01	105.17	110.05
31	6	309	CLA	C11-C12-C13	-2.01	109.43	115.92
43	2	304	A86	C7-C6-C8	2.01	121.24	118.08
31	c	513	CLA	O2D-CGD-CBD	2.01	114.83	111.27
31	c	508	CLA	CAA-C2A-C3A	-2.01	107.28	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	18	313	KC1	C2A-C1A-CHA	-2.01	120.80	127.44
31	b	607	CLA	CHC-C1C-NC	2.01	127.25	124.20
31	c	507	CLA	O1D-CGD-CBD	2.01	128.59	124.48
31	C	506	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	B	601	CLA	CAA-C2A-C1A	2.01	118.55	111.97
43	7	303	A86	C36-C31-C32	-2.01	117.70	119.70
31	16	309	CLA	C11-C12-C13	-2.01	109.44	115.92
33	Y	101	BCR	C31-C1-C6	2.01	113.55	110.30
31	12	312	CLA	O1D-CGD-CBD	2.01	128.59	124.48
31	D	401	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
42	p	609	KC1	CED-O2D-CGD	2.01	120.47	115.94
43	2	303	A86	C26-C25-C24	-2.00	116.96	123.22
43	2	305	A86	O-C13-C14	2.00	125.73	121.66
38	n	701	LMG	O6-C1-C2	-2.00	106.11	110.35
31	14	306	CLA	CHD-C1D-C2D	2.00	129.68	125.48
45	10	310	KC2	O1D-CGD-CBD	-2.00	120.38	124.48
31	b	604	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
31	14	311	CLA	CHA-C4D-ND	2.00	136.69	132.50
33	C	516	BCR	C2-C1-C6	2.00	113.57	110.48
43	11	303	A86	C3-C4-C5	-2.00	119.37	123.47
39	c	520	DGD	O5E-C6E-C5E	-2.00	104.42	111.29
31	C	513	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	b	617	CLA	CHD-C1D-ND	-2.00	122.61	124.45
43	8	301	A86	O2-C18-C17	-2.00	105.82	109.80
31	b	610	CLA	C2A-C1A-CHA	2.00	127.36	123.86
32	D	402	PHO	O1D-CGD-CBD	2.00	128.07	124.74
45	6	312	KC2	CMB-C2B-C1B	2.00	128.24	124.71
31	3	316	CLA	C2A-C1A-CHA	2.00	127.36	123.86
45	18	310	KC2	C3C-C2C-C1C	-2.00	105.00	106.49
43	2	302	A86	C40-C32-C33	2.00	118.04	109.05
31	19	308	CLA	CMC-C2C-C1C	2.00	128.09	125.04
43	18	303	A86	C41-C32-C31	-2.00	108.68	110.47
43	18	301	A86	C10-C9-C8	-2.00	116.97	123.22
43	12	306	A86	C-C1-C24	2.00	121.23	118.08
36	z	102	LHG	O10-C23-C24	-2.00	115.92	123.73
31	c	505	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
31	3	308	CLA	O2D-CGD-O1D	-2.00	119.93	123.84
31	P	605	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
31	18	307	CLA	C4-C3-C5	2.00	118.64	115.27
38	c	522	LMG	O3-C3-C2	-2.00	105.72	110.35
31	8	309	CLA	CHD-C1D-ND	-2.00	122.62	124.45
31	7	313	CLA	C3C-C4C-NC	-2.00	108.33	110.57

All (204) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	403	CLA	ND
31	A	404	CLA	ND
31	A	406	CLA	ND
31	B	601	CLA	ND
31	B	602	CLA	ND
31	B	603	CLA	ND
31	B	604	CLA	ND
31	B	605	CLA	ND
31	B	606	CLA	ND
31	B	607	CLA	ND
31	B	608	CLA	ND
31	B	611	CLA	ND
31	B	612	CLA	ND
31	B	613	CLA	ND
31	B	614	CLA	ND
31	B	615	CLA	ND
31	B	616	CLA	ND
31	C	502	CLA	ND
31	C	503	CLA	ND
31	C	504	CLA	ND
31	C	505	CLA	ND
31	C	506	CLA	ND
31	C	507	CLA	ND
31	C	508	CLA	ND
31	C	509	CLA	ND
31	C	510	CLA	ND
31	C	511	CLA	ND
31	C	512	CLA	ND
31	C	513	CLA	ND
31	C	514	CLA	ND
31	D	401	CLA	ND
31	D	404	CLA	ND
31	D	405	CLA	ND
31	P	601	CLA	ND
31	P	602	CLA	ND
31	P	603	CLA	ND
31	P	604	CLA	ND
31	P	605	CLA	ND
31	P	606	CLA	ND
31	P	607	CLA	ND
31	P	608	CLA	ND
31	P	610	CLA	ND

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Mol	Chain	Res	Type	Atom
31	R	101	CLA	ND
31	W	202	CLA	ND
31	Z	101	CLA	ND
31	a	403	CLA	ND
31	a	404	CLA	ND
31	a	406	CLA	ND
31	b	602	CLA	ND
31	b	603	CLA	ND
31	b	604	CLA	ND
31	b	605	CLA	ND
31	b	606	CLA	ND
31	b	607	CLA	ND
31	b	608	CLA	ND
31	b	609	CLA	ND
31	b	612	CLA	ND
31	b	613	CLA	ND
31	b	614	CLA	ND
31	b	615	CLA	ND
31	b	616	CLA	ND
31	b	617	CLA	ND
31	c	502	CLA	ND
31	c	503	CLA	ND
31	c	504	CLA	ND
31	c	505	CLA	ND
31	c	506	CLA	ND
31	c	507	CLA	ND
31	c	508	CLA	ND
31	c	509	CLA	ND
31	c	510	CLA	ND
31	c	511	CLA	ND
31	c	512	CLA	ND
31	c	513	CLA	ND
31	c	514	CLA	ND
31	d	401	CLA	ND
31	d	404	CLA	ND
31	d	405	CLA	ND
31	p	601	CLA	ND
31	p	602	CLA	ND
31	p	603	CLA	ND
31	p	604	CLA	ND
31	p	605	CLA	ND
31	p	606	CLA	ND

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Mol	Chain	Res	Type	Atom
31	p	607	CLA	ND
31	p	608	CLA	ND
31	p	610	CLA	ND
31	r	101	CLA	ND
31	w	203	CLA	ND
31	z	101	CLA	ND
31	z	103	CLA	ND
31	0	307	CLA	ND
31	0	308	CLA	ND
31	0	311	CLA	ND
31	0	312	CLA	ND
31	0	313	CLA	ND
31	0	316	CLA	ND
31	1	307	CLA	ND
31	1	310	CLA	ND
31	1	312	CLA	ND
31	1	313	CLA	ND
31	1	316	CLA	ND
31	1	321	CLA	ND
31	2	306	CLA	ND
31	2	307	CLA	ND
31	2	309	CLA	ND
31	3	307	CLA	ND
31	3	308	CLA	ND
31	3	310	CLA	ND
31	3	313	CLA	ND
31	3	315	CLA	ND
31	4	307	CLA	ND
31	4	309	CLA	ND
31	4	311	CLA	ND
31	4	312	CLA	ND
31	4	314	CLA	ND
31	4	315	CLA	ND
31	5	306	CLA	ND
31	5	307	CLA	ND
31	5	309	CLA	ND
31	5	311	CLA	ND
31	5	314	CLA	ND
31	6	308	CLA	ND
31	6	309	CLA	ND
31	6	311	CLA	ND
31	6	313	CLA	ND

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Mol	Chain	Res	Type	Atom
31	6	314	CLA	ND
31	6	316	CLA	ND
31	7	307	CLA	ND
31	7	310	CLA	ND
31	7	312	CLA	ND
31	7	313	CLA	ND
31	7	315	CLA	ND
31	8	306	CLA	ND
31	8	307	CLA	ND
31	8	309	CLA	ND
31	8	312	CLA	ND
31	8	314	CLA	ND
31	9	307	CLA	ND
31	9	308	CLA	ND
31	9	310	CLA	ND
31	9	311	CLA	ND
31	9	312	CLA	ND
31	9	313	CLA	ND
31	9	315	CLA	ND
31	10	307	CLA	ND
31	10	308	CLA	ND
31	10	311	CLA	ND
31	10	312	CLA	ND
31	10	313	CLA	ND
31	10	314	CLA	ND
31	10	316	CLA	ND
31	10	317	CLA	ND
31	11	307	CLA	ND
31	11	308	CLA	ND
31	11	310	CLA	ND
31	11	312	CLA	ND
31	11	313	CLA	ND
31	11	315	CLA	ND
31	11	316	CLA	ND
31	12	307	CLA	ND
31	12	308	CLA	ND
31	12	310	CLA	ND
31	12	312	CLA	ND
31	12	316	CLA	ND
31	13	307	CLA	ND
31	13	308	CLA	ND
31	13	310	CLA	ND

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Mol	Chain	Res	Type	Atom
31	13	312	CLA	ND
31	14	306	CLA	ND
31	14	307	CLA	ND
31	14	309	CLA	ND
31	14	311	CLA	ND
31	14	312	CLA	ND
31	14	314	CLA	ND
31	14	315	CLA	ND
31	15	306	CLA	ND
31	15	307	CLA	ND
31	15	309	CLA	ND
31	15	311	CLA	ND
31	15	313	CLA	ND
31	16	308	CLA	ND
31	16	309	CLA	ND
31	16	311	CLA	ND
31	16	313	CLA	ND
31	16	314	CLA	ND
31	16	316	CLA	ND
31	17	307	CLA	ND
31	17	310	CLA	ND
31	17	312	CLA	ND
31	17	313	CLA	ND
31	17	315	CLA	ND
31	18	306	CLA	ND
31	18	307	CLA	ND
31	18	309	CLA	ND
31	18	312	CLA	ND
31	18	314	CLA	ND
31	19	307	CLA	ND
31	19	308	CLA	ND
31	19	310	CLA	ND
31	19	311	CLA	ND
31	19	312	CLA	ND
31	19	313	CLA	ND
31	19	315	CLA	ND

All (5474) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	403	CLA	CBD-CGD-O2D-CED
31	B	601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C3A-C2A-CAA-CBA
31	B	601	CLA	CHA-CBD-CGD-O1D
31	B	601	CLA	CHA-CBD-CGD-O2D
31	B	601	CLA	CAD-CBD-CGD-O1D
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	C3A-C2A-CAA-CBA
31	B	602	CLA	C4-C3-C5-C6
31	B	604	CLA	C14-C13-C15-C16
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	C2A-CAA-CBA-CGA
31	B	609	CLA	CHA-CBD-CGD-O1D
31	B	609	CLA	CHA-CBD-CGD-O2D
31	B	609	CLA	CAD-CBD-CGD-O1D
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C3A-C2A-CAA-CBA
31	B	614	CLA	CHA-CBD-CGD-O1D
31	B	614	CLA	CHA-CBD-CGD-O2D
31	B	614	CLA	CAD-CBD-CGD-O1D
31	B	616	CLA	C1A-C2A-CAA-CBA
31	B	616	CLA	CBD-CGD-O2D-CED
31	C	502	CLA	CHA-CBD-CGD-O1D
31	C	502	CLA	CHA-CBD-CGD-O2D
31	C	504	CLA	C11-C10-C8-C7
31	C	505	CLA	CBD-CGD-O2D-CED
31	C	507	CLA	C1A-C2A-CAA-CBA
31	C	507	CLA	CHA-CBD-CGD-O1D
31	C	507	CLA	CHA-CBD-CGD-O2D
31	C	507	CLA	CAD-CBD-CGD-O1D
31	C	507	CLA	CAD-CBD-CGD-O2D
31	D	401	CLA	CHA-CBD-CGD-O1D
31	D	401	CLA	CHA-CBD-CGD-O2D
31	D	405	CLA	C2-C3-C5-C6
31	D	405	CLA	C4-C3-C5-C6
31	P	601	CLA	CHA-CBD-CGD-O1D
31	P	601	CLA	CAD-CBD-CGD-O1D
31	P	601	CLA	CAD-CBD-CGD-O2D
31	P	601	CLA	CBD-CGD-O2D-CED
31	P	602	CLA	CHA-CBD-CGD-O1D
31	P	602	CLA	CHA-CBD-CGD-O2D
31	P	603	CLA	CHA-CBD-CGD-O1D
31	P	604	CLA	CBD-CGD-O2D-CED
31	P	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	P	606	CLA	CBD-CGD-O2D-CED
31	P	608	CLA	CBD-CGD-O2D-CED
31	W	202	CLA	C2A-CAA-CBA-CGA
31	W	202	CLA	CHA-CBD-CGD-O1D
31	W	202	CLA	CHA-CBD-CGD-O2D
31	Z	101	CLA	C2-C3-C5-C6
31	Z	101	CLA	C4-C3-C5-C6
31	a	403	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C3A-C2A-CAA-CBA
31	b	602	CLA	CHA-CBD-CGD-O1D
31	b	602	CLA	CHA-CBD-CGD-O2D
31	b	602	CLA	CAD-CBD-CGD-O1D
31	b	602	CLA	C14-C13-C15-C16
31	b	603	CLA	C1A-C2A-CAA-CBA
31	b	603	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C4-C3-C5-C6
31	b	605	CLA	C14-C13-C15-C16
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	C2A-CAA-CBA-CGA
31	b	610	CLA	CHA-CBD-CGD-O1D
31	b	610	CLA	CHA-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	613	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	b	615	CLA	CHA-CBD-CGD-O1D
31	b	615	CLA	CHA-CBD-CGD-O2D
31	b	615	CLA	CAD-CBD-CGD-O1D
31	b	617	CLA	C1A-C2A-CAA-CBA
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	502	CLA	CHA-CBD-CGD-O1D
31	c	502	CLA	CHA-CBD-CGD-O2D
31	c	504	CLA	C11-C10-C8-C7
31	c	505	CLA	CBD-CGD-O2D-CED
31	c	507	CLA	C1A-C2A-CAA-CBA
31	c	507	CLA	CHA-CBD-CGD-O1D
31	c	507	CLA	CHA-CBD-CGD-O2D
31	c	507	CLA	CAD-CBD-CGD-O1D
31	c	507	CLA	CAD-CBD-CGD-O2D
31	d	401	CLA	CHA-CBD-CGD-O1D
31	d	401	CLA	CHA-CBD-CGD-O2D
31	d	405	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	d	405	CLA	C4-C3-C5-C6
31	p	601	CLA	CHA-CBD-CGD-O1D
31	p	601	CLA	CAD-CBD-CGD-O1D
31	p	601	CLA	CAD-CBD-CGD-O2D
31	p	601	CLA	CBD-CGD-O2D-CED
31	p	602	CLA	CHA-CBD-CGD-O1D
31	p	602	CLA	CHA-CBD-CGD-O2D
31	p	603	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CBD-CGD-O2D-CED
31	p	606	CLA	C1A-C2A-CAA-CBA
31	p	606	CLA	CBD-CGD-O2D-CED
31	p	608	CLA	CBD-CGD-O2D-CED
31	p	608	CLA	O1D-CGD-O2D-CED
31	w	203	CLA	C2A-CAA-CBA-CGA
31	w	203	CLA	CHA-CBD-CGD-O1D
31	w	203	CLA	CHA-CBD-CGD-O2D
31	z	101	CLA	C2-C3-C5-C6
31	z	101	CLA	C4-C3-C5-C6
31	z	103	CLA	CBD-CGD-O2D-CED
31	0	308	CLA	CHA-CBD-CGD-O1D
31	0	308	CLA	CHA-CBD-CGD-O2D
31	0	309	CLA	CHA-CBD-CGD-O1D
31	0	312	CLA	CBA-CGA-O2A-C1
31	0	312	CLA	O1A-CGA-O2A-C1
31	0	313	CLA	C1A-C2A-CAA-CBA
31	0	313	CLA	C3A-C2A-CAA-CBA
31	0	313	CLA	CHA-CBD-CGD-O1D
31	0	313	CLA	CHA-CBD-CGD-O2D
31	0	314	CLA	C1A-C2A-CAA-CBA
31	0	314	CLA	C3A-C2A-CAA-CBA
31	0	316	CLA	CBD-CGD-O2D-CED
31	1	308	CLA	CBD-CGD-O2D-CED
31	1	312	CLA	C1A-C2A-CAA-CBA
31	1	312	CLA	CBA-CGA-O2A-C1
31	1	312	CLA	O1A-CGA-O2A-C1
31	1	316	CLA	C1A-C2A-CAA-CBA
31	1	321	CLA	CHA-CBD-CGD-O1D
31	1	321	CLA	CHA-CBD-CGD-O2D
31	2	306	CLA	CAD-CBD-CGD-O2D
31	2	307	CLA	C1A-C2A-CAA-CBA
31	2	307	CLA	C2-C3-C5-C6
31	2	307	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	2	309	CLA	C1A-C2A-CAA-CBA
31	2	309	CLA	CBD-CGD-O2D-CED
31	2	312	CLA	CBD-CGD-O2D-CED
31	2	314	CLA	CHA-CBD-CGD-O2D
31	2	315	CLA	C1A-C2A-CAA-CBA
31	3	308	CLA	C1A-C2A-CAA-CBA
31	3	310	CLA	CBD-CGD-O2D-CED
31	3	312	CLA	C1A-C2A-CAA-CBA
31	3	313	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	C1A-C2A-CAA-CBA
31	3	315	CLA	C3A-C2A-CAA-CBA
31	3	315	CLA	CHA-CBD-CGD-O1D
31	3	315	CLA	CHA-CBD-CGD-O2D
31	3	316	CLA	C1A-C2A-CAA-CBA
31	3	316	CLA	C3A-C2A-CAA-CBA
31	3	316	CLA	C11-C12-C13-C14
31	4	311	CLA	C1A-C2A-CAA-CBA
31	4	311	CLA	C3A-C2A-CAA-CBA
31	4	315	CLA	C1A-C2A-CAA-CBA
31	4	315	CLA	CBD-CGD-O2D-CED
31	5	306	CLA	C1A-C2A-CAA-CBA
31	5	306	CLA	CHA-CBD-CGD-O1D
31	5	306	CLA	CHA-CBD-CGD-O2D
31	5	307	CLA	C1A-C2A-CAA-CBA
31	5	307	CLA	C2-C3-C5-C6
31	5	307	CLA	C4-C3-C5-C6
31	5	309	CLA	CHA-CBD-CGD-O1D
31	5	311	CLA	CHA-CBD-CGD-O1D
31	5	311	CLA	CHA-CBD-CGD-O2D
31	5	312	CLA	CBD-CGD-O2D-CED
31	6	308	CLA	C1A-C2A-CAA-CBA
31	6	308	CLA	C3A-C2A-CAA-CBA
31	6	308	CLA	CAD-CBD-CGD-O2D
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	313	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	CBD-CGD-O2D-CED
31	7	307	CLA	CAD-CBD-CGD-O2D
31	7	310	CLA	CBD-CGD-O2D-CED
31	7	312	CLA	C1A-C2A-CAA-CBA
31	7	313	CLA	CBD-CGD-O2D-CED
31	8	307	CLA	C2-C3-C5-C6
31	8	307	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	8	309	CLA	CBD-CGD-O2D-CED
31	8	311	CLA	C1A-C2A-CAA-CBA
31	8	311	CLA	CBA-CGA-O2A-C1
31	8	312	CLA	C1A-C2A-CAA-CBA
31	8	312	CLA	CBD-CGD-O2D-CED
31	8	314	CLA	CHA-CBD-CGD-O1D
31	8	314	CLA	CHA-CBD-CGD-O2D
31	9	308	CLA	O2A-C1-C2-C3
31	9	308	CLA	C2-C3-C5-C6
31	9	308	CLA	C4-C3-C5-C6
31	9	308	CLA	C6-C7-C8-C9
31	9	311	CLA	C1A-C2A-CAA-CBA
31	9	313	CLA	C1A-C2A-CAA-CBA
31	10	308	CLA	CHA-CBD-CGD-O2D
31	10	312	CLA	CBA-CGA-O2A-C1
31	10	312	CLA	O1A-CGA-O2A-C1
31	10	313	CLA	C1A-C2A-CAA-CBA
31	10	313	CLA	C3A-C2A-CAA-CBA
31	10	313	CLA	CHA-CBD-CGD-O1D
31	10	313	CLA	CHA-CBD-CGD-O2D
31	10	314	CLA	C1A-C2A-CAA-CBA
31	10	316	CLA	CBD-CGD-O2D-CED
31	10	317	CLA	CBD-CGD-O2D-CED
31	11	308	CLA	C14-C13-C15-C16
31	11	310	CLA	CBD-CGD-O2D-CED
31	11	312	CLA	CBA-CGA-O2A-C1
31	12	310	CLA	C1A-C2A-CAA-CBA
31	12	310	CLA	CBD-CGD-O2D-CED
31	12	312	CLA	CHA-CBD-CGD-O1D
31	12	312	CLA	CHA-CBD-CGD-O2D
31	12	312	CLA	CBD-CGD-O2D-CED
31	12	312	CLA	O1D-CGD-O2D-CED
31	12	313	CLA	CBD-CGD-O2D-CED
31	13	310	CLA	CBD-CGD-O2D-CED
31	13	312	CLA	CHA-CBD-CGD-O1D
31	13	312	CLA	CHA-CBD-CGD-O2D
31	13	312	CLA	CBD-CGD-O2D-CED
31	13	313	CLA	CBA-CGA-O2A-C1
31	13	313	CLA	O1A-CGA-O2A-C1
31	13	313	CLA	CBD-CGD-O2D-CED
31	13	313	CLA	O2A-C1-C2-C3
31	13	315	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	13	316	CLA	C1A-C2A-CAA-CBA
31	13	316	CLA	C3A-C2A-CAA-CBA
31	13	316	CLA	CBD-CGD-O2D-CED
31	14	306	CLA	CHA-CBD-CGD-O1D
31	14	306	CLA	CHA-CBD-CGD-O2D
31	14	311	CLA	C1A-C2A-CAA-CBA
31	14	311	CLA	C3A-C2A-CAA-CBA
31	14	312	CLA	CBD-CGD-O2D-CED
31	14	315	CLA	C1A-C2A-CAA-CBA
31	14	315	CLA	CBD-CGD-O2D-CED
31	15	306	CLA	C1A-C2A-CAA-CBA
31	15	306	CLA	CHA-CBD-CGD-O1D
31	15	306	CLA	CHA-CBD-CGD-O2D
31	15	307	CLA	C1A-C2A-CAA-CBA
31	15	307	CLA	C2-C3-C5-C6
31	15	307	CLA	C4-C3-C5-C6
31	15	309	CLA	CHA-CBD-CGD-O1D
31	15	309	CLA	CHA-CBD-CGD-O2D
31	15	311	CLA	CHA-CBD-CGD-O1D
31	15	311	CLA	CHA-CBD-CGD-O2D
31	15	312	CLA	CBD-CGD-O2D-CED
31	16	308	CLA	C3A-C2A-CAA-CBA
31	16	309	CLA	C2-C3-C5-C6
31	16	309	CLA	C4-C3-C5-C6
31	16	311	CLA	CBD-CGD-O2D-CED
31	16	313	CLA	C1A-C2A-CAA-CBA
31	16	314	CLA	C1A-C2A-CAA-CBA
31	16	314	CLA	CBD-CGD-O2D-CED
31	16	314	CLA	O1D-CGD-O2D-CED
31	16	316	CLA	CHA-CBD-CGD-O1D
31	16	316	CLA	CHA-CBD-CGD-O2D
31	17	307	CLA	CAD-CBD-CGD-O2D
31	17	310	CLA	CBD-CGD-O2D-CED
31	17	312	CLA	C1A-C2A-CAA-CBA
31	17	313	CLA	C2A-CAA-CBA-CGA
31	17	315	CLA	CHA-CBD-CGD-O1D
31	17	315	CLA	CHA-CBD-CGD-O2D
31	18	306	CLA	CAD-CBD-CGD-O2D
31	18	311	CLA	CBD-CGD-O2D-CED
31	18	312	CLA	C1A-C2A-CAA-CBA
31	18	314	CLA	CHA-CBD-CGD-O1D
31	18	314	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	19	308	CLA	O2A-C1-C2-C3
31	19	308	CLA	C4-C3-C5-C6
31	19	311	CLA	C3A-C2A-CAA-CBA
31	19	313	CLA	C1A-C2A-CAA-CBA
33	A	407	BCR	C1-C6-C7-C8
33	A	407	BCR	C7-C8-C9-C34
33	A	407	BCR	C35-C13-C14-C15
33	A	407	BCR	C23-C24-C25-C30
33	B	617	BCR	C7-C8-C9-C34
33	B	617	BCR	C10-C11-C12-C13
33	B	617	BCR	C11-C12-C13-C14
33	B	618	BCR	C7-C8-C9-C10
33	B	618	BCR	C7-C8-C9-C34
33	B	619	BCR	C1-C6-C7-C8
33	B	619	BCR	C17-C18-C19-C20
33	B	619	BCR	C21-C22-C23-C24
33	B	619	BCR	C22-C23-C24-C25
33	C	516	BCR	C1-C6-C7-C8
33	C	516	BCR	C23-C24-C25-C26
33	C	517	BCR	C1-C6-C7-C8
33	C	517	BCR	C11-C12-C13-C14
33	F	101	BCR	C11-C12-C13-C14
33	F	101	BCR	C35-C13-C14-C15
33	F	101	BCR	C20-C21-C22-C23
33	F	101	BCR	C20-C21-C22-C37
33	F	101	BCR	C37-C22-C23-C24
33	F	101	BCR	C22-C23-C24-C25
33	H	101	BCR	C1-C6-C7-C8
33	H	101	BCR	C7-C8-C9-C10
33	H	101	BCR	C7-C8-C9-C34
33	Y	101	BCR	C10-C11-C12-C13
33	Y	101	BCR	C12-C13-C14-C15
33	Y	101	BCR	C35-C13-C14-C15
33	a	407	BCR	C1-C6-C7-C8
33	a	407	BCR	C7-C8-C9-C34
33	a	407	BCR	C35-C13-C14-C15
33	b	618	BCR	C7-C8-C9-C34
33	b	618	BCR	C10-C11-C12-C13
33	b	618	BCR	C11-C12-C13-C14
33	b	619	BCR	C7-C8-C9-C10
33	b	619	BCR	C7-C8-C9-C34
33	b	620	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	b	620	BCR	C17-C18-C19-C20
33	b	620	BCR	C21-C22-C23-C24
33	b	620	BCR	C22-C23-C24-C25
33	c	516	BCR	C1-C6-C7-C8
33	c	516	BCR	C23-C24-C25-C26
33	c	517	BCR	C1-C6-C7-C8
33	c	517	BCR	C11-C12-C13-C14
33	f	101	BCR	C11-C12-C13-C14
33	f	101	BCR	C35-C13-C14-C15
33	f	101	BCR	C20-C21-C22-C23
33	f	101	BCR	C20-C21-C22-C37
33	f	101	BCR	C37-C22-C23-C24
33	f	101	BCR	C22-C23-C24-C25
33	h	101	BCR	C1-C6-C7-C8
33	h	101	BCR	C7-C8-C9-C10
33	h	101	BCR	C7-C8-C9-C34
33	y	101	BCR	C10-C11-C12-C13
33	y	101	BCR	C12-C13-C14-C15
33	y	101	BCR	C35-C13-C14-C15
34	A	411	SQD	C2-C1-O6-C44
34	A	411	SQD	O5-C1-O6-C44
34	A	411	SQD	O49-C7-O47-C45
34	A	411	SQD	C8-C7-O47-C45
34	A	411	SQD	C5-C6-S-O7
34	A	411	SQD	C5-C6-S-O8
34	B	623	SQD	C2-C1-O6-C44
34	B	623	SQD	O5-C1-O6-C44
34	B	623	SQD	O49-C7-O47-C45
34	B	623	SQD	C8-C7-O47-C45
34	B	623	SQD	O5-C5-C6-S
34	L	102	SQD	C5-C6-S-O7
34	L	102	SQD	C5-C6-S-O8
34	L	102	SQD	C5-C6-S-O9
34	b	601	SQD	C2-C1-O6-C44
34	b	601	SQD	O5-C1-O6-C44
34	b	601	SQD	O49-C7-O47-C45
34	b	601	SQD	C8-C7-O47-C45
34	b	601	SQD	O5-C5-C6-S
34	i	101	SQD	C2-C1-O6-C44
34	i	101	SQD	O5-C1-O6-C44
34	i	101	SQD	O49-C7-O47-C45
34	i	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
34	i	101	SQD	C5-C6-S-O7
34	i	101	SQD	C5-C6-S-O8
34	l	101	SQD	C5-C6-S-O7
34	l	101	SQD	C5-C6-S-O8
34	l	101	SQD	C5-C6-S-O9
34	0	318	SQD	C2-C1-O6-C44
34	0	318	SQD	O5-C5-C6-S
34	0	318	SQD	C5-C6-S-O9
34	10	320	SQD	C2-C1-O6-C44
34	10	320	SQD	O5-C1-O6-C44
34	10	320	SQD	O5-C5-C6-S
34	10	320	SQD	C5-C6-S-O9
35	A	409	PL9	C12-C13-C14-C16
35	A	409	PL9	C17-C18-C19-C21
35	A	409	PL9	C22-C23-C24-C25
35	A	409	PL9	C22-C23-C24-C26
35	a	409	PL9	C12-C13-C14-C16
35	a	409	PL9	C17-C18-C19-C21
35	a	409	PL9	C22-C23-C24-C25
35	a	409	PL9	C22-C23-C24-C26
36	B	622	LHG	O1-C1-C2-O2
36	B	622	LHG	O1-C1-C2-C3
36	B	622	LHG	C3-O3-P-O4
36	B	622	LHG	C4-O6-P-O5
36	C	521	LHG	O1-C1-C2-C3
36	C	521	LHG	C3-O3-P-O4
36	C	521	LHG	C3-O3-P-O5
36	C	521	LHG	C3-O3-P-O6
36	C	521	LHG	C8-C7-O7-C5
36	D	407	LHG	O1-C1-C2-C3
36	D	407	LHG	C3-O3-P-O4
36	D	407	LHG	C3-O3-P-O5
36	L	101	LHG	O1-C1-C2-O2
36	L	101	LHG	O1-C1-C2-C3
36	L	101	LHG	C3-O3-P-O4
36	P	615	LHG	O1-C1-C2-O2
36	P	615	LHG	O1-C1-C2-C3
36	P	615	LHG	C3-O3-P-O4
36	Z	103	LHG	O1-C1-C2-O2
36	Z	103	LHG	O1-C1-C2-C3
36	Z	103	LHG	C4-O6-P-O5
36	b	623	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
36	b	623	LHG	O1-C1-C2-C3
36	b	623	LHG	C3-O3-P-O4
36	b	623	LHG	C4-O6-P-O5
36	d	407	LHG	O1-C1-C2-C3
36	d	407	LHG	C3-O3-P-O4
36	d	407	LHG	C3-O3-P-O5
36	l	102	LHG	O1-C1-C2-O2
36	l	102	LHG	O1-C1-C2-C3
36	l	102	LHG	C3-O3-P-O4
36	p	615	LHG	O1-C1-C2-O2
36	p	615	LHG	O1-C1-C2-C3
36	p	615	LHG	C3-O3-P-O4
36	w	202	LHG	O1-C1-C2-C3
36	w	202	LHG	C3-O3-P-O4
36	w	202	LHG	C3-O3-P-O5
36	w	202	LHG	C3-O3-P-O6
36	w	202	LHG	C8-C7-O7-C5
36	z	102	LHG	O1-C1-C2-O2
36	z	102	LHG	O1-C1-C2-C3
36	z	102	LHG	C4-O6-P-O5
36	4	317	LHG	O1-C1-C2-C3
36	4	317	LHG	C4-O6-P-O3
36	4	317	LHG	C4-O6-P-O5
36	4	317	LHG	C5-C4-O6-P
36	4	317	LHG	O9-C7-O7-C5
36	4	317	LHG	C8-C7-O7-C5
36	5	317	LHG	O1-C1-C2-O2
36	5	317	LHG	O1-C1-C2-C3
36	5	317	LHG	C3-O3-P-O5
36	5	317	LHG	C4-O6-P-O3
36	5	317	LHG	C4-O6-P-O5
36	8	315	LHG	C1-C2-C3-O3
36	8	315	LHG	C3-O3-P-O4
36	8	316	LHG	O1-C1-C2-C3
36	8	316	LHG	C4-O6-P-O3
36	8	316	LHG	C5-C4-O6-P
36	8	316	LHG	O9-C7-O7-C5
36	8	316	LHG	C8-C7-O7-C5
36	14	317	LHG	O1-C1-C2-C3
36	14	317	LHG	C4-O6-P-O3
36	14	317	LHG	C4-O6-P-O5
36	14	317	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
36	15	316	LHG	O1-C1-C2-O2
36	15	316	LHG	O1-C1-C2-C3
36	15	316	LHG	C4-O6-P-O5
36	18	315	LHG	C3-O3-P-O4
36	18	316	LHG	C4-O6-P-O3
36	18	316	LHG	C5-C4-O6-P
36	18	316	LHG	O9-C7-O7-C5
36	18	316	LHG	C8-C7-O7-C5
38	B	620	LMG	O6-C1-O1-C7
38	C	522	LMG	C11-C10-O7-C8
38	D	408	LMG	O9-C10-O7-C8
38	D	408	LMG	C11-C10-O7-C8
38	F	102	LMG	O9-C10-O7-C8
38	F	102	LMG	C11-C10-O7-C8
38	J	101	LMG	C2-C1-O1-C7
38	J	101	LMG	O6-C1-O1-C7
38	b	621	LMG	O6-C1-O1-C7
38	c	521	LMG	C11-C10-O7-C8
38	d	408	LMG	O9-C10-O7-C8
38	d	408	LMG	C11-C10-O7-C8
38	f	102	LMG	O9-C10-O7-C8
38	f	102	LMG	C11-C10-O7-C8
38	j	101	LMG	C2-C1-O1-C7
38	j	101	LMG	O6-C1-O1-C7
38	1	301	LMG	C2-C1-O1-C7
38	1	301	LMG	O6-C1-O1-C7
38	1	301	LMG	O7-C8-C9-O8
38	1	317	LMG	O6-C1-O1-C7
38	4	316	LMG	O9-C10-O7-C8
38	4	316	LMG	C11-C10-O7-C8
38	5	315	LMG	C2-C1-O1-C7
38	5	315	LMG	O6-C1-O1-C7
38	5	316	LMG	C2-C1-O1-C7
38	5	316	LMG	O6-C1-O1-C7
38	11	301	LMG	C2-C1-O1-C7
38	11	301	LMG	O6-C1-O1-C7
38	11	301	LMG	O7-C8-C9-O8
38	11	317	LMG	C2-C1-O1-C7
38	11	317	LMG	O6-C1-O1-C7
38	14	316	LMG	O9-C10-O7-C8
38	14	316	LMG	C11-C10-O7-C8
38	15	314	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
38	15	314	LMG	O6-C1-O1-C7
38	15	315	LMG	C2-C1-O1-C7
38	15	315	LMG	O6-C1-O1-C7
38	15	315	LMG	O7-C8-C9-O8
39	B	621	DGD	C2D-C1D-O3G-C3G
39	B	621	DGD	C2E-C1E-O5D-C6D
39	B	621	DGD	O6E-C1E-O5D-C6D
39	C	520	DGD	C2D-C1D-O3G-C3G
39	C	520	DGD	O6D-C1D-O3G-C3G
39	H	102	DGD	C2E-C1E-O5D-C6D
39	H	102	DGD	O6E-C1E-O5D-C6D
39	W	203	DGD	C2D-C1D-O3G-C3G
39	W	203	DGD	O6D-C1D-O3G-C3G
39	W	203	DGD	O6E-C1E-O5D-C6D
39	b	622	DGD	C2D-C1D-O3G-C3G
39	b	622	DGD	C2E-C1E-O5D-C6D
39	b	622	DGD	O6E-C1E-O5D-C6D
39	c	520	DGD	C2D-C1D-O3G-C3G
39	c	520	DGD	O6D-C1D-O3G-C3G
39	h	102	DGD	C2E-C1E-O5D-C6D
39	h	102	DGD	O6E-C1E-O5D-C6D
39	w	204	DGD	C2D-C1D-O3G-C3G
39	w	204	DGD	O6D-C1D-O3G-C3G
39	w	204	DGD	O6E-C1E-O5D-C6D
39	1	318	DGD	C2B-C1B-O2G-C2G
39	1	318	DGD	O1B-C1B-O2G-C2G
39	1	318	DGD	O1G-C1G-C2G-O2G
39	1	318	DGD	C2D-C1D-O3G-C3G
39	1	318	DGD	O6D-C1D-O3G-C3G
39	1	318	DGD	C2E-C1E-O5D-C6D
39	1	318	DGD	O6E-C1E-O5D-C6D
39	11	318	DGD	C2B-C1B-O2G-C2G
39	11	318	DGD	O1B-C1B-O2G-C2G
39	11	318	DGD	O1G-C1G-C2G-O2G
39	11	318	DGD	C2D-C1D-O3G-C3G
39	11	318	DGD	O6D-C1D-O3G-C3G
39	11	318	DGD	O6E-C1E-O5D-C6D
41	V	201	HEM	C1A-C2A-CAA-CBA
41	V	201	HEM	C3A-C2A-CAA-CBA
41	v	201	HEM	C1A-C2A-CAA-CBA
41	v	201	HEM	C3A-C2A-CAA-CBA
42	P	609	KC1	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
42	P	609	KC1	C3A-C2A-CAA-CBA
42	P	609	KC1	C2B-C3B-CAB-CBB
42	P	609	KC1	C4B-C3B-CAB-CBB
42	P	609	KC1	CBD-CGD-O2D-CED
42	p	609	KC1	C1A-C2A-CAA-CBA
42	p	609	KC1	C3A-C2A-CAA-CBA
42	p	609	KC1	C2B-C3B-CAB-CBB
42	p	609	KC1	C4B-C3B-CAB-CBB
42	p	609	KC1	CBD-CGD-O2D-CED
42	0	315	KC1	C1A-C2A-CAA-CBA
42	0	315	KC1	C3A-C2A-CAA-CBA
42	0	315	KC1	CAA-CBA-CGA-O1A
42	0	315	KC1	CAA-CBA-CGA-O2A
42	1	314	KC1	C1A-C2A-CAA-CBA
42	1	314	KC1	C3A-C2A-CAA-CBA
42	4	313	KC1	C1A-C2A-CAA-CBA
42	4	313	KC1	C3A-C2A-CAA-CBA
42	9	314	KC1	C1A-C2A-CAA-CBA
42	9	314	KC1	C3A-C2A-CAA-CBA
42	10	315	KC1	C1A-C2A-CAA-CBA
42	11	314	KC1	C1A-C2A-CAA-CBA
42	11	314	KC1	C3A-C2A-CAA-CBA
42	14	313	KC1	C3A-C2A-CAA-CBA
42	14	313	KC1	CBD-CGD-O2D-CED
42	19	314	KC1	C1A-C2A-CAA-CBA
42	19	314	KC1	C3A-C2A-CAA-CBA
43	P	611	A86	C13-C14-C15-C20
43	P	611	A86	C33-C34-O4-C38
43	P	613	A86	C10-C11-C13-O
43	P	613	A86	C12-C11-C13-O
43	P	613	A86	C13-C14-C15-O1
43	p	611	A86	C13-C14-C15-C20
43	p	611	A86	C33-C34-O4-C38
43	p	613	A86	C10-C11-C13-O
43	p	613	A86	C12-C11-C13-O
43	p	613	A86	C13-C14-C15-O1
43	0	302	A86	C39-C38-O4-C34
43	0	304	A86	C39-C38-O4-C34
43	0	305	A86	C12-C11-C13-C14
43	0	305	A86	C13-C14-C15-O1
43	0	306	A86	C12-C11-C13-C14
43	1	302	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
43	1	302	A86	C11-C13-C14-C15
43	1	302	A86	C13-C14-C15-C16
43	1	302	A86	C39-C38-O4-C34
43	1	303	A86	C12-C11-C13-C14
43	1	303	A86	C13-C14-C15-C20
43	1	305	A86	O-C13-C14-C15
43	1	305	A86	C11-C13-C14-C15
43	1	305	A86	C13-C14-C15-C16
43	1	306	A86	C12-C11-C13-O
43	1	306	A86	C39-C38-O4-C34
43	1	319	A86	C12-C11-C13-C14
43	1	319	A86	C13-C14-C15-C20
43	2	301	A86	C13-C14-C15-C16
43	2	301	A86	C13-C14-C15-O1
43	2	305	A86	C13-C14-C15-O1
43	3	301	A86	C39-C38-O4-C34
43	3	303	A86	C12-C11-C13-C14
43	3	303	A86	C13-C14-C15-C20
43	3	305	A86	C13-C14-C15-C20
43	3	305	A86	C13-C14-C15-O1
43	3	306	A86	C13-C14-C15-O1
43	4	301	A86	C12-C11-C13-C14
43	4	302	A86	C33-C34-O4-C38
43	4	302	A86	C39-C38-O4-C34
43	4	303	A86	C13-C14-C15-C20
43	4	303	A86	C13-C14-C15-O1
43	4	303	A86	C24-C25-C26-C27
43	4	303	A86	C35-C34-O4-C38
43	4	303	A86	C7-C6-C8-C9
43	4	304	A86	C13-C14-C15-O1
43	4	305	A86	C39-C38-O4-C34
43	4	306	A86	C13-C14-C15-C16
43	4	306	A86	C13-C14-C15-O1
43	5	302	A86	C13-C14-C15-O1
43	5	302	A86	C39-C38-O4-C34
43	5	304	A86	O-C13-C14-C15
43	5	304	A86	C11-C13-C14-C15
43	5	304	A86	C13-C14-C15-C16
43	5	304	A86	C33-C34-O4-C38
43	5	304	A86	C39-C38-O4-C34
43	5	318	A86	C10-C11-C13-O
43	5	318	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	5	318	A86	C11-C13-C14-C15
43	6	301	A86	C12-C11-C13-O
43	6	301	A86	C13-C14-C15-O1
43	6	301	A86	C39-C38-O4-C34
43	6	303	A86	C10-C11-C13-O
43	6	303	A86	C12-C11-C13-O
43	6	303	A86	C12-C11-C13-C14
43	6	303	A86	C13-C14-C15-C16
43	6	303	A86	C13-C14-C15-O1
43	6	303	A86	C39-C38-O4-C34
43	6	305	A86	C13-C14-C15-C20
43	6	305	A86	C13-C14-C15-O1
43	6	306	A86	C12-C11-C13-O
43	6	306	A86	C12-C11-C13-C14
43	6	306	A86	C13-C14-C15-O1
43	6	307	A86	C11-C10-C9-C8
43	6	307	A86	C10-C11-C13-O
43	6	307	A86	C12-C11-C13-C14
43	6	307	A86	C13-C14-C15-C16
43	6	307	A86	C35-C34-O4-C38
43	6	307	A86	C39-C38-O4-C34
43	7	302	A86	C13-C14-C15-C16
43	7	302	A86	C13-C14-C15-O1
43	7	304	A86	C13-C14-C15-C20
43	7	304	A86	C13-C14-C15-O1
43	7	305	A86	C13-C14-C15-O1
43	7	306	A86	C13-C14-C15-O1
43	8	301	A86	C10-C11-C13-O
43	8	301	A86	O-C13-C14-C15
43	8	301	A86	C11-C13-C14-C15
43	8	301	A86	C13-C14-C15-C16
43	8	302	A86	C13-C14-C15-C16
43	8	302	A86	C13-C14-C15-O1
43	8	303	A86	C33-C34-O4-C38
43	8	303	A86	C39-C38-O4-C34
43	8	304	A86	C33-C34-O4-C38
43	8	304	A86	C39-C38-O4-C34
43	8	305	A86	C13-C14-C15-O1
43	9	302	A86	C39-C38-O4-C34
43	9	305	A86	C13-C14-C15-C20
43	9	305	A86	C39-C38-O4-C34
43	9	306	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	10	302	A86	C39-C38-O4-C34
43	10	304	A86	C39-C38-O4-C34
43	10	305	A86	C12-C11-C13-C14
43	10	305	A86	C13-C14-C15-O1
43	10	305	A86	C39-C38-O4-C34
43	10	306	A86	C10-C11-C13-O
43	10	306	A86	C12-C11-C13-C14
43	10	318	A86	C13-C14-C15-O1
43	11	303	A86	C12-C11-C13-C14
43	11	303	A86	C13-C14-C15-C20
43	11	304	A86	C7-C6-C8-C9
43	11	305	A86	C12-C11-C13-O
43	11	305	A86	O-C13-C14-C15
43	11	305	A86	C11-C13-C14-C15
43	11	305	A86	C13-C14-C15-C16
43	11	306	A86	C13-C14-C15-C20
43	11	306	A86	C39-C38-O4-C34
43	11	320	A86	C13-C14-C15-C16
43	12	302	A86	C12-C11-C13-C14
43	12	302	A86	C13-C14-C15-C20
43	12	304	A86	C39-C38-O4-C34
43	12	305	A86	C39-C38-O4-C34
43	12	306	A86	C13-C14-C15-O1
43	12	306	A86	C39-C38-O4-C34
43	13	302	A86	C12-C11-C13-C14
43	13	302	A86	C13-C14-C15-C20
43	13	302	A86	C39-C38-O4-C34
43	13	304	A86	C13-C14-C15-C20
43	13	304	A86	C13-C14-C15-O1
43	13	304	A86	C39-C38-O4-C34
43	13	305	A86	C12-C11-C13-C14
43	13	305	A86	C39-C38-O4-C34
43	13	306	A86	C12-C11-C13-O
43	13	306	A86	C13-C14-C15-O1
43	14	301	A86	C2-C1-C24-C25
43	14	301	A86	C13-C14-C15-O1
43	14	301	A86	C35-C34-O4-C38
43	14	301	A86	C5-C6-C8-C9
43	14	301	A86	C7-C6-C8-C9
43	14	302	A86	C35-C34-O4-C38
43	14	302	A86	C39-C38-O4-C34
43	14	302	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	14	303	A86	C13-C14-C15-O1
43	14	305	A86	C39-C38-O4-C34
43	15	302	A86	C13-C14-C15-O1
43	15	304	A86	C11-C13-C14-C15
43	15	304	A86	C13-C14-C15-C16
43	15	305	A86	C33-C34-O4-C38
43	16	302	A86	C10-C11-C13-O
43	16	302	A86	C12-C11-C13-O
43	16	302	A86	C13-C14-C15-O1
43	16	302	A86	C39-C38-O4-C34
43	16	304	A86	C13-C14-C15-O1
43	16	306	A86	C13-C14-C15-C20
43	16	306	A86	C13-C14-C15-O1
43	16	307	A86	C12-C11-C13-O
43	16	307	A86	C12-C11-C13-C14
43	16	307	A86	C13-C14-C15-O1
43	17	301	A86	C12-C11-C13-O
43	17	301	A86	C13-C14-C15-O1
43	17	301	A86	C39-C38-O4-C34
43	17	303	A86	C33-C34-O4-C38
43	17	303	A86	C35-C34-O4-C38
43	17	305	A86	C13-C14-C15-C20
43	17	305	A86	C13-C14-C15-O1
43	17	306	A86	C13-C14-C15-O1
43	17	316	A86	C12-C11-C13-C14
43	17	316	A86	C13-C14-C15-C20
43	18	302	A86	C35-C34-O4-C38
43	18	302	A86	C39-C38-O4-C34
43	18	302	A86	O5-C38-O4-C34
43	18	302	A86	C5-C6-C8-C9
43	18	302	A86	C7-C6-C8-C9
43	18	303	A86	C33-C34-O4-C38
43	18	303	A86	C39-C38-O4-C34
43	18	303	A86	O5-C38-O4-C34
43	18	304	A86	C33-C34-O4-C38
43	18	304	A86	C39-C38-O4-C34
43	18	305	A86	C-C1-C24-C25
43	18	305	A86	C2-C1-C24-C25
43	18	305	A86	C12-C11-C13-O
43	18	305	A86	C13-C14-C15-C16
43	18	305	A86	C35-C34-O4-C38
43	18	305	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	18	305	A86	O5-C38-O4-C34
43	19	302	A86	C25-C26-C27-C29
43	19	305	A86	C13-C14-C15-C20
43	19	306	A86	C39-C38-O4-C34
44	P	612	DD6	C10-C11-C13-C14
44	P	612	DD6	C12-C11-C13-C14
44	P	612	DD6	C13-C14-C15-O1
44	P	612	DD6	C5-C6-C8-C9
44	P	612	DD6	C7-C6-C8-C9
44	p	612	DD6	C10-C11-C13-C14
44	p	612	DD6	C12-C11-C13-C14
44	p	612	DD6	C13-C14-C15-C16
44	p	612	DD6	C13-C14-C15-C20
44	p	612	DD6	C13-C14-C15-O1
44	p	612	DD6	C5-C6-C8-C9
44	p	612	DD6	C7-C6-C8-C9
45	0	310	KC2	C1A-C2A-CAA-CBA
45	0	310	KC2	C2B-C3B-CAB-CBB
45	0	310	KC2	C2C-C3C-CAC-CBC
45	0	310	KC2	C4C-C3C-CAC-CBC
45	1	309	KC2	C1A-C2A-CAA-CBA
45	1	309	KC2	C3A-C2A-CAA-CBA
45	1	311	KC2	C2C-C3C-CAC-CBC
45	1	311	KC2	C4C-C3C-CAC-CBC
45	1	311	KC2	CAA-CBA-CGA-O1A
45	1	311	KC2	CAA-CBA-CGA-O2A
45	2	308	KC2	C1A-C2A-CAA-CBA
45	2	308	KC2	C3A-C2A-CAA-CBA
45	2	308	KC2	C2B-C3B-CAB-CBB
45	2	308	KC2	C2C-C3C-CAC-CBC
45	2	308	KC2	C4C-C3C-CAC-CBC
45	2	308	KC2	CBD-CGD-O2D-CED
45	2	310	KC2	C1A-C2A-CAA-CBA
45	2	310	KC2	C3A-C2A-CAA-CBA
45	2	310	KC2	C2B-C3B-CAB-CBB
45	2	310	KC2	C4B-C3B-CAB-CBB
45	2	310	KC2	C2C-C3C-CAC-CBC
45	3	309	KC2	C1A-C2A-CAA-CBA
45	3	309	KC2	C3A-C2A-CAA-CBA
45	3	309	KC2	C2B-C3B-CAB-CBB
45	3	309	KC2	C4B-C3B-CAB-CBB
45	3	309	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
45	3	309	KC2	C4C-C3C-CAC-CBC
45	3	309	KC2	CBD-CGD-O2D-CED
45	3	311	KC2	C1A-C2A-CAA-CBA
45	3	311	KC2	C3A-C2A-CAA-CBA
45	3	311	KC2	C2B-C3B-CAB-CBB
45	3	311	KC2	C4B-C3B-CAB-CBB
45	3	311	KC2	C2C-C3C-CAC-CBC
45	4	308	KC2	C1A-C2A-CAA-CBA
45	4	308	KC2	C3A-C2A-CAA-CBA
45	4	308	KC2	C2C-C3C-CAC-CBC
45	4	308	KC2	C4C-C3C-CAC-CBC
45	4	310	KC2	C2C-C3C-CAC-CBC
45	4	310	KC2	C4C-C3C-CAC-CBC
45	5	308	KC2	C1A-C2A-CAA-CBA
45	5	308	KC2	C3A-C2A-CAA-CBA
45	5	310	KC2	C1A-C2A-CAA-CBA
45	5	310	KC2	C3A-C2A-CAA-CBA
45	5	310	KC2	C2C-C3C-CAC-CBC
45	5	310	KC2	C4C-C3C-CAC-CBC
45	6	310	KC2	C1A-C2A-CAA-CBA
45	6	310	KC2	C3A-C2A-CAA-CBA
45	6	310	KC2	C2B-C3B-CAB-CBB
45	6	310	KC2	C2C-C3C-CAC-CBC
45	6	310	KC2	C4C-C3C-CAC-CBC
45	6	310	KC2	CBD-CGD-O2D-CED
45	6	312	KC2	C1A-C2A-CAA-CBA
45	6	312	KC2	C3A-C2A-CAA-CBA
45	6	312	KC2	C2B-C3B-CAB-CBB
45	6	312	KC2	C4B-C3B-CAB-CBB
45	6	312	KC2	C2C-C3C-CAC-CBC
45	7	309	KC2	C1A-C2A-CAA-CBA
45	7	309	KC2	C3A-C2A-CAA-CBA
45	7	309	KC2	C2B-C3B-CAB-CBB
45	7	309	KC2	C4B-C3B-CAB-CBB
45	7	309	KC2	C2C-C3C-CAC-CBC
45	7	309	KC2	C4C-C3C-CAC-CBC
45	7	309	KC2	CBD-CGD-O2D-CED
45	7	311	KC2	C1A-C2A-CAA-CBA
45	7	311	KC2	C3A-C2A-CAA-CBA
45	7	311	KC2	C2B-C3B-CAB-CBB
45	7	311	KC2	C4B-C3B-CAB-CBB
45	7	311	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
45	7	311	KC2	C4C-C3C-CAC-CBC
45	8	308	KC2	C1A-C2A-CAA-CBA
45	8	308	KC2	C3A-C2A-CAA-CBA
45	8	308	KC2	C2B-C3B-CAB-CBB
45	8	308	KC2	C4B-C3B-CAB-CBB
45	8	308	KC2	C2C-C3C-CAC-CBC
45	8	308	KC2	C4C-C3C-CAC-CBC
45	8	308	KC2	CBD-CGD-O2D-CED
45	8	310	KC2	C1A-C2A-CAA-CBA
45	8	310	KC2	C3A-C2A-CAA-CBA
45	8	310	KC2	C2B-C3B-CAB-CBB
45	8	310	KC2	C4B-C3B-CAB-CBB
45	8	310	KC2	C2C-C3C-CAC-CBC
45	9	309	KC2	C2C-C3C-CAC-CBC
45	10	310	KC2	C1A-C2A-CAA-CBA
45	10	310	KC2	C2B-C3B-CAB-CBB
45	10	310	KC2	C2C-C3C-CAC-CBC
45	11	309	KC2	C1A-C2A-CAA-CBA
45	11	309	KC2	C3A-C2A-CAA-CBA
45	11	309	KC2	C2C-C3C-CAC-CBC
45	11	309	KC2	C4C-C3C-CAC-CBC
45	11	309	KC2	CBD-CGD-O2D-CED
45	11	309	KC2	O1D-CGD-O2D-CED
45	11	311	KC2	C2C-C3C-CAC-CBC
45	11	311	KC2	C4C-C3C-CAC-CBC
45	12	309	KC2	C1A-C2A-CAA-CBA
45	12	309	KC2	C3A-C2A-CAA-CBA
45	12	309	KC2	C2C-C3C-CAC-CBC
45	12	309	KC2	C4C-C3C-CAC-CBC
45	12	311	KC2	C1A-C2A-CAA-CBA
45	12	311	KC2	C3A-C2A-CAA-CBA
45	13	309	KC2	C1A-C2A-CAA-CBA
45	13	309	KC2	C3A-C2A-CAA-CBA
45	13	309	KC2	C2B-C3B-CAB-CBB
45	13	309	KC2	C4B-C3B-CAB-CBB
45	13	309	KC2	C2C-C3C-CAC-CBC
45	13	309	KC2	C4C-C3C-CAC-CBC
45	13	311	KC2	C1A-C2A-CAA-CBA
45	13	311	KC2	C3A-C2A-CAA-CBA
45	13	311	KC2	C2C-C3C-CAC-CBC
45	13	311	KC2	C4C-C3C-CAC-CBC
45	14	308	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
45	14	308	KC2	C3A-C2A-CAA-CBA
45	14	308	KC2	C2C-C3C-CAC-CBC
45	14	308	KC2	C4C-C3C-CAC-CBC
45	14	310	KC2	C2C-C3C-CAC-CBC
45	14	310	KC2	C4C-C3C-CAC-CBC
45	15	308	KC2	C1A-C2A-CAA-CBA
45	15	308	KC2	C3A-C2A-CAA-CBA
45	15	308	KC2	CAA-CBA-CGA-O2A
45	15	310	KC2	C1A-C2A-CAA-CBA
45	15	310	KC2	C3A-C2A-CAA-CBA
45	15	310	KC2	C2C-C3C-CAC-CBC
45	15	310	KC2	C4C-C3C-CAC-CBC
45	15	310	KC2	CAA-CBA-CGA-O1A
45	15	310	KC2	CAA-CBA-CGA-O2A
45	16	310	KC2	C1A-C2A-CAA-CBA
45	16	310	KC2	C3A-C2A-CAA-CBA
45	16	310	KC2	C2B-C3B-CAB-CBB
45	16	310	KC2	C2C-C3C-CAC-CBC
45	16	310	KC2	C4C-C3C-CAC-CBC
45	16	310	KC2	CBD-CGD-O2D-CED
45	16	312	KC2	C1A-C2A-CAA-CBA
45	16	312	KC2	C3A-C2A-CAA-CBA
45	16	312	KC2	C2B-C3B-CAB-CBB
45	16	312	KC2	C4B-C3B-CAB-CBB
45	16	312	KC2	C2C-C3C-CAC-CBC
45	17	309	KC2	C1A-C2A-CAA-CBA
45	17	309	KC2	C3A-C2A-CAA-CBA
45	17	309	KC2	C2B-C3B-CAB-CBB
45	17	309	KC2	C2C-C3C-CAC-CBC
45	17	309	KC2	C4C-C3C-CAC-CBC
45	17	309	KC2	CBD-CGD-O2D-CED
45	17	311	KC2	C2B-C3B-CAB-CBB
45	17	311	KC2	C4B-C3B-CAB-CBB
45	17	311	KC2	C2C-C3C-CAC-CBC
45	17	311	KC2	C4C-C3C-CAC-CBC
45	17	311	KC2	CAA-CBA-CGA-O1A
45	17	311	KC2	CAA-CBA-CGA-O2A
45	18	308	KC2	C1A-C2A-CAA-CBA
45	18	308	KC2	C3A-C2A-CAA-CBA
45	18	308	KC2	C2B-C3B-CAB-CBB
45	18	308	KC2	C4B-C3B-CAB-CBB
45	18	308	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
45	18	308	KC2	C4C-C3C-CAC-CBC
45	18	308	KC2	CBD-CGD-O2D-CED
45	18	310	KC2	C2B-C3B-CAB-CBB
45	18	310	KC2	C4B-C3B-CAB-CBB
45	18	310	KC2	C2C-C3C-CAC-CBC
45	19	309	KC2	C2C-C3C-CAC-CBC
43	P	611	A86	C39-C38-O4-C34
43	P	613	A86	C39-C38-O4-C34
43	p	611	A86	C39-C38-O4-C34
43	p	613	A86	C39-C38-O4-C34
43	0	305	A86	C39-C38-O4-C34
43	0	306	A86	C39-C38-O4-C34
43	1	303	A86	C39-C38-O4-C34
43	1	304	A86	C39-C38-O4-C34
43	1	305	A86	C39-C38-O4-C34
43	1	319	A86	C39-C38-O4-C34
43	2	303	A86	C39-C38-O4-C34
43	2	304	A86	C39-C38-O4-C34
43	3	303	A86	C39-C38-O4-C34
43	3	304	A86	C39-C38-O4-C34
43	4	301	A86	C39-C38-O4-C34
43	4	304	A86	C39-C38-O4-C34
43	4	306	A86	C39-C38-O4-C34
43	5	305	A86	C39-C38-O4-C34
43	5	318	A86	C39-C38-O4-C34
43	6	304	A86	C39-C38-O4-C34
43	6	305	A86	C39-C38-O4-C34
43	7	302	A86	C39-C38-O4-C34
43	7	303	A86	C39-C38-O4-C34
43	7	304	A86	C39-C38-O4-C34
43	7	306	A86	C39-C38-O4-C34
43	8	301	A86	C39-C38-O4-C34
43	8	302	A86	C39-C38-O4-C34
43	8	303	A86	O5-C38-O4-C34
43	10	306	A86	C39-C38-O4-C34
43	11	303	A86	C39-C38-O4-C34
43	11	304	A86	C39-C38-O4-C34
43	11	305	A86	C39-C38-O4-C34
43	12	302	A86	C39-C38-O4-C34
43	12	303	A86	C39-C38-O4-C34
43	13	303	A86	C39-C38-O4-C34
43	13	306	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	14	301	A86	C39-C38-O4-C34
43	14	301	A86	O5-C38-O4-C34
43	14	303	A86	C39-C38-O4-C34
43	14	304	A86	C39-C38-O4-C34
43	15	301	A86	C39-C38-O4-C34
43	15	304	A86	C39-C38-O4-C34
43	15	305	A86	C39-C38-O4-C34
43	16	304	A86	C39-C38-O4-C34
43	16	305	A86	C39-C38-O4-C34
43	17	303	A86	C39-C38-O4-C34
43	17	304	A86	C39-C38-O4-C34
43	17	305	A86	C39-C38-O4-C34
43	18	301	A86	C39-C38-O4-C34
43	19	302	A86	C39-C38-O4-C34
43	19	303	A86	C39-C38-O4-C34
43	19	305	A86	C39-C38-O4-C34
31	C	504	CLA	O1D-CGD-O2D-CED
31	P	608	CLA	O1D-CGD-O2D-CED
31	c	504	CLA	O1D-CGD-O2D-CED
31	1	312	CLA	O1D-CGD-O2D-CED
31	2	306	CLA	O1D-CGD-O2D-CED
31	3	307	CLA	O1D-CGD-O2D-CED
31	3	316	CLA	O1D-CGD-O2D-CED
31	4	312	CLA	O1D-CGD-O2D-CED
31	4	315	CLA	O1D-CGD-O2D-CED
31	6	308	CLA	O1D-CGD-O2D-CED
31	6	314	CLA	O1D-CGD-O2D-CED
31	7	307	CLA	O1D-CGD-O2D-CED
31	8	306	CLA	O1D-CGD-O2D-CED
31	13	312	CLA	O1D-CGD-O2D-CED
31	13	313	CLA	O1D-CGD-O2D-CED
31	14	315	CLA	O1D-CGD-O2D-CED
31	15	312	CLA	O1D-CGD-O2D-CED
31	17	307	CLA	O1D-CGD-O2D-CED
31	18	306	CLA	O1D-CGD-O2D-CED
42	P	609	KC1	O1D-CGD-O2D-CED
42	p	609	KC1	O1D-CGD-O2D-CED
42	4	313	KC1	O1D-CGD-O2D-CED
42	14	313	KC1	O1D-CGD-O2D-CED
45	7	309	KC2	O1D-CGD-O2D-CED
45	17	309	KC2	O1D-CGD-O2D-CED
45	18	308	KC2	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
43	3	305	A86	C39-C38-O4-C34
43	5	301	A86	C39-C38-O4-C34
43	5	303	A86	C39-C38-O4-C34
43	9	303	A86	C39-C38-O4-C34
43	10	306	A86	O5-C38-O4-C34
43	12	304	A86	O5-C38-O4-C34
43	15	302	A86	C39-C38-O4-C34
43	16	306	A86	C39-C38-O4-C34
31	A	403	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	O1D-CGD-O2D-CED
31	B	609	CLA	O1D-CGD-O2D-CED
31	B	611	CLA	O1D-CGD-O2D-CED
31	P	601	CLA	O1D-CGD-O2D-CED
31	a	403	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	p	601	CLA	O1D-CGD-O2D-CED
31	0	316	CLA	O1D-CGD-O2D-CED
31	1	315	CLA	O1D-CGD-O2D-CED
31	3	313	CLA	O1D-CGD-O2D-CED
31	5	312	CLA	O1D-CGD-O2D-CED
31	7	313	CLA	O1D-CGD-O2D-CED
31	10	316	CLA	O1D-CGD-O2D-CED
31	11	312	CLA	O1D-CGD-O2D-CED
31	14	311	CLA	O1D-CGD-O2D-CED
31	18	311	CLA	O1D-CGD-O2D-CED
45	2	308	KC2	O1D-CGD-O2D-CED
45	3	309	KC2	O1D-CGD-O2D-CED
45	6	310	KC2	O1D-CGD-O2D-CED
45	8	308	KC2	O1D-CGD-O2D-CED
45	16	310	KC2	O1D-CGD-O2D-CED
31	A	404	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED
31	B	609	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	C	504	CLA	CBD-CGD-O2D-CED
31	C	507	CLA	CBD-CGD-O2D-CED
31	C	509	CLA	CBD-CGD-O2D-CED
31	C	514	CLA	CBD-CGD-O2D-CED
31	D	404	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	P	603	CLA	CBD-CGD-O2D-CED
31	a	404	CLA	CBD-CGD-O2D-CED
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	CBD-CGD-O2D-CED
31	c	504	CLA	CBD-CGD-O2D-CED
31	c	507	CLA	CBD-CGD-O2D-CED
31	c	509	CLA	CBD-CGD-O2D-CED
31	c	514	CLA	CBD-CGD-O2D-CED
31	d	404	CLA	CBD-CGD-O2D-CED
31	p	603	CLA	CBD-CGD-O2D-CED
31	1	310	CLA	CBD-CGD-O2D-CED
31	1	312	CLA	CBD-CGD-O2D-CED
31	1	313	CLA	CBD-CGD-O2D-CED
31	1	315	CLA	CBD-CGD-O2D-CED
31	2	306	CLA	CBD-CGD-O2D-CED
31	3	307	CLA	CBD-CGD-O2D-CED
31	3	316	CLA	CBD-CGD-O2D-CED
31	4	307	CLA	CBD-CGD-O2D-CED
31	4	309	CLA	CBD-CGD-O2D-CED
31	4	311	CLA	CBD-CGD-O2D-CED
31	4	312	CLA	CBD-CGD-O2D-CED
31	6	308	CLA	CBD-CGD-O2D-CED
31	7	307	CLA	CBD-CGD-O2D-CED
31	8	306	CLA	CBD-CGD-O2D-CED
31	9	315	CLA	CBD-CGD-O2D-CED
31	11	308	CLA	CBD-CGD-O2D-CED
31	11	312	CLA	CBD-CGD-O2D-CED
31	11	313	CLA	CBD-CGD-O2D-CED
31	11	315	CLA	CBD-CGD-O2D-CED
31	14	307	CLA	CBD-CGD-O2D-CED
31	14	309	CLA	CBD-CGD-O2D-CED
31	14	311	CLA	CBD-CGD-O2D-CED
31	16	308	CLA	CBD-CGD-O2D-CED
31	17	307	CLA	CBD-CGD-O2D-CED
31	18	306	CLA	CBD-CGD-O2D-CED
31	18	309	CLA	CBD-CGD-O2D-CED
31	18	312	CLA	CBD-CGD-O2D-CED
42	4	313	KC1	CBD-CGD-O2D-CED
42	11	314	KC1	CBD-CGD-O2D-CED
45	1	309	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	5	308	KC2	CBD-CGD-O2D-CED
45	15	308	KC2	CBD-CGD-O2D-CED
31	A	403	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	O1A-CGA-O2A-C1
31	a	403	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	O1A-CGA-O2A-C1
31	3	316	CLA	O1A-CGA-O2A-C1
31	10	307	CLA	O1A-CGA-O2A-C1
31	11	313	CLA	O1A-CGA-O2A-C1
31	13	316	CLA	O1A-CGA-O2A-C1
31	18	307	CLA	O1A-CGA-O2A-C1
36	5	317	LHG	O10-C23-O8-C6
38	D	408	LMG	O10-C28-O8-C9
38	M	101	LMG	O10-C28-O8-C9
38	d	408	LMG	O10-C28-O8-C9
38	m	101	LMG	O10-C28-O8-C9
39	B	621	DGD	O1A-C1A-O1G-C1G
39	C	519	DGD	O1A-C1A-O1G-C1G
39	b	622	DGD	O1A-C1A-O1G-C1G
39	c	519	DGD	O1A-C1A-O1G-C1G
31	8	311	CLA	O1A-CGA-O2A-C1
31	11	315	CLA	C4C-C3C-CAC-CBC
43	0	306	A86	O5-C38-O4-C34
43	7	302	A86	O5-C38-O4-C34
43	11	320	A86	C39-C38-O4-C34
43	12	302	A86	O5-C38-O4-C34
43	15	305	A86	O5-C38-O4-C34
31	P	606	CLA	O1D-CGD-O2D-CED
31	p	606	CLA	O1D-CGD-O2D-CED
31	4	311	CLA	O1D-CGD-O2D-CED
31	12	310	CLA	O1D-CGD-O2D-CED
31	14	312	CLA	O1D-CGD-O2D-CED
31	16	308	CLA	O1D-CGD-O2D-CED
39	H	102	DGD	C4D-C5D-C6D-O5D
39	h	102	DGD	C4D-C5D-C6D-O5D
31	0	312	CLA	C4C-C3C-CAC-CBC
31	10	312	CLA	C4C-C3C-CAC-CBC
43	6	304	A86	C35-C34-O4-C38
43	12	305	A86	C35-C34-O4-C38
43	15	302	A86	C35-C34-O4-C38
43	16	305	A86	C35-C34-O4-C38
43	17	316	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
31	B	605	CLA	O1D-CGD-O2D-CED
31	B	616	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
31	z	103	CLA	O1D-CGD-O2D-CED
31	3	310	CLA	O1D-CGD-O2D-CED
31	8	312	CLA	O1D-CGD-O2D-CED
31	10	317	CLA	O1D-CGD-O2D-CED
31	13	316	CLA	O1D-CGD-O2D-CED
45	1	309	KC2	O1D-CGD-O2D-CED
45	5	308	KC2	O1D-CGD-O2D-CED
45	15	308	KC2	O1D-CGD-O2D-CED
31	B	602	CLA	CBA-CGA-O2A-C1
31	b	603	CLA	CBA-CGA-O2A-C1
31	3	316	CLA	CBA-CGA-O2A-C1
31	13	316	CLA	CBA-CGA-O2A-C1
31	18	307	CLA	CBA-CGA-O2A-C1
38	M	101	LMG	C29-C28-O8-C9
31	C	508	CLA	CBD-CGD-O2D-CED
31	C	511	CLA	CBD-CGD-O2D-CED
31	P	610	CLA	CBD-CGD-O2D-CED
31	c	508	CLA	CBD-CGD-O2D-CED
31	c	511	CLA	CBD-CGD-O2D-CED
31	p	610	CLA	CBD-CGD-O2D-CED
31	0	308	CLA	CBD-CGD-O2D-CED
31	0	309	CLA	CBD-CGD-O2D-CED
31	0	314	CLA	CBD-CGD-O2D-CED
31	4	314	CLA	CBD-CGD-O2D-CED
31	5	309	CLA	CBD-CGD-O2D-CED
31	9	307	CLA	CBD-CGD-O2D-CED
31	10	308	CLA	CBD-CGD-O2D-CED
31	10	309	CLA	CBD-CGD-O2D-CED
31	14	314	CLA	CBD-CGD-O2D-CED
31	15	309	CLA	CBD-CGD-O2D-CED
31	17	313	CLA	CBD-CGD-O2D-CED
31	17	315	CLA	CBD-CGD-O2D-CED
31	19	307	CLA	CBD-CGD-O2D-CED
31	19	315	CLA	CBD-CGD-O2D-CED
42	2	313	KC1	CBD-CGD-O2D-CED
45	14	308	KC2	CBD-CGD-O2D-CED
31	2	315	CLA	C4C-C3C-CAC-CBC
31	11	315	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
43	1	319	A86	O5-C38-O4-C34
43	3	303	A86	O5-C38-O4-C34
43	6	303	A86	O5-C38-O4-C34
43	8	302	A86	O5-C38-O4-C34
43	10	304	A86	O5-C38-O4-C34
31	P	603	CLA	O1A-CGA-O2A-C1
31	R	101	CLA	O1A-CGA-O2A-C1
31	p	603	CLA	O1A-CGA-O2A-C1
31	r	101	CLA	O1A-CGA-O2A-C1
31	0	307	CLA	O1A-CGA-O2A-C1
31	0	309	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	O1A-CGA-O2A-C1
31	7	313	CLA	O1A-CGA-O2A-C1
31	8	307	CLA	O1A-CGA-O2A-C1
31	10	309	CLA	O1A-CGA-O2A-C1
31	17	313	CLA	O1A-CGA-O2A-C1
31	19	308	CLA	O1A-CGA-O2A-C1
32	A	405	PHO	O1A-CGA-O2A-C1
32	a	405	PHO	O1A-CGA-O2A-C1
36	8	315	LHG	O10-C23-O8-C6
36	18	315	LHG	O10-C23-O8-C6
38	D	403	LMG	O10-C28-O8-C9
38	W	201	LMG	O10-C28-O8-C9
38	w	201	LMG	O10-C28-O8-C9
39	W	203	DGD	O1A-C1A-O1G-C1G
39	w	204	DGD	O1A-C1A-O1G-C1G
31	11	312	CLA	O1A-CGA-O2A-C1
31	1	308	CLA	O1D-CGD-O2D-CED
42	4	313	KC1	CAA-CBA-CGA-O2A
43	P	611	A86	O5-C38-O4-C34
43	p	611	A86	O5-C38-O4-C34
43	0	304	A86	O5-C38-O4-C34
43	0	305	A86	O5-C38-O4-C34
43	1	302	A86	O5-C38-O4-C34
43	1	303	A86	O5-C38-O4-C34
43	1	304	A86	O5-C38-O4-C34
43	2	303	A86	O5-C38-O4-C34
43	2	304	A86	O5-C38-O4-C34
43	3	304	A86	O5-C38-O4-C34
43	4	301	A86	O5-C38-O4-C34
43	4	302	A86	O5-C38-O4-C34
43	4	304	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	4	306	A86	O5-C38-O4-C34
43	5	302	A86	O5-C38-O4-C34
43	5	305	A86	O5-C38-O4-C34
43	5	318	A86	O5-C38-O4-C34
43	6	304	A86	O5-C38-O4-C34
43	7	303	A86	O5-C38-O4-C34
43	7	306	A86	O5-C38-O4-C34
43	8	301	A86	O5-C38-O4-C34
43	9	302	A86	O5-C38-O4-C34
43	9	305	A86	O5-C38-O4-C34
43	9	306	A86	O5-C38-O4-C34
43	10	305	A86	O5-C38-O4-C34
43	11	303	A86	O5-C38-O4-C34
43	11	304	A86	O5-C38-O4-C34
43	12	303	A86	O5-C38-O4-C34
43	12	306	A86	O5-C38-O4-C34
43	13	303	A86	O5-C38-O4-C34
43	13	304	A86	O5-C38-O4-C34
43	13	305	A86	O5-C38-O4-C34
43	13	306	A86	O5-C38-O4-C34
43	14	303	A86	O5-C38-O4-C34
43	14	304	A86	O5-C38-O4-C34
43	15	304	A86	O5-C38-O4-C34
43	16	302	A86	O5-C38-O4-C34
43	16	304	A86	O5-C38-O4-C34
43	16	305	A86	O5-C38-O4-C34
43	17	301	A86	O5-C38-O4-C34
43	17	303	A86	O5-C38-O4-C34
43	17	304	A86	O5-C38-O4-C34
43	17	305	A86	O5-C38-O4-C34
43	18	301	A86	O5-C38-O4-C34
43	19	302	A86	O5-C38-O4-C34
43	19	305	A86	O5-C38-O4-C34
43	19	306	A86	O5-C38-O4-C34
31	P	604	CLA	O1D-CGD-O2D-CED
31	p	604	CLA	O1D-CGD-O2D-CED
31	2	309	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	O1D-CGD-O2D-CED
31	11	310	CLA	O1D-CGD-O2D-CED
31	12	313	CLA	O1D-CGD-O2D-CED
31	13	310	CLA	O1D-CGD-O2D-CED
31	16	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
43	1	306	A86	O5-C38-O4-C34
43	3	301	A86	O5-C38-O4-C34
43	8	304	A86	O5-C38-O4-C34
43	11	306	A86	O5-C38-O4-C34
43	13	302	A86	O5-C38-O4-C34
43	18	304	A86	O5-C38-O4-C34
31	B	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	CBD-CGD-O2D-CED
31	2	312	CLA	O1D-CGD-O2D-CED
31	7	310	CLA	O1D-CGD-O2D-CED
31	17	310	CLA	O1D-CGD-O2D-CED
34	10	320	SQD	O49-C7-O47-C45
36	C	521	LHG	O9-C7-O7-C5
36	P	615	LHG	O9-C7-O7-C5
36	p	615	LHG	O9-C7-O7-C5
36	w	202	LHG	O9-C7-O7-C5
36	5	317	LHG	O9-C7-O7-C5
36	15	316	LHG	O9-C7-O7-C5
38	C	522	LMG	O9-C10-O7-C8
38	D	403	LMG	O9-C10-O7-C8
38	M	101	LMG	O9-C10-O7-C8
38	c	521	LMG	O9-C10-O7-C8
38	m	101	LMG	O9-C10-O7-C8
38	11	317	LMG	O9-C10-O7-C8
31	9	308	CLA	O1A-CGA-O2A-C1
31	18	311	CLA	CBA-CGA-O2A-C1
31	0	312	CLA	C2C-C3C-CAC-CBC
43	0	302	A86	O5-C38-O4-C34
43	5	304	A86	O5-C38-O4-C34
43	10	302	A86	O5-C38-O4-C34
43	12	305	A86	O5-C38-O4-C34
31	18	311	CLA	O1A-CGA-O2A-C1
43	19	306	A86	C35-C34-O4-C38
31	C	505	CLA	O1D-CGD-O2D-CED
31	c	505	CLA	O1D-CGD-O2D-CED
31	A	406	CLA	C3-C5-C6-C7
31	B	604	CLA	C3-C5-C6-C7
31	B	614	CLA	C3-C5-C6-C7
31	C	503	CLA	C3-C5-C6-C7
31	C	510	CLA	C3-C5-C6-C7
31	a	406	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	b	615	CLA	C3-C5-C6-C7
31	c	503	CLA	C3-C5-C6-C7
31	c	510	CLA	C3-C5-C6-C7
31	4	307	CLA	C3-C5-C6-C7
31	10	309	CLA	C3-C5-C6-C7
31	14	307	CLA	C3-C5-C6-C7
32	A	405	PHO	C3-C5-C6-C7
32	D	402	PHO	C3-C5-C6-C7
32	a	405	PHO	C3-C5-C6-C7
32	d	402	PHO	C3-C5-C6-C7
31	A	403	CLA	CBA-CGA-O2A-C1
31	P	603	CLA	CBA-CGA-O2A-C1
31	R	101	CLA	CBA-CGA-O2A-C1
31	a	403	CLA	CBA-CGA-O2A-C1
31	p	603	CLA	CBA-CGA-O2A-C1
31	r	101	CLA	CBA-CGA-O2A-C1
31	0	307	CLA	CBA-CGA-O2A-C1
31	10	307	CLA	CBA-CGA-O2A-C1
31	11	313	CLA	CBA-CGA-O2A-C1
31	17	313	CLA	CBA-CGA-O2A-C1
32	A	405	PHO	CBA-CGA-O2A-C1
32	a	405	PHO	CBA-CGA-O2A-C1
36	8	315	LHG	C24-C23-O8-C6
36	18	315	LHG	C24-C23-O8-C6
38	D	403	LMG	C29-C28-O8-C9
38	D	408	LMG	C29-C28-O8-C9
38	d	408	LMG	C29-C28-O8-C9
38	m	101	LMG	C29-C28-O8-C9
38	4	316	LMG	C29-C28-O8-C9
39	B	621	DGD	C2A-C1A-O1G-C1G
39	C	519	DGD	C2A-C1A-O1G-C1G
39	W	203	DGD	C2A-C1A-O1G-C1G
39	b	622	DGD	C2A-C1A-O1G-C1G
39	c	519	DGD	C2A-C1A-O1G-C1G
39	w	204	DGD	C2A-C1A-O1G-C1G
43	14	305	A86	O5-C38-O4-C34
36	14	317	LHG	C8-C7-O7-C5
31	1	310	CLA	O1D-CGD-O2D-CED
31	8	309	CLA	O1D-CGD-O2D-CED
31	11	308	CLA	O1D-CGD-O2D-CED
31	14	307	CLA	O1D-CGD-O2D-CED
42	7	314	KC1	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	10	312	CLA	C2C-C3C-CAC-CBC
43	P	613	A86	O5-C38-O4-C34
43	p	613	A86	O5-C38-O4-C34
43	4	305	A86	O5-C38-O4-C34
43	6	301	A86	O5-C38-O4-C34
43	6	306	A86	C39-C38-O4-C34
43	6	307	A86	O5-C38-O4-C34
43	7	304	A86	O5-C38-O4-C34
43	11	305	A86	O5-C38-O4-C34
36	15	316	LHG	O10-C23-O8-C6
39	1	318	DGD	O6D-C5D-C6D-O5D
39	1	318	DGD	C4D-C5D-C6D-O5D
43	3	305	A86	O5-C38-O4-C34
43	15	302	A86	O5-C38-O4-C34
42	1	314	KC1	CAA-CBA-CGA-O1A
42	1	314	KC1	CAA-CBA-CGA-O2A
42	8	313	KC1	CAA-CBA-CGA-O1A
42	8	313	KC1	CAA-CBA-CGA-O2A
45	1	309	KC2	CAA-CBA-CGA-O1A
45	1	309	KC2	CAA-CBA-CGA-O2A
45	2	308	KC2	CAA-CBA-CGA-O1A
45	2	308	KC2	CAA-CBA-CGA-O2A
45	3	309	KC2	CAA-CBA-CGA-O1A
45	3	309	KC2	CAA-CBA-CGA-O2A
45	5	310	KC2	CAA-CBA-CGA-O1A
45	5	310	KC2	CAA-CBA-CGA-O2A
45	7	309	KC2	CAA-CBA-CGA-O1A
45	7	309	KC2	CAA-CBA-CGA-O2A
45	8	308	KC2	CAA-CBA-CGA-O1A
45	8	308	KC2	CAA-CBA-CGA-O2A
45	11	309	KC2	CAA-CBA-CGA-O1A
45	12	311	KC2	CAA-CBA-CGA-O1A
45	12	311	KC2	CAA-CBA-CGA-O2A
45	18	308	KC2	CAA-CBA-CGA-O1A
45	18	308	KC2	CAA-CBA-CGA-O2A
45	18	310	KC2	CAA-CBA-CGA-O1A
45	18	310	KC2	CAA-CBA-CGA-O2A
31	0	316	CLA	CBA-CGA-O2A-C1
31	2	315	CLA	C2C-C3C-CAC-CBC
43	11	302	A86	C39-C38-O4-C34
31	B	608	CLA	C4-C3-C5-C6
31	P	601	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	b	609	CLA	C4-C3-C5-C6
31	p	601	CLA	C4-C3-C5-C6
31	12	308	CLA	C4-C3-C5-C6
31	B	602	CLA	C2-C3-C5-C6
31	b	603	CLA	C2-C3-C5-C6
31	12	308	CLA	C2-C3-C5-C6
31	19	308	CLA	C2-C3-C5-C6
31	B	606	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2A-CAA-CBA-CGA
31	C	508	CLA	C2A-CAA-CBA-CGA
31	b	607	CLA	C2A-CAA-CBA-CGA
31	b	611	CLA	C2A-CAA-CBA-CGA
31	c	508	CLA	C2A-CAA-CBA-CGA
31	1	313	CLA	C2A-CAA-CBA-CGA
31	14	312	CLA	C2A-CAA-CBA-CGA
31	A	404	CLA	O1D-CGD-O2D-CED
31	a	404	CLA	O1D-CGD-O2D-CED
31	B	601	CLA	C3-C5-C6-C7
31	C	504	CLA	C3-C5-C6-C7
31	b	602	CLA	C3-C5-C6-C7
31	c	504	CLA	C3-C5-C6-C7
31	8	312	CLA	C3-C5-C6-C7
31	18	312	CLA	C3-C5-C6-C7
31	P	601	CLA	CBA-CGA-O2A-C1
31	p	601	CLA	CBA-CGA-O2A-C1
31	0	309	CLA	CBA-CGA-O2A-C1
31	1	313	CLA	CBA-CGA-O2A-C1
31	3	313	CLA	CBA-CGA-O2A-C1
31	4	307	CLA	CBA-CGA-O2A-C1
31	7	313	CLA	CBA-CGA-O2A-C1
31	8	307	CLA	CBA-CGA-O2A-C1
31	9	312	CLA	CBA-CGA-O2A-C1
31	10	309	CLA	CBA-CGA-O2A-C1
31	14	312	CLA	CBA-CGA-O2A-C1
31	19	308	CLA	CBA-CGA-O2A-C1
34	L	102	SQD	C24-C23-O48-C46
34	l	101	SQD	C24-C23-O48-C46
38	J	101	LMG	C29-C28-O8-C9
38	j	101	LMG	C29-C28-O8-C9
34	B	623	SQD	C9-C10-C11-C12
34	b	601	SQD	C9-C10-C11-C12
31	11	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	18	309	CLA	O1D-CGD-O2D-CED
31	18	312	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	CBD-CGD-O2D-CED
31	1	313	CLA	O1D-CGD-O2D-CED
38	d	403	LMG	O9-C10-O7-C8
38	1	317	LMG	O9-C10-O7-C8
39	C	519	DGD	O1B-C1B-O2G-C2G
39	c	519	DGD	O1B-C1B-O2G-C2G
31	C	511	CLA	O1A-CGA-O2A-C1
31	c	511	CLA	O1A-CGA-O2A-C1
31	1	313	CLA	O1A-CGA-O2A-C1
31	9	312	CLA	O1A-CGA-O2A-C1
31	14	312	CLA	O1A-CGA-O2A-C1
31	18	306	CLA	O1A-CGA-O2A-C1
31	19	312	CLA	O1A-CGA-O2A-C1
36	Z	103	LHG	O10-C23-O8-C6
36	z	102	LHG	O10-C23-O8-C6
38	J	101	LMG	O10-C28-O8-C9
38	j	101	LMG	O10-C28-O8-C9
38	1	317	LMG	O10-C28-O8-C9
39	11	318	DGD	O1A-C1A-O1G-C1G
31	10	316	CLA	CBA-CGA-O2A-C1
36	8	316	LHG	C24-C23-O8-C6
43	15	303	A86	C39-C38-O4-C34
31	0	316	CLA	O1A-CGA-O2A-C1
43	14	301	A86	C1-C2-C3-C4
43	1	305	A86	O5-C38-O4-C34
43	9	301	A86	C39-C38-O4-C34
43	16	307	A86	C39-C38-O4-C34
43	19	301	A86	C39-C38-O4-C34
42	10	315	KC1	CAA-CBA-CGA-O1A
42	10	315	KC1	CAA-CBA-CGA-O2A
45	0	310	KC2	CAA-CBA-CGA-O2A
45	10	310	KC2	CAA-CBA-CGA-O1A
45	10	310	KC2	CAA-CBA-CGA-O2A
45	17	309	KC2	CAA-CBA-CGA-O1A
45	17	309	KC2	CAA-CBA-CGA-O2A
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	613	CLA	CBD-CGD-O2D-CED
31	P	605	CLA	CBD-CGD-O2D-CED
31	W	202	CLA	CBD-CGD-O2D-CED
31	b	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	615	CLA	CBD-CGD-O2D-CED
31	p	605	CLA	CBD-CGD-O2D-CED
31	w	203	CLA	CBD-CGD-O2D-CED
31	16	316	CLA	CBD-CGD-O2D-CED
42	17	314	KC1	CBD-CGD-O2D-CED
31	D	404	CLA	O1D-CGD-O2D-CED
31	d	404	CLA	O1D-CGD-O2D-CED
36	8	315	LHG	O2-C2-C3-O3
36	18	315	LHG	O2-C2-C3-O3
31	C	513	CLA	C3-C5-C6-C7
31	c	513	CLA	C3-C5-C6-C7
31	0	309	CLA	C3-C5-C6-C7
31	5	307	CLA	C3-C5-C6-C7
31	15	307	CLA	C3-C5-C6-C7
31	19	308	CLA	C3-C5-C6-C7
31	C	506	CLA	CBA-CGA-O2A-C1
31	D	405	CLA	CBA-CGA-O2A-C1
31	c	506	CLA	CBA-CGA-O2A-C1
31	d	405	CLA	CBA-CGA-O2A-C1
31	4	312	CLA	CBA-CGA-O2A-C1
31	9	308	CLA	CBA-CGA-O2A-C1
31	11	308	CLA	CBA-CGA-O2A-C1
31	14	307	CLA	CBA-CGA-O2A-C1
31	19	312	CLA	CBA-CGA-O2A-C1
36	5	317	LHG	C24-C23-O8-C6
36	15	316	LHG	C24-C23-O8-C6
38	W	201	LMG	C29-C28-O8-C9
38	w	201	LMG	C29-C28-O8-C9
43	0	301	A86	C39-C38-O4-C34
43	0	303	A86	C39-C38-O4-C34
43	1	320	A86	C39-C38-O4-C34
43	2	301	A86	C39-C38-O4-C34
43	2	302	A86	C39-C38-O4-C34
43	2	305	A86	C39-C38-O4-C34
43	2	305	A86	O5-C38-O4-C34
43	3	302	A86	C39-C38-O4-C34
43	3	306	A86	C39-C38-O4-C34
43	6	302	A86	C39-C38-O4-C34
43	7	301	A86	C39-C38-O4-C34
43	7	305	A86	C39-C38-O4-C34
43	7	305	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	8	305	A86	C39-C38-O4-C34
43	9	304	A86	C39-C38-O4-C34
43	10	301	A86	C39-C38-O4-C34
43	10	303	A86	C39-C38-O4-C34
43	10	318	A86	C39-C38-O4-C34
43	11	319	A86	C39-C38-O4-C34
43	12	301	A86	C39-C38-O4-C34
43	13	301	A86	C39-C38-O4-C34
43	16	303	A86	C39-C38-O4-C34
43	17	302	A86	C39-C38-O4-C34
43	17	306	A86	C39-C38-O4-C34
43	17	306	A86	O5-C38-O4-C34
43	17	316	A86	C39-C38-O4-C34
43	19	301	A86	O5-C38-O4-C34
43	19	304	A86	C39-C38-O4-C34
31	D	405	CLA	O1A-CGA-O2A-C1
31	d	405	CLA	O1A-CGA-O2A-C1
38	4	316	LMG	O6-C5-C6-O5
31	C	507	CLA	O1D-CGD-O2D-CED
31	c	507	CLA	O1D-CGD-O2D-CED
31	11	313	CLA	O1D-CGD-O2D-CED
42	11	314	KC1	O1D-CGD-O2D-CED
36	P	615	LHG	C8-C7-O7-C5
36	p	615	LHG	C8-C7-O7-C5
36	18	315	LHG	C8-C7-O7-C5
38	d	403	LMG	C11-C10-O7-C8
38	1	317	LMG	C11-C10-O7-C8
38	11	317	LMG	C11-C10-O7-C8
39	C	519	DGD	C2B-C1B-O2G-C2G
39	c	519	DGD	C2B-C1B-O2G-C2G
43	0	301	A86	O5-C38-O4-C34
43	0	303	A86	O5-C38-O4-C34
43	1	320	A86	O5-C38-O4-C34
43	2	301	A86	O5-C38-O4-C34
43	2	302	A86	O5-C38-O4-C34
43	3	302	A86	O5-C38-O4-C34
43	3	306	A86	O5-C38-O4-C34
43	5	301	A86	O5-C38-O4-C34
43	5	303	A86	O5-C38-O4-C34
43	6	302	A86	O5-C38-O4-C34
43	6	305	A86	O5-C38-O4-C34
43	6	306	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	7	301	A86	O5-C38-O4-C34
43	8	305	A86	O5-C38-O4-C34
43	9	301	A86	O5-C38-O4-C34
43	9	303	A86	O5-C38-O4-C34
43	9	304	A86	O5-C38-O4-C34
43	10	301	A86	O5-C38-O4-C34
43	10	303	A86	O5-C38-O4-C34
43	10	318	A86	O5-C38-O4-C34
43	11	302	A86	O5-C38-O4-C34
43	11	319	A86	O5-C38-O4-C34
43	11	320	A86	O5-C38-O4-C34
43	12	301	A86	O5-C38-O4-C34
43	13	301	A86	O5-C38-O4-C34
43	15	301	A86	O5-C38-O4-C34
43	15	303	A86	O5-C38-O4-C34
43	16	303	A86	O5-C38-O4-C34
43	16	306	A86	O5-C38-O4-C34
43	16	307	A86	O5-C38-O4-C34
43	17	302	A86	O5-C38-O4-C34
43	17	316	A86	O5-C38-O4-C34
43	19	303	A86	O5-C38-O4-C34
43	19	304	A86	O5-C38-O4-C34
31	4	311	CLA	CBA-CGA-O2A-C1
31	14	311	CLA	CBA-CGA-O2A-C1
31	19	311	CLA	CBA-CGA-O2A-C1
31	6	316	CLA	CBD-CGD-O2D-CED
31	15	307	CLA	CBD-CGD-O2D-CED
38	J	101	LMG	C11-C12-C13-C14
38	j	101	LMG	C11-C12-C13-C14
43	3	301	A86	C35-C34-O4-C38
43	17	301	A86	C35-C34-O4-C38
31	14	307	CLA	O1A-CGA-O2A-C1
38	K	101	LMG	C11-C12-C13-C14
38	k	101	LMG	C11-C12-C13-C14
38	4	316	LMG	C32-C33-C34-C35
38	14	316	LMG	O6-C5-C6-O5
31	9	315	CLA	O1D-CGD-O2D-CED
31	C	511	CLA	CBA-CGA-O2A-C1
31	c	511	CLA	CBA-CGA-O2A-C1
31	18	306	CLA	CBA-CGA-O2A-C1
38	14	316	LMG	C29-C28-O8-C9
31	B	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	608	CLA	O1D-CGD-O2D-CED
39	W	203	DGD	O6E-C5E-C6E-O5E
39	w	204	DGD	O6E-C5E-C6E-O5E
45	0	310	KC2	CAA-CBA-CGA-O1A
45	11	309	KC2	CAA-CBA-CGA-O2A
45	15	308	KC2	CAA-CBA-CGA-O1A
34	A	411	SQD	C26-C27-C28-C29
34	i	101	SQD	C26-C27-C28-C29
36	14	317	LHG	C5-C4-O6-P
31	C	506	CLA	O1A-CGA-O2A-C1
31	P	601	CLA	O1A-CGA-O2A-C1
31	c	506	CLA	O1A-CGA-O2A-C1
31	p	601	CLA	O1A-CGA-O2A-C1
31	4	312	CLA	O1A-CGA-O2A-C1
38	5	315	LMG	O10-C28-O8-C9
38	15	314	LMG	O10-C28-O8-C9
39	1	318	DGD	O1A-C1A-O1G-C1G
41	V	201	HEM	C3D-CAD-CBD-CGD
41	v	201	HEM	C3D-CAD-CBD-CGD
38	11	317	LMG	C29-C30-C31-C32
31	14	311	CLA	O1A-CGA-O2A-C1
38	P	614	LMG	O6-C5-C6-O5
38	p	614	LMG	O6-C5-C6-O5
39	H	102	DGD	O6E-C5E-C6E-O5E
39	h	102	DGD	O6E-C5E-C6E-O5E
31	C	503	CLA	C4-C3-C5-C6
31	C	505	CLA	C4-C3-C5-C6
31	C	508	CLA	C4-C3-C5-C6
31	C	513	CLA	C4-C3-C5-C6
31	c	503	CLA	C4-C3-C5-C6
31	c	505	CLA	C4-C3-C5-C6
31	c	508	CLA	C4-C3-C5-C6
31	c	513	CLA	C4-C3-C5-C6
31	C	503	CLA	C2-C3-C5-C6
31	C	505	CLA	C2-C3-C5-C6
31	C	508	CLA	C2-C3-C5-C6
31	C	513	CLA	C2-C3-C5-C6
31	c	503	CLA	C2-C3-C5-C6
31	c	505	CLA	C2-C3-C5-C6
31	c	508	CLA	C2-C3-C5-C6
31	c	513	CLA	C2-C3-C5-C6
43	2	303	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
43	9	306	A86	C35-C34-O4-C38
31	B	601	CLA	C2A-CAA-CBA-CGA
31	R	101	CLA	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	r	101	CLA	C2A-CAA-CBA-CGA
31	4	307	CLA	O1D-CGD-O2D-CED
31	4	309	CLA	O1D-CGD-O2D-CED
31	4	307	CLA	O1A-CGA-O2A-C1
34	l	101	SQD	O10-C23-O48-C46
38	0	317	LMG	O10-C28-O8-C9
38	C	522	LMG	O6-C1-O1-C7
38	c	521	LMG	O6-C1-O1-C7
38	w	201	LMG	O6-C1-O1-C7
35	A	409	PL9	C14-C16-C17-C18
35	A	409	PL9	C19-C21-C22-C23
35	a	409	PL9	C14-C16-C17-C18
35	a	409	PL9	C19-C21-C22-C23
43	4	303	A86	C39-C38-O4-C34
31	4	311	CLA	O1A-CGA-O2A-C1
36	Z	103	LHG	C24-C23-O8-C6
38	1	317	LMG	C29-C28-O8-C9
39	11	318	DGD	C2A-C1A-O1G-C1G
31	c	509	CLA	O1D-CGD-O2D-CED
31	9	311	CLA	CBA-CGA-O2A-C1
39	B	621	DGD	O6D-C5D-C6D-O5D
39	b	622	DGD	O6D-C5D-C6D-O5D
31	C	509	CLA	O1D-CGD-O2D-CED
31	C	514	CLA	O1D-CGD-O2D-CED
31	c	514	CLA	O1D-CGD-O2D-CED
31	10	308	CLA	O1D-CGD-O2D-CED
31	14	309	CLA	O1D-CGD-O2D-CED
31	19	315	CLA	O1D-CGD-O2D-CED
31	11	308	CLA	O1A-CGA-O2A-C1
34	L	102	SQD	O10-C23-O48-C46
38	D	403	LMG	C11-C10-O7-C8
42	P	609	KC1	CAA-CBA-CGA-O2A
42	p	609	KC1	CAA-CBA-CGA-O2A
42	4	313	KC1	CAA-CBA-CGA-O1A
42	14	313	KC1	CAA-CBA-CGA-O1A
45	4	310	KC2	CAA-CBA-CGA-O2A
45	5	308	KC2	CAA-CBA-CGA-O2A
45	9	309	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	13	311	KC2	CAA-CBA-CGA-O2A
45	14	310	KC2	CAA-CBA-CGA-O1A
45	14	310	KC2	CAA-CBA-CGA-O2A
45	19	309	KC2	CAA-CBA-CGA-O2A
43	0	306	A86	C35-C34-O4-C38
43	5	318	A86	C35-C34-O4-C38
43	9	301	A86	C35-C34-O4-C38
43	11	302	A86	C33-C34-O4-C38
43	12	303	A86	C35-C34-O4-C38
43	12	306	A86	C33-C34-O4-C38
43	19	301	A86	C35-C34-O4-C38
35	A	409	PL9	C17-C18-C19-C20
35	a	409	PL9	C17-C18-C19-C20
31	P	603	CLA	O1D-CGD-O2D-CED
31	p	603	CLA	O1D-CGD-O2D-CED
31	B	608	CLA	CBD-CGD-O2D-CED
31	4	314	CLA	O1D-CGD-O2D-CED
36	18	315	LHG	C1-C2-C3-O3
38	J	101	LMG	O9-C10-O7-C8
38	j	101	LMG	O9-C10-O7-C8
31	P	610	CLA	O1D-CGD-O2D-CED
31	p	610	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	CBA-CGA-O2A-C1
31	b	611	CLA	CBA-CGA-O2A-C1
31	1	308	CLA	CBA-CGA-O2A-C1
31	2	312	CLA	CBA-CGA-O2A-C1
31	9	313	CLA	CBA-CGA-O2A-C1
31	12	313	CLA	CBA-CGA-O2A-C1
31	19	313	CLA	CBA-CGA-O2A-C1
36	z	102	LHG	C24-C23-O8-C6
38	5	315	LMG	C29-C28-O8-C9
38	15	315	LMG	C29-C28-O8-C9
39	C	520	DGD	C2A-C1A-O1G-C1G
39	c	520	DGD	C2A-C1A-O1G-C1G
39	1	318	DGD	C2A-C1A-O1G-C1G
36	18	316	LHG	C24-C23-O8-C6
39	C	518	DGD	O6E-C5E-C6E-O5E
39	c	518	DGD	O6E-C5E-C6E-O5E
31	b	609	CLA	CBD-CGD-O2D-CED
38	4	316	LMG	C4-C5-C6-O5
31	10	316	CLA	O1A-CGA-O2A-C1
33	B	618	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
43	14	302	A86	C24-C25-C26-C27
43	18	302	A86	C3-C4-C5-C6
43	0	302	A86	C35-C34-O4-C38
43	3	304	A86	C35-C34-O4-C38
43	5	305	A86	C35-C34-O4-C38
36	18	315	LHG	C7-C8-C9-C10
38	10	319	LMG	C28-C29-C30-C31
31	B	613	CLA	C13-C15-C16-C17
31	P	602	CLA	C10-C11-C12-C13
31	p	602	CLA	C10-C11-C12-C13
38	14	316	LMG	C4-C5-C6-O5
39	H	102	DGD	C4E-C5E-C6E-O5E
39	h	102	DGD	C4E-C5E-C6E-O5E
36	C	521	LHG	C29-C30-C31-C32
36	w	202	LHG	C29-C30-C31-C32
42	P	609	KC1	CAA-CBA-CGA-O1A
42	p	609	KC1	CAA-CBA-CGA-O1A
42	9	314	KC1	CAA-CBA-CGA-O2A
42	11	314	KC1	CAA-CBA-CGA-O2A
42	14	313	KC1	CAA-CBA-CGA-O2A
42	19	314	KC1	CAA-CBA-CGA-O1A
42	19	314	KC1	CAA-CBA-CGA-O2A
45	5	308	KC2	CAA-CBA-CGA-O1A
45	6	310	KC2	CAA-CBA-CGA-O1A
45	13	309	KC2	CAA-CBA-CGA-O2A
45	13	311	KC2	CAA-CBA-CGA-O1A
45	16	310	KC2	CAA-CBA-CGA-O2A
45	19	309	KC2	CAA-CBA-CGA-O1A
36	P	615	LHG	O6-C4-C5-O7
36	p	615	LHG	O6-C4-C5-O7
38	P	614	LMG	C4-C5-C6-O5
38	p	614	LMG	C4-C5-C6-O5
31	B	604	CLA	C13-C15-C16-C17
31	W	202	CLA	C10-C11-C12-C13
31	b	605	CLA	C13-C15-C16-C17
31	b	614	CLA	C13-C15-C16-C17
31	w	203	CLA	C10-C11-C12-C13
31	0	309	CLA	C5-C6-C7-C8
31	3	316	CLA	C5-C6-C7-C8
31	4	309	CLA	C5-C6-C7-C8
31	9	313	CLA	C8-C10-C11-C12
31	11	308	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	13	316	CLA	C5-C6-C7-C8
31	9	308	CLA	C3-C5-C6-C7
39	C	520	DGD	C1A-C2A-C3A-C4A
39	c	520	DGD	C1A-C2A-C3A-C4A
38	C	522	LMG	C2-C1-O1-C7
38	c	521	LMG	C2-C1-O1-C7
38	1	317	LMG	C2-C1-O1-C7
39	11	318	DGD	C2E-C1E-O5D-C6D
38	B	620	LMG	O7-C8-C9-O8
38	K	101	LMG	O7-C8-C9-O8
38	b	621	LMG	O7-C8-C9-O8
38	k	101	LMG	O7-C8-C9-O8
38	5	316	LMG	O7-C8-C9-O8
36	18	316	LHG	C12-C13-C14-C15
31	19	313	CLA	O1A-CGA-O2A-C1
38	n	701	LMG	O10-C28-O8-C9
31	19	307	CLA	C4-C3-C5-C6
31	P	601	CLA	C2-C3-C5-C6
31	p	601	CLA	C2-C3-C5-C6
31	B	601	CLA	C11-C10-C8-C9
31	B	601	CLA	C14-C13-C15-C16
31	B	605	CLA	C6-C7-C8-C9
31	B	605	CLA	C14-C13-C15-C16
31	B	614	CLA	C11-C10-C8-C9
31	C	504	CLA	C11-C12-C13-C14
31	C	505	CLA	C11-C12-C13-C14
31	C	513	CLA	C6-C7-C8-C9
31	b	602	CLA	C11-C10-C8-C9
31	b	606	CLA	C6-C7-C8-C9
31	b	606	CLA	C14-C13-C15-C16
31	b	615	CLA	C11-C10-C8-C9
31	c	504	CLA	C11-C12-C13-C14
31	c	505	CLA	C11-C12-C13-C14
31	c	513	CLA	C6-C7-C8-C9
31	0	309	CLA	C6-C7-C8-C9
31	1	308	CLA	C14-C13-C15-C16
31	1	321	CLA	C11-C10-C8-C9
31	10	309	CLA	C6-C7-C8-C9
31	12	308	CLA	C6-C7-C8-C9
31	13	316	CLA	C11-C12-C13-C14
31	14	306	CLA	C6-C7-C8-C9
31	14	306	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	19	308	CLA	C6-C7-C8-C9
31	0	308	CLA	O1D-CGD-O2D-CED
31	0	309	CLA	O1D-CGD-O2D-CED
31	5	309	CLA	O1D-CGD-O2D-CED
31	14	314	CLA	O1D-CGD-O2D-CED
31	15	309	CLA	O1D-CGD-O2D-CED
43	3	305	A86	C35-C34-O4-C38
43	4	304	A86	C35-C34-O4-C38
43	18	304	A86	C35-C34-O4-C38
31	C	504	CLA	C2A-CAA-CBA-CGA
31	c	504	CLA	C2A-CAA-CBA-CGA
31	11	313	CLA	C2A-CAA-CBA-CGA
33	F	101	BCR	C11-C12-C13-C35
33	f	101	BCR	C11-C12-C13-C35
43	1	304	A86	C7-C6-C8-C9
43	3	302	A86	C7-C6-C8-C9
43	6	307	A86	C7-C6-C8-C9
43	14	301	A86	C-C1-C24-C25
43	16	303	A86	C7-C6-C8-C9
43	17	302	A86	C7-C6-C8-C9
33	B	617	BCR	C7-C8-C9-C10
33	b	618	BCR	C7-C8-C9-C10
31	9	307	CLA	O1D-CGD-O2D-CED
38	K	101	LMG	O9-C10-O7-C8
38	k	101	LMG	O9-C10-O7-C8
36	A	410	LHG	C7-C8-C9-C10
36	D	407	LHG	C23-C24-C25-C26
36	a	410	LHG	C7-C8-C9-C10
36	d	407	LHG	C23-C24-C25-C26
38	B	620	LMG	C28-C29-C30-C31
38	b	621	LMG	C28-C29-C30-C31
38	d	403	LMG	C10-C11-C12-C13
38	m	101	LMG	C10-C11-C12-C13
38	1	317	LMG	C28-C29-C30-C31
39	H	102	DGD	O6D-C5D-C6D-O5D
39	h	102	DGD	O6D-C5D-C6D-O5D
31	1	308	CLA	O1A-CGA-O2A-C1
31	9	313	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	C5-C6-C7-C8
31	B	605	CLA	C8-C10-C11-C12
31	C	504	CLA	C13-C15-C16-C17
31	b	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	b	606	CLA	C8-C10-C11-C12
31	b	608	CLA	C15-C16-C17-C18
31	c	504	CLA	C13-C15-C16-C17
31	3	313	CLA	C5-C6-C7-C8
31	19	313	CLA	C8-C10-C11-C12
42	9	314	KC1	CAA-CBA-CGA-O1A
42	11	314	KC1	CAA-CBA-CGA-O1A
45	4	310	KC2	CAA-CBA-CGA-O1A
45	6	310	KC2	CAA-CBA-CGA-O2A
45	11	311	KC2	CAA-CBA-CGA-O1A
45	11	311	KC2	CAA-CBA-CGA-O2A
45	13	309	KC2	CAA-CBA-CGA-O1A
45	16	310	KC2	CAA-CBA-CGA-O1A
31	17	315	CLA	O1D-CGD-O2D-CED
31	4	315	CLA	C2A-CAA-CBA-CGA
31	14	315	CLA	C2A-CAA-CBA-CGA
34	10	320	SQD	C24-C23-O48-C46
38	K	101	LMG	C29-C28-O8-C9
38	d	403	LMG	C29-C28-O8-C9
38	k	101	LMG	C29-C28-O8-C9
38	0	317	LMG	C29-C28-O8-C9
38	5	316	LMG	C29-C28-O8-C9
31	B	611	CLA	C10-C11-C12-C13
31	B	616	CLA	C13-C15-C16-C17
31	C	506	CLA	C15-C16-C17-C18
31	c	503	CLA	C10-C11-C12-C13
31	c	506	CLA	C15-C16-C17-C18
31	1	321	CLA	C8-C10-C11-C12
31	3	316	CLA	C8-C10-C11-C12
31	9	310	CLA	C8-C10-C11-C12
31	10	309	CLA	C5-C6-C7-C8
31	13	313	CLA	C5-C6-C7-C8
31	14	306	CLA	C5-C6-C7-C8
38	W	201	LMG	O6-C5-C6-O5
38	w	201	LMG	O6-C5-C6-O5
43	1	304	A86	C35-C34-O4-C38
43	14	303	A86	C35-C34-O4-C38
36	8	315	LHG	C7-C8-C9-C10
39	B	621	DGD	C1A-C2A-C3A-C4A
39	W	203	DGD	C1B-C2B-C3B-C4B
39	b	622	DGD	C1A-C2A-C3A-C4A
39	w	204	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
31	10	309	CLA	O1D-CGD-O2D-CED
31	19	307	CLA	O1D-CGD-O2D-CED
33	F	101	BCR	C14-C15-C16-C17
33	f	101	BCR	C14-C15-C16-C17
31	C	511	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	C5-C6-C7-C8
31	B	612	CLA	C13-C15-C16-C17
31	C	503	CLA	C10-C11-C12-C13
31	C	506	CLA	C10-C11-C12-C13
31	C	508	CLA	C15-C16-C17-C18
31	C	511	CLA	C5-C6-C7-C8
31	b	604	CLA	C5-C6-C7-C8
31	b	612	CLA	C10-C11-C12-C13
31	b	613	CLA	C13-C15-C16-C17
31	c	506	CLA	C10-C11-C12-C13
31	c	508	CLA	C15-C16-C17-C18
31	c	511	CLA	C5-C6-C7-C8
31	9	308	CLA	C15-C16-C17-C18
31	14	306	CLA	C10-C11-C12-C13
31	19	308	CLA	C15-C16-C17-C18
31	14	311	CLA	C2C-C3C-CAC-CBC
31	C	508	CLA	O1D-CGD-O2D-CED
31	c	508	CLA	O1D-CGD-O2D-CED
31	c	511	CLA	O1D-CGD-O2D-CED
31	17	313	CLA	O1D-CGD-O2D-CED
35	A	409	PL9	C12-C13-C14-C15
35	a	409	PL9	C12-C13-C14-C15
36	C	521	LHG	C23-C24-C25-C26
36	w	202	LHG	C23-C24-C25-C26
38	C	522	LMG	C10-C11-C12-C13
38	D	408	LMG	C10-C11-C12-C13
38	D	408	LMG	C28-C29-C30-C31
38	F	102	LMG	C10-C11-C12-C13
38	J	101	LMG	C10-C11-C12-C13
38	M	101	LMG	C10-C11-C12-C13
38	Z	102	LMG	C28-C29-C30-C31
38	c	521	LMG	C10-C11-C12-C13
38	c	522	LMG	C28-C29-C30-C31
38	d	408	LMG	C10-C11-C12-C13
38	d	408	LMG	C28-C29-C30-C31
38	f	102	LMG	C10-C11-C12-C13
38	j	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	m	101	LMG	C28-C29-C30-C31
38	11	317	LMG	C28-C29-C30-C31
38	15	314	LMG	C10-C11-C12-C13
39	C	519	DGD	C1A-C2A-C3A-C4A
39	c	519	DGD	C1A-C2A-C3A-C4A
31	b	607	CLA	C15-C16-C17-C18
31	Z	101	CLA	CBA-CGA-O2A-C1
31	z	101	CLA	CBA-CGA-O2A-C1
34	0	318	SQD	C24-C23-O48-C46
38	15	314	LMG	C29-C28-O8-C9
36	D	407	LHG	C32-C33-C34-C35
36	d	407	LHG	C32-C33-C34-C35
43	P	613	A86	C35-C34-O4-C38
43	p	613	A86	C35-C34-O4-C38
43	1	306	A86	C35-C34-O4-C38
43	4	306	A86	C35-C34-O4-C38
43	5	304	A86	C35-C34-O4-C38
43	6	301	A86	C33-C34-O4-C38
43	6	301	A86	C35-C34-O4-C38
43	12	304	A86	C35-C34-O4-C38
43	16	304	A86	C35-C34-O4-C38
43	17	301	A86	C33-C34-O4-C38
31	0	314	CLA	O1D-CGD-O2D-CED
45	9	309	KC2	CAA-CBA-CGA-O1A
31	4	312	CLA	C2-C1-O2A-CGA
31	B	607	CLA	C15-C16-C17-C18
31	B	609	CLA	C5-C6-C7-C8
31	C	502	CLA	C15-C16-C17-C18
31	b	610	CLA	C5-C6-C7-C8
31	b	610	CLA	C13-C15-C16-C17
31	b	617	CLA	C13-C15-C16-C17
31	c	502	CLA	C15-C16-C17-C18
31	1	321	CLA	C10-C11-C12-C13
31	14	306	CLA	C8-C10-C11-C12
31	19	310	CLA	C8-C10-C11-C12
32	A	405	PHO	C5-C6-C7-C8
32	a	405	PHO	C5-C6-C7-C8
36	L	101	LHG	C7-C8-C9-C10
36	l	102	LHG	C7-C8-C9-C10
38	k	101	LMG	C10-C11-C12-C13
39	H	102	DGD	C1A-C2A-C3A-C4A
39	h	102	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
32	A	405	PHO	CBD-CGD-O2D-CED
32	a	405	PHO	CBD-CGD-O2D-CED
42	18	313	KC1	CBD-CGD-O2D-CED
45	12	311	KC2	CBD-CGD-O2D-CED
38	J	101	LMG	C11-C10-O7-C8
38	j	101	LMG	C11-C10-O7-C8
31	B	606	CLA	C15-C16-C17-C18
31	B	609	CLA	C13-C15-C16-C17
31	C	504	CLA	C5-C6-C7-C8
31	c	504	CLA	C5-C6-C7-C8
31	B	611	CLA	C12-C13-C15-C16
31	b	612	CLA	C12-C13-C15-C16
31	14	306	CLA	C6-C7-C8-C10
31	14	309	CLA	C6-C7-C8-C10
31	2	312	CLA	O1A-CGA-O2A-C1
31	12	313	CLA	O1A-CGA-O2A-C1
38	N	101	LMG	O10-C28-O8-C9
39	C	520	DGD	O1A-C1A-O1G-C1G
39	c	520	DGD	O1A-C1A-O1G-C1G
33	b	619	BCR	C13-C14-C15-C16
43	14	301	A86	C24-C25-C26-C27
43	18	302	A86	C11-C10-C9-C8
38	K	101	LMG	C10-C11-C12-C13
31	0	312	CLA	C2A-CAA-CBA-CGA
31	3	313	CLA	C2A-CAA-CBA-CGA
42	2	313	KC1	O1D-CGD-O2D-CED
45	14	308	KC2	O1D-CGD-O2D-CED
39	b	622	DGD	C4D-C5D-C6D-O5D
31	B	601	CLA	C5-C6-C7-C8
31	B	601	CLA	C13-C15-C16-C17
31	C	504	CLA	C10-C11-C12-C13
31	C	509	CLA	C10-C11-C12-C13
31	W	202	CLA	C8-C10-C11-C12
31	b	602	CLA	C5-C6-C7-C8
31	b	602	CLA	C13-C15-C16-C17
31	c	504	CLA	C10-C11-C12-C13
31	c	509	CLA	C10-C11-C12-C13
31	w	203	CLA	C8-C10-C11-C12
31	1	308	CLA	C10-C11-C12-C13
31	12	308	CLA	C8-C10-C11-C12
31	19	313	CLA	C5-C6-C7-C8
31	B	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	b	611	CLA	O1A-CGA-O2A-C1
34	0	318	SQD	O5-C1-O6-C44
38	W	201	LMG	O6-C1-O1-C7
39	C	519	DGD	O6E-C1E-O5D-C6D
39	C	520	DGD	O6E-C1E-O5D-C6D
39	c	519	DGD	O6E-C1E-O5D-C6D
39	c	520	DGD	O6E-C1E-O5D-C6D
31	C	505	CLA	C10-C11-C12-C13
31	c	505	CLA	C10-C11-C12-C13
31	19	308	CLA	C8-C10-C11-C12
36	B	622	LHG	C7-C8-C9-C10
38	M	101	LMG	C28-C29-C30-C31
33	B	619	BCR	C18-C19-C20-C21
33	b	620	BCR	C18-C19-C20-C21
36	D	407	LHG	O2-C2-C3-O3
36	d	407	LHG	O2-C2-C3-O3
36	18	315	LHG	O9-C7-O7-C5
39	B	621	DGD	O1B-C1B-O2G-C2G
39	W	203	DGD	C4E-C5E-C6E-O5E
39	w	204	DGD	C4E-C5E-C6E-O5E
43	9	305	A86	C35-C34-O4-C38
43	10	302	A86	C35-C34-O4-C38
31	19	311	CLA	O1A-CGA-O2A-C1
31	B	608	CLA	C5-C6-C7-C8
31	B	611	CLA	C5-C6-C7-C8
31	B	612	CLA	C10-C11-C12-C13
31	b	609	CLA	C5-C6-C7-C8
31	b	612	CLA	C5-C6-C7-C8
31	b	613	CLA	C10-C11-C12-C13
31	3	313	CLA	C15-C16-C17-C18
31	9	312	CLA	C15-C16-C17-C18
31	9	313	CLA	C5-C6-C7-C8
31	11	308	CLA	C13-C15-C16-C17
38	11	317	LMG	C29-C28-O8-C9
31	18	314	CLA	C2C-C3C-CAC-CBC
38	4	316	LMG	O10-C28-O8-C9
31	A	403	CLA	C15-C16-C17-C18
31	B	605	CLA	C5-C6-C7-C8
31	B	611	CLA	C8-C10-C11-C12
31	C	506	CLA	C5-C6-C7-C8
31	a	403	CLA	C15-C16-C17-C18
31	b	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	b	612	CLA	C8-C10-C11-C12
31	b	616	CLA	C10-C11-C12-C13
31	c	506	CLA	C5-C6-C7-C8
31	3	316	CLA	C15-C16-C17-C18
31	9	308	CLA	C13-C15-C16-C17
38	14	316	LMG	C32-C33-C34-C35
31	B	604	CLA	O1D-CGD-O2D-CED
31	b	605	CLA	O1D-CGD-O2D-CED
31	Z	101	CLA	O1A-CGA-O2A-C1
31	z	101	CLA	O1A-CGA-O2A-C1
36	8	315	LHG	C8-C7-O7-C5
39	B	621	DGD	C4D-C5D-C6D-O5D
31	B	608	CLA	C15-C16-C17-C18
31	B	613	CLA	C15-C16-C17-C18
31	B	615	CLA	C10-C11-C12-C13
31	D	401	CLA	C10-C11-C12-C13
31	P	601	CLA	C13-C15-C16-C17
31	b	609	CLA	C15-C16-C17-C18
31	b	614	CLA	C15-C16-C17-C18
31	d	401	CLA	C10-C11-C12-C13
31	p	601	CLA	C13-C15-C16-C17
31	1	313	CLA	C5-C6-C7-C8
31	9	308	CLA	C8-C10-C11-C12
31	14	309	CLA	C5-C6-C7-C8
31	19	308	CLA	C13-C15-C16-C17
43	13	303	A86	C35-C34-O4-C38
36	A	410	LHG	C3-O3-P-O6
36	D	407	LHG	C3-O3-P-O6
36	D	407	LHG	C4-O6-P-O3
36	L	101	LHG	C3-O3-P-O6
36	P	615	LHG	C3-O3-P-O6
36	Z	103	LHG	C4-O6-P-O3
36	a	410	LHG	C3-O3-P-O6
36	d	407	LHG	C3-O3-P-O6
36	d	407	LHG	C4-O6-P-O3
36	l	102	LHG	C3-O3-P-O6
36	p	615	LHG	C3-O3-P-O6
36	z	102	LHG	C4-O6-P-O3
36	8	315	LHG	C3-O3-P-O6
36	15	316	LHG	C4-O6-P-O3
36	18	315	LHG	C3-O3-P-O6
36	b	623	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
38	15	314	LMG	C28-C29-C30-C31
31	C	512	CLA	CBA-CGA-O2A-C1
31	C	513	CLA	CBA-CGA-O2A-C1
31	W	202	CLA	CBA-CGA-O2A-C1
31	c	512	CLA	CBA-CGA-O2A-C1
31	c	513	CLA	CBA-CGA-O2A-C1
31	w	203	CLA	CBA-CGA-O2A-C1
42	7	314	KC1	O1D-CGD-O2D-CED
31	B	613	CLA	C8-C10-C11-C12
31	b	614	CLA	C8-C10-C11-C12
31	0	311	CLA	C5-C6-C7-C8
31	10	311	CLA	C5-C6-C7-C8
31	14	314	CLA	C2A-CAA-CBA-CGA
39	W	203	DGD	C4D-C5D-C6D-O5D
39	w	204	DGD	C4D-C5D-C6D-O5D
31	7	315	CLA	O1D-CGD-O2D-CED
36	D	407	LHG	C1-C2-C3-O3
36	d	407	LHG	C1-C2-C3-O3
34	0	318	SQD	O49-C7-O47-C45
31	6	309	CLA	C4-C3-C5-C6
31	14	307	CLA	C4-C3-C5-C6
31	18	307	CLA	C4-C3-C5-C6
31	p	602	CLA	C15-C16-C17-C18
43	7	303	A86	C35-C34-O4-C38
43	10	306	A86	C35-C34-O4-C38
43	14	305	A86	C35-C34-O4-C38
43	17	304	A86	C35-C34-O4-C38
39	1	318	DGD	C6B-C7B-C8B-C9B
31	C	502	CLA	C2A-CAA-CBA-CGA
31	c	502	CLA	C2A-CAA-CBA-CGA
31	4	312	CLA	C2A-CAA-CBA-CGA
31	c	507	CLA	C16-C17-C18-C20
31	11	308	CLA	C16-C17-C18-C19
31	15	307	CLA	CBA-CGA-O2A-C1
36	L	101	LHG	C24-C23-O8-C6
36	l	102	LHG	C24-C23-O8-C6
38	Z	102	LMG	C29-C28-O8-C9
38	c	522	LMG	C29-C28-O8-C9
31	P	602	CLA	C15-C16-C17-C18
43	11	304	A86	C35-C34-O4-C38
43	15	305	A86	C35-C34-O4-C38
36	B	622	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
36	b	623	LHG	C25-C26-C27-C28
38	J	101	LMG	C17-C18-C19-C20
38	4	316	LMG	C36-C37-C38-C39
36	5	317	LHG	C8-C7-O7-C5
36	15	316	LHG	C8-C7-O7-C5
38	M	101	LMG	C11-C10-O7-C8
38	m	101	LMG	C11-C10-O7-C8
31	4	307	CLA	C10-C11-C12-C13
31	11	313	CLA	C5-C6-C7-C8
31	14	307	CLA	C10-C11-C12-C13
33	B	619	BCR	C16-C17-C18-C36
33	B	619	BCR	C20-C21-C22-C37
33	C	515	BCR	C16-C17-C18-C36
33	C	517	BCR	C11-C10-C9-C34
33	H	101	BCR	C11-C10-C9-C34
33	b	620	BCR	C16-C17-C18-C36
33	b	620	BCR	C20-C21-C22-C37
33	c	515	BCR	C16-C17-C18-C36
33	c	517	BCR	C11-C10-C9-C34
33	h	101	BCR	C11-C10-C9-C34
34	L	102	SQD	C16-C17-C18-C19
34	10	320	SQD	C9-C10-C11-C12
34	10	320	SQD	C24-C25-C26-C27
36	D	407	LHG	C9-C10-C11-C12
36	d	407	LHG	C9-C10-C11-C12
36	4	317	LHG	C14-C15-C16-C17
36	14	317	LHG	C12-C13-C14-C15
38	D	403	LMG	C30-C31-C32-C33
38	D	408	LMG	C31-C32-C33-C34
38	D	408	LMG	C32-C33-C34-C35
38	J	101	LMG	C30-C31-C32-C33
38	d	408	LMG	C31-C32-C33-C34
38	d	408	LMG	C32-C33-C34-C35
38	j	101	LMG	C17-C18-C19-C20
38	j	101	LMG	C30-C31-C32-C33
38	0	317	LMG	C11-C12-C13-C14
38	14	316	LMG	C16-C17-C18-C19
39	B	621	DGD	C6B-C7B-C8B-C9B
39	H	102	DGD	C6A-C7A-C8A-C9A
39	c	518	DGD	C2B-C3B-C4B-C5B
39	1	318	DGD	C2B-C3B-C4B-C5B
31	C	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	P	602	CLA	C16-C17-C18-C20
31	p	602	CLA	C16-C17-C18-C20
31	4	309	CLA	C16-C17-C18-C20
31	B	612	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	5	307	CLA	CBA-CGA-O2A-C1
34	l	101	SQD	C16-C17-C18-C19
34	0	318	SQD	C24-C25-C26-C27
36	B	622	LHG	C29-C30-C31-C32
36	D	407	LHG	C31-C32-C33-C34
36	b	623	LHG	C29-C30-C31-C32
36	d	407	LHG	C31-C32-C33-C34
38	C	522	LMG	C18-C19-C20-C21
38	D	403	LMG	C11-C12-C13-C14
38	c	521	LMG	C16-C17-C18-C19
38	c	521	LMG	C18-C19-C20-C21
38	c	521	LMG	C31-C32-C33-C34
38	1	317	LMG	C29-C30-C31-C32
38	4	316	LMG	C16-C17-C18-C19
38	11	317	LMG	C14-C15-C16-C17
38	15	315	LMG	C33-C34-C35-C36
39	C	518	DGD	C2B-C3B-C4B-C5B
39	H	102	DGD	CBA-CCA-CDA-CEA
39	b	622	DGD	C5A-C6A-C7A-C8A
39	h	102	DGD	C6A-C7A-C8A-C9A
39	h	102	DGD	CBA-CCA-CDA-CEA
34	L	102	SQD	O49-C7-O47-C45
34	l	101	SQD	O49-C7-O47-C45
39	b	622	DGD	O1B-C1B-O2G-C2G
45	12	309	KC2	CAA-CBA-CGA-O2A
31	19	312	CLA	C15-C16-C17-C18
34	0	318	SQD	C11-C12-C13-C14
38	C	522	LMG	C31-C32-C33-C34
38	w	201	LMG	C37-C38-C39-C40
38	1	317	LMG	C14-C15-C16-C17
38	14	316	LMG	C36-C37-C38-C39
38	15	314	LMG	C16-C17-C18-C19
31	W	202	CLA	O1D-CGD-O2D-CED
31	w	203	CLA	O1D-CGD-O2D-CED
43	13	305	A86	C35-C34-O4-C38
43	15	304	A86	C35-C34-O4-C38
34	A	408	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	a	408	SQD	C18-C19-C20-C21
36	18	316	LHG	C9-C10-C11-C12
38	C	522	LMG	C16-C17-C18-C19
38	W	201	LMG	C37-C38-C39-C40
39	B	621	DGD	C5A-C6A-C7A-C8A
39	C	519	DGD	C2B-C3B-C4B-C5B
39	C	519	DGD	CBB-CCB-CDB-CEB
39	C	520	DGD	CCA-CDA-CEA-CFA
39	c	519	DGD	C2B-C3B-C4B-C5B
39	c	519	DGD	CBB-CCB-CDB-CEB
39	c	520	DGD	CCA-CDA-CEA-CFA
39	11	318	DGD	C7B-C8B-C9B-CAB
38	J	101	LMG	C4-C5-C6-O5
38	j	101	LMG	C4-C5-C6-O5
31	B	604	CLA	C10-C11-C12-C13
31	b	605	CLA	C10-C11-C12-C13
31	2	307	CLA	C8-C10-C11-C12
31	13	316	CLA	C8-C10-C11-C12
34	B	623	SQD	C11-C12-C13-C14
34	a	408	SQD	C34-C35-C36-C37
34	b	601	SQD	C11-C12-C13-C14
36	8	315	LHG	C11-C12-C13-C14
36	14	317	LHG	C15-C16-C17-C18
38	5	315	LMG	C16-C17-C18-C19
38	5	315	LMG	C28-C29-C30-C31
33	A	407	BCR	C12-C13-C14-C15
33	C	515	BCR	C11-C10-C9-C8
33	H	101	BCR	C11-C10-C9-C8
33	a	407	BCR	C12-C13-C14-C15
33	c	515	BCR	C11-C10-C9-C8
33	h	101	BCR	C11-C10-C9-C8
38	B	620	LMG	C2-C1-O1-C7
38	D	403	LMG	C2-C1-O1-C7
38	P	614	LMG	C2-C1-O1-C7
38	Z	102	LMG	C2-C1-O1-C7
38	b	621	LMG	C2-C1-O1-C7
38	c	522	LMG	C2-C1-O1-C7
38	d	403	LMG	C2-C1-O1-C7
38	p	614	LMG	C2-C1-O1-C7
39	C	519	DGD	C2E-C1E-O5D-C6D
39	C	520	DGD	C2E-C1E-O5D-C6D
39	c	519	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
39	c	520	DGD	C2E-C1E-O5D-C6D
38	f	102	LMG	C29-C28-O8-C9
34	A	408	SQD	C34-C35-C36-C37
38	4	316	LMG	C31-C32-C33-C34
38	14	316	LMG	C12-C13-C14-C15
39	C	520	DGD	C5B-C6B-C7B-C8B
39	c	520	DGD	C5B-C6B-C7B-C8B
31	19	313	CLA	C10-C11-C12-C13
31	B	611	CLA	C4-C3-C5-C6
31	C	504	CLA	C4-C3-C5-C6
31	b	612	CLA	C4-C3-C5-C6
31	c	504	CLA	C4-C3-C5-C6
34	l	101	SQD	C11-C10-C9-C8
36	A	410	LHG	C28-C29-C30-C31
36	a	410	LHG	C28-C29-C30-C31
36	8	315	LHG	C27-C28-C29-C30
36	18	315	LHG	C27-C28-C29-C30
38	J	101	LMG	C16-C17-C18-C19
38	j	101	LMG	C16-C17-C18-C19
38	4	316	LMG	C12-C13-C14-C15
39	C	518	DGD	C2A-C3A-C4A-C5A
39	C	519	DGD	CAB-CBB-CCB-CDB
39	b	622	DGD	C5B-C6B-C7B-C8B
39	c	518	DGD	C2A-C3A-C4A-C5A
39	c	519	DGD	CAB-CBB-CCB-CDB
39	h	102	DGD	C7A-C8A-C9A-CAA
31	B	607	CLA	C11-C10-C8-C9
31	b	608	CLA	C11-C10-C8-C9
31	9	310	CLA	C11-C12-C13-C14
31	B	606	CLA	O1D-CGD-O2D-CED
43	2	302	A86	C35-C34-O4-C38
43	8	301	A86	C33-C34-O4-C38
43	12	301	A86	C35-C34-O4-C38
38	1	317	LMG	C10-C11-C12-C13
34	l	101	SQD	C15-C16-C17-C18
38	B	620	LMG	C30-C31-C32-C33
38	b	621	LMG	C31-C32-C33-C34
38	d	403	LMG	C30-C31-C32-C33
39	B	621	DGD	C4B-C5B-C6B-C7B
39	H	102	DGD	C7A-C8A-C9A-CAA
39	H	102	DGD	C4B-C5B-C6B-C7B
39	h	102	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
39	1	318	DGD	C7B-C8B-C9B-CAB
31	B	616	CLA	C15-C16-C17-C18
45	12	309	KC2	CAA-CBA-CGA-O1A
31	5	311	CLA	C2A-CAA-CBA-CGA
31	7	313	CLA	C2A-CAA-CBA-CGA
31	C	513	CLA	O1A-CGA-O2A-C1
31	c	513	CLA	O1A-CGA-O2A-C1
38	14	316	LMG	O10-C28-O8-C9
33	C	516	BCR	C37-C22-C23-C24
33	c	515	BCR	C11-C12-C13-C35
33	c	516	BCR	C37-C22-C23-C24
34	B	623	SQD	C30-C31-C32-C33
34	L	102	SQD	C15-C16-C17-C18
34	b	601	SQD	C30-C31-C32-C33
38	B	620	LMG	C31-C32-C33-C34
38	15	314	LMG	C30-C31-C32-C33
39	C	520	DGD	CAB-CBB-CCB-CDB
39	11	318	DGD	C2B-C3B-C4B-C5B
36	A	410	LHG	O1-C1-C2-C3
36	a	410	LHG	O1-C1-C2-C3
33	Y	101	BCR	C7-C8-C9-C10
33	y	101	BCR	C7-C8-C9-C10
43	4	303	A86	C5-C6-C8-C9
43	6	307	A86	C5-C6-C8-C9
38	15	314	LMG	C11-C10-O7-C8
34	L	102	SQD	C11-C10-C9-C8
36	A	410	LHG	C25-C26-C27-C28
36	C	521	LHG	C27-C28-C29-C30
36	a	410	LHG	C25-C26-C27-C28
36	4	317	LHG	C12-C13-C14-C15
38	F	102	LMG	C30-C31-C32-C33
38	f	102	LMG	C30-C31-C32-C33
38	5	316	LMG	C33-C34-C35-C36
38	10	319	LMG	C11-C12-C13-C14
38	14	316	LMG	C15-C16-C17-C18
39	H	102	DGD	CCA-CDA-CEA-CFA
39	c	520	DGD	CAB-CBB-CCB-CDB
38	J	101	LMG	C28-C29-C30-C31
38	W	201	LMG	C28-C29-C30-C31
38	j	101	LMG	C28-C29-C30-C31
38	w	201	LMG	C28-C29-C30-C31
38	11	317	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	15	315	LMG	C28-C29-C30-C31
34	A	411	SQD	C27-C28-C29-C30
34	i	101	SQD	C27-C28-C29-C30
34	10	320	SQD	C11-C12-C13-C14
36	D	407	LHG	C27-C28-C29-C30
36	L	101	LHG	C27-C28-C29-C30
36	d	407	LHG	C27-C28-C29-C30
36	l	102	LHG	C27-C28-C29-C30
36	w	202	LHG	C27-C28-C29-C30
38	C	522	LMG	C37-C38-C39-C40
38	F	102	LMG	C16-C17-C18-C19
38	K	101	LMG	C32-C33-C34-C35
38	W	201	LMG	C30-C31-C32-C33
38	b	621	LMG	C30-C31-C32-C33
38	c	521	LMG	C12-C13-C14-C15
38	c	521	LMG	C37-C38-C39-C40
38	d	403	LMG	C32-C33-C34-C35
38	f	102	LMG	C16-C17-C18-C19
38	k	101	LMG	C32-C33-C34-C35
38	w	201	LMG	C30-C31-C32-C33
38	1	317	LMG	C30-C31-C32-C33
38	4	316	LMG	C33-C34-C35-C36
39	B	621	DGD	CBB-CCB-CDB-CEB
39	C	519	DGD	C3B-C4B-C5B-C6B
39	C	520	DGD	C5A-C6A-C7A-C8A
39	H	102	DGD	C3A-C4A-C5A-C6A
39	b	622	DGD	C6B-C7B-C8B-C9B
39	c	519	DGD	C3B-C4B-C5B-C6B
39	c	520	DGD	C5A-C6A-C7A-C8A
39	h	102	DGD	C5A-C6A-C7A-C8A
39	h	102	DGD	CCA-CDA-CEA-CFA
38	M	101	LMG	O6-C5-C6-O5
31	B	615	CLA	C16-C17-C18-C19
31	B	615	CLA	C16-C17-C18-C20
31	b	616	CLA	C16-C17-C18-C19
38	D	403	LMG	O6-C1-O1-C7
38	P	614	LMG	O6-C1-O1-C7
38	d	403	LMG	O6-C1-O1-C7
38	p	614	LMG	O6-C1-O1-C7
39	B	621	DGD	O6D-C1D-O3G-C3G
39	C	518	DGD	O6D-C1D-O3G-C3G
39	c	518	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C8-C10-C11-C12
31	C	509	CLA	C13-C15-C16-C17
31	b	608	CLA	C13-C15-C16-C17
31	c	509	CLA	C13-C15-C16-C17
31	9	313	CLA	C10-C11-C12-C13
36	Z	103	LHG	O6-C4-C5-C6
43	11	306	A86	C35-C34-O4-C38
34	B	623	SQD	C18-C19-C20-C21
34	b	601	SQD	C18-C19-C20-C21
38	W	201	LMG	C18-C19-C20-C21
38	w	201	LMG	C18-C19-C20-C21
38	4	316	LMG	C13-C14-C15-C16
39	H	102	DGD	C5A-C6A-C7A-C8A
39	H	102	DGD	C8A-C9A-CAA-CBA
39	h	102	DGD	C3A-C4A-C5A-C6A
39	h	102	DGD	C8A-C9A-CAA-CBA
31	16	316	CLA	O1D-CGD-O2D-CED
34	B	623	SQD	C12-C13-C14-C15
34	b	601	SQD	C12-C13-C14-C15
36	D	407	LHG	C16-C17-C18-C19
36	a	410	LHG	C26-C27-C28-C29
36	d	407	LHG	C16-C17-C18-C19
38	5	315	LMG	C12-C13-C14-C15
39	B	621	DGD	C8B-C9B-CAB-CBB
39	c	520	DGD	C6A-C7A-C8A-C9A
34	0	318	SQD	C23-C24-C25-C26
34	10	320	SQD	C23-C24-C25-C26
31	b	602	CLA	C8-C10-C11-C12
31	18	312	CLA	C5-C6-C7-C8
34	A	408	SQD	C12-C13-C14-C15
34	B	623	SQD	C14-C15-C16-C17
34	a	408	SQD	C12-C13-C14-C15
34	b	601	SQD	C14-C15-C16-C17
36	A	410	LHG	C11-C10-C9-C8
36	A	410	LHG	C26-C27-C28-C29
36	D	407	LHG	C13-C14-C15-C16
36	a	410	LHG	C11-C10-C9-C8
36	d	407	LHG	C13-C14-C15-C16
38	1	317	LMG	C15-C16-C17-C18
38	5	315	LMG	C30-C31-C32-C33
38	15	315	LMG	C31-C32-C33-C34
39	C	519	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
39	C	520	DGD	C6A-C7A-C8A-C9A
39	H	102	DGD	C9A-CAA-CBA-CCA
39	c	519	DGD	C6A-C7A-C8A-C9A
39	h	102	DGD	C9A-CAA-CBA-CCA
31	9	311	CLA	O1A-CGA-O2A-C1
31	P	601	CLA	C3-C5-C6-C7
31	p	601	CLA	C3-C5-C6-C7
31	12	308	CLA	CBA-CGA-O2A-C1
34	A	408	SQD	C24-C23-O48-C46
34	a	408	SQD	C24-C23-O48-C46
38	F	102	LMG	C29-C28-O8-C9
38	K	101	LMG	C29-C30-C31-C32
38	k	101	LMG	C29-C30-C31-C32
39	w	204	DGD	C6A-C7A-C8A-C9A
31	B	613	CLA	O1D-CGD-O2D-CED
31	b	607	CLA	O1D-CGD-O2D-CED
31	15	307	CLA	O1D-CGD-O2D-CED
42	17	314	KC1	O1D-CGD-O2D-CED
31	A	403	CLA	C3A-C2A-CAA-CBA
31	C	507	CLA	C3A-C2A-CAA-CBA
31	D	404	CLA	C3A-C2A-CAA-CBA
31	P	606	CLA	C3A-C2A-CAA-CBA
31	P	607	CLA	C3A-C2A-CAA-CBA
31	a	403	CLA	C3A-C2A-CAA-CBA
31	c	507	CLA	C3A-C2A-CAA-CBA
31	d	404	CLA	C3A-C2A-CAA-CBA
31	p	606	CLA	C3A-C2A-CAA-CBA
31	p	607	CLA	C3A-C2A-CAA-CBA
31	1	312	CLA	C3A-C2A-CAA-CBA
31	2	311	CLA	C3A-C2A-CAA-CBA
31	2	312	CLA	C3A-C2A-CAA-CBA
31	2	315	CLA	C3A-C2A-CAA-CBA
31	3	312	CLA	C3A-C2A-CAA-CBA
31	6	313	CLA	C3A-C2A-CAA-CBA
31	7	312	CLA	C3A-C2A-CAA-CBA
31	8	311	CLA	C3A-C2A-CAA-CBA
31	9	311	CLA	C3A-C2A-CAA-CBA
31	10	307	CLA	C3A-C2A-CAA-CBA
31	10	314	CLA	C3A-C2A-CAA-CBA
31	11	312	CLA	C3A-C2A-CAA-CBA
31	12	313	CLA	C3A-C2A-CAA-CBA
31	13	315	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	16	313	CLA	C3A-C2A-CAA-CBA
31	17	312	CLA	C3A-C2A-CAA-CBA
41	V	201	HEM	C2A-CAA-CBA-CGA
41	v	201	HEM	C2A-CAA-CBA-CGA
31	B	607	CLA	C13-C15-C16-C17
36	C	521	LHG	C25-C26-C27-C28
36	w	202	LHG	C25-C26-C27-C28
36	18	315	LHG	C14-C15-C16-C17
38	W	201	LMG	C11-C12-C13-C14
38	c	521	LMG	C19-C20-C21-C22
38	w	201	LMG	C11-C12-C13-C14
38	5	316	LMG	C31-C32-C33-C34
39	C	520	DGD	C2B-C3B-C4B-C5B
39	W	203	DGD	C6A-C7A-C8A-C9A
39	c	520	DGD	C2B-C3B-C4B-C5B
43	16	302	A86	C35-C34-O4-C38
31	b	614	CLA	O1D-CGD-O2D-CED
31	b	615	CLA	O1D-CGD-O2D-CED
31	6	316	CLA	O1D-CGD-O2D-CED
31	C	512	CLA	O1A-CGA-O2A-C1
31	c	512	CLA	O1A-CGA-O2A-C1
31	C	504	CLA	C16-C17-C18-C20
31	b	616	CLA	C16-C17-C18-C20
31	c	504	CLA	C16-C17-C18-C20
38	d	403	LMG	C11-C12-C13-C14
38	1	317	LMG	C31-C32-C33-C34
38	4	316	LMG	C15-C16-C17-C18
39	B	621	DGD	C5B-C6B-C7B-C8B
31	8	309	CLA	C3-C5-C6-C7
34	10	320	SQD	C44-C45-C46-O48
38	1	301	LMG	O9-C10-O7-C8
38	11	301	LMG	O9-C10-O7-C8
31	19	308	CLA	CBD-CGD-O2D-CED
38	C	522	LMG	C12-C13-C14-C15
38	C	522	LMG	C19-C20-C21-C22
39	C	519	DGD	C2A-C3A-C4A-C5A
39	b	622	DGD	C3B-C4B-C5B-C6B
39	c	519	DGD	C2A-C3A-C4A-C5A
31	D	401	CLA	C3-C5-C6-C7
31	d	401	CLA	C3-C5-C6-C7
36	d	407	LHG	C14-C15-C16-C17
31	B	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	b	606	CLA	C15-C16-C17-C18
31	5	309	CLA	C4-C3-C5-C6
31	15	309	CLA	C4-C3-C5-C6
31	0	308	CLA	CBA-CGA-O2A-C1
31	B	608	CLA	C2-C3-C5-C6
31	B	611	CLA	C2-C3-C5-C6
31	b	609	CLA	C2-C3-C5-C6
31	b	612	CLA	C2-C3-C5-C6
31	4	309	CLA	C2-C3-C5-C6
31	5	309	CLA	C2-C3-C5-C6
31	15	309	CLA	C2-C3-C5-C6
36	D	407	LHG	C14-C15-C16-C17
36	L	101	LHG	C12-C13-C14-C15
36	l	102	LHG	C12-C13-C14-C15
38	14	316	LMG	C13-C14-C15-C16
43	7	304	A86	C33-C34-O4-C38
43	12	306	A86	C35-C34-O4-C38
43	17	305	A86	C35-C34-O4-C38
43	19	305	A86	C35-C34-O4-C38
36	A	410	LHG	O1-C1-C2-O2
36	C	521	LHG	O1-C1-C2-O2
36	a	410	LHG	O1-C1-C2-O2
36	w	202	LHG	O1-C1-C2-O2
31	5	307	CLA	C8-C10-C11-C12
34	10	320	SQD	C25-C26-C27-C28
36	L	101	LHG	C29-C30-C31-C32
36	l	102	LHG	C29-C30-C31-C32
38	14	316	LMG	C18-C19-C20-C21
39	W	203	DGD	C3A-C4A-C5A-C6A
39	w	204	DGD	C3A-C4A-C5A-C6A
39	11	318	DGD	CBB-CCB-CDB-CEB
36	5	317	LHG	C7-C8-C9-C10
36	15	316	LHG	C7-C8-C9-C10
31	5	307	CLA	O1A-CGA-O2A-C1
36	B	622	LHG	C23-C24-C25-C26
36	b	623	LHG	C23-C24-C25-C26
31	14	311	CLA	C4C-C3C-CAC-CBC
36	D	407	LHG	C25-C26-C27-C28
36	d	407	LHG	C25-C26-C27-C28
38	J	101	LMG	C31-C32-C33-C34
38	j	101	LMG	C31-C32-C33-C34
31	B	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	614	CLA	C10-C11-C12-C13
31	14	309	CLA	C13-C15-C16-C17
36	L	101	LHG	C16-C17-C18-C19
38	K	101	LMG	C33-C34-C35-C36
31	B	616	CLA	CBA-CGA-O2A-C1
34	L	102	SQD	C25-C26-C27-C28
36	l	102	LHG	C16-C17-C18-C19
38	M	101	LMG	C32-C33-C34-C35
38	k	101	LMG	C33-C34-C35-C36
31	15	307	CLA	O1A-CGA-O2A-C1
43	11	303	A86	C33-C34-O4-C38
43	11	319	A86	C33-C34-O4-C38
36	Z	103	LHG	C1-C2-C3-O3
34	l	101	SQD	C25-C26-C27-C28
36	D	407	LHG	C15-C16-C17-C18
36	L	101	LHG	C24-C25-C26-C27
36	d	407	LHG	C15-C16-C17-C18
36	l	102	LHG	C24-C25-C26-C27
38	K	101	LMG	C38-C39-C40-C41
38	K	101	LMG	C39-C40-C41-C42
38	j	101	LMG	C19-C20-C21-C22
38	k	101	LMG	C38-C39-C40-C41
38	k	101	LMG	C39-C40-C41-C42
38	11	317	LMG	C15-C16-C17-C18
38	Z	102	LMG	O9-C10-O7-C8
38	c	522	LMG	O9-C10-O7-C8
39	W	203	DGD	O1B-C1B-O2G-C2G
39	w	204	DGD	O1B-C1B-O2G-C2G
31	14	312	CLA	C2-C1-O2A-CGA
34	A	408	SQD	C31-C32-C33-C34
34	L	102	SQD	C32-C33-C34-C35
34	a	408	SQD	C31-C32-C33-C34
38	J	101	LMG	C19-C20-C21-C22
39	C	518	DGD	C3A-C4A-C5A-C6A
39	C	520	DGD	CBA-CCA-CDA-CEA
39	W	203	DGD	CAB-CBB-CCB-CDB
39	c	518	DGD	C3A-C4A-C5A-C6A
39	c	520	DGD	CBA-CCA-CDA-CEA
39	w	204	DGD	CAB-CBB-CCB-CDB
38	j	101	LMG	O6-C5-C6-O5
31	W	202	CLA	O1A-CGA-O2A-C1
31	w	203	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	11	317	LMG	O10-C28-O8-C9
36	B	622	LHG	C12-C13-C14-C15
36	C	521	LHG	C26-C27-C28-C29
36	b	623	LHG	C12-C13-C14-C15
36	w	202	LHG	C26-C27-C28-C29
38	D	403	LMG	C10-C11-C12-C13
31	8	307	CLA	C3-C5-C6-C7
33	A	407	BCR	C5-C6-C7-C8
33	A	407	BCR	C23-C24-C25-C26
33	B	617	BCR	C1-C6-C7-C8
33	B	617	BCR	C5-C6-C7-C8
33	B	619	BCR	C5-C6-C7-C8
33	C	516	BCR	C5-C6-C7-C8
33	C	516	BCR	C23-C24-C25-C30
33	C	517	BCR	C5-C6-C7-C8
33	F	101	BCR	C1-C6-C7-C8
33	F	101	BCR	C5-C6-C7-C8
33	F	101	BCR	C23-C24-C25-C26
33	F	101	BCR	C23-C24-C25-C30
33	H	101	BCR	C5-C6-C7-C8
33	a	407	BCR	C5-C6-C7-C8
33	a	407	BCR	C23-C24-C25-C26
33	a	407	BCR	C23-C24-C25-C30
33	b	618	BCR	C1-C6-C7-C8
33	b	618	BCR	C5-C6-C7-C8
33	b	620	BCR	C5-C6-C7-C8
33	c	516	BCR	C5-C6-C7-C8
33	c	516	BCR	C23-C24-C25-C30
33	c	517	BCR	C5-C6-C7-C8
33	f	101	BCR	C1-C6-C7-C8
33	f	101	BCR	C5-C6-C7-C8
33	f	101	BCR	C23-C24-C25-C26
33	f	101	BCR	C23-C24-C25-C30
33	h	101	BCR	C5-C6-C7-C8
38	d	403	LMG	C12-C13-C14-C15
38	11	317	LMG	C31-C32-C33-C34
39	C	518	DGD	C6B-C7B-C8B-C9B
39	c	518	DGD	C6B-C7B-C8B-C9B
31	C	504	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	CBA-CGA-O2A-C1
31	c	504	CLA	CBA-CGA-O2A-C1
43	4	302	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
43	7	302	A86	C33-C34-O4-C38
31	B	608	CLA	C10-C11-C12-C13
31	P	601	CLA	C8-C10-C11-C12
31	p	601	CLA	C8-C10-C11-C12
31	9	312	CLA	C13-C15-C16-C17
31	19	312	CLA	C13-C15-C16-C17
38	K	101	LMG	C11-C10-O7-C8
38	k	101	LMG	C11-C10-O7-C8
31	18	314	CLA	C4C-C3C-CAC-CBC
31	B	612	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
38	J	101	LMG	O6-C5-C6-O5
39	C	520	DGD	O6E-C5E-C6E-O5E
39	c	520	DGD	O6E-C5E-C6E-O5E
36	18	315	LHG	C23-C24-C25-C26
34	B	623	SQD	C25-C26-C27-C28
34	b	601	SQD	C25-C26-C27-C28
36	18	315	LHG	C26-C27-C28-C29
38	m	101	LMG	C29-C30-C31-C32
31	A	403	CLA	C13-C15-C16-C17
31	a	403	CLA	C13-C15-C16-C17
31	11	313	CLA	C15-C16-C17-C18
38	K	101	LMG	O6-C5-C6-O5
38	M	101	LMG	C33-C34-C35-C36
39	W	203	DGD	C2B-C3B-C4B-C5B
39	w	204	DGD	C2B-C3B-C4B-C5B
31	4	309	CLA	C4-C3-C5-C6
31	8	309	CLA	C4-C3-C5-C6
31	18	309	CLA	C4-C3-C5-C6
31	P	605	CLA	O1D-CGD-O2D-CED
31	p	605	CLA	O1D-CGD-O2D-CED
31	B	607	CLA	C11-C12-C13-C15
31	B	612	CLA	C6-C7-C8-C10
31	C	503	CLA	C12-C13-C15-C16
31	C	504	CLA	C2-C3-C5-C6
31	C	504	CLA	C6-C7-C8-C10
31	C	506	CLA	C11-C12-C13-C15
31	b	608	CLA	C11-C12-C13-C15
31	b	613	CLA	C6-C7-C8-C10
31	b	615	CLA	C11-C10-C8-C7
31	c	503	CLA	C12-C13-C15-C16
31	c	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	c	504	CLA	C6-C7-C8-C10
31	c	506	CLA	C11-C12-C13-C15
31	3	316	CLA	C11-C12-C13-C15
31	4	307	CLA	C11-C10-C8-C7
31	4	309	CLA	C6-C7-C8-C10
31	9	310	CLA	C11-C12-C13-C15
31	14	306	CLA	C11-C10-C8-C7
31	14	307	CLA	C11-C10-C8-C7
31	14	309	CLA	C2-C3-C5-C6
31	14	309	CLA	C11-C10-C8-C7
31	18	309	CLA	C2-C3-C5-C6
31	19	307	CLA	C2-C3-C5-C6
31	19	310	CLA	C11-C12-C13-C15
32	A	405	PHO	C11-C10-C8-C7
32	a	405	PHO	C11-C10-C8-C7
31	0	308	CLA	O1A-CGA-O2A-C1
31	12	308	CLA	O1A-CGA-O2A-C1
31	D	404	CLA	C2C-C3C-CAC-CBC
31	d	404	CLA	C2C-C3C-CAC-CBC
38	1	317	LMG	C34-C35-C36-C37
31	D	404	CLA	C8-C10-C11-C12
31	b	609	CLA	C10-C11-C12-C13
31	b	617	CLA	C15-C16-C17-C18
31	d	404	CLA	C8-C10-C11-C12
31	4	309	CLA	C15-C16-C17-C18
33	B	618	BCR	C15-C16-C17-C18
33	F	101	BCR	C9-C10-C11-C12
33	b	618	BCR	C9-C10-C11-C12
33	b	619	BCR	C15-C16-C17-C18
33	f	101	BCR	C9-C10-C11-C12
43	4	303	A86	C11-C10-C9-C8
43	18	303	A86	C11-C10-C9-C8
31	B	614	CLA	CBD-CGD-O2D-CED
45	13	309	KC2	CBD-CGD-O2D-CED
31	11	308	CLA	C16-C17-C18-C20
43	1	302	A86	C35-C34-O4-C38
43	8	304	A86	C35-C34-O4-C38
38	k	101	LMG	O6-C5-C6-O5
39	11	318	DGD	O6E-C5E-C6E-O5E
36	D	407	LHG	O9-C7-O7-C5
36	Z	103	LHG	O9-C7-O7-C5
36	d	407	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
36	z	102	LHG	O9-C7-O7-C5
38	n	701	LMG	C29-C28-O8-C9
34	l	101	SQD	C32-C33-C34-C35
39	11	318	DGD	C6B-C7B-C8B-C9B
31	C	506	CLA	C2A-CAA-CBA-CGA
31	c	506	CLA	C2A-CAA-CBA-CGA
31	2	312	CLA	C2A-CAA-CBA-CGA
31	10	312	CLA	C2A-CAA-CBA-CGA
31	14	306	CLA	C2A-CAA-CBA-CGA
31	13	313	CLA	C15-C16-C17-C18
34	L	102	SQD	C24-C25-C26-C27
38	B	620	LMG	C33-C34-C35-C36
38	15	314	LMG	C15-C16-C17-C18
34	0	318	SQD	C26-C27-C28-C29
38	k	101	LMG	C15-C16-C17-C18
39	C	518	DGD	C1A-C2A-C3A-C4A
39	c	518	DGD	C1A-C2A-C3A-C4A
39	1	318	DGD	C1A-C2A-C3A-C4A
38	K	101	LMG	C15-C16-C17-C18
38	4	316	LMG	C18-C19-C20-C21
38	5	315	LMG	C15-C16-C17-C18
42	1	314	KC1	C2B-C3B-CAB-CBB
42	11	314	KC1	C2B-C3B-CAB-CBB
42	13	314	KC1	C2B-C3B-CAB-CBB
45	11	309	KC2	C2B-C3B-CAB-CBB
45	12	311	KC2	C2C-C3C-CAC-CBC
38	D	403	LMG	C32-C33-C34-C35
38	d	408	LMG	C11-C12-C13-C14
43	4	303	A86	O5-C38-O4-C34
33	Y	101	BCR	C22-C23-C24-C25
33	y	101	BCR	C22-C23-C24-C25
31	19	310	CLA	CBD-CGD-O2D-CED
31	9	307	CLA	CBA-CGA-O2A-C1
31	C	507	CLA	C16-C17-C18-C19
31	c	507	CLA	C16-C17-C18-C19
39	b	622	DGD	O6D-C1D-O3G-C3G
34	a	408	SQD	C28-C29-C30-C31
34	0	318	SQD	C12-C13-C14-C15
36	D	407	LHG	C24-C25-C26-C27
36	d	407	LHG	C24-C25-C26-C27
36	8	315	LHG	C26-C27-C28-C29
38	D	408	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
39	H	102	DGD	C3B-C4B-C5B-C6B
39	h	102	DGD	C3B-C4B-C5B-C6B
34	A	408	SQD	C8-C7-O47-C45
34	a	408	SQD	C8-C7-O47-C45
38	N	101	LMG	C11-C10-O7-C8
38	W	201	LMG	C11-C10-O7-C8
38	n	701	LMG	C11-C10-O7-C8
38	w	201	LMG	C11-C10-O7-C8
38	5	315	LMG	C11-C10-O7-C8
38	5	316	LMG	C11-C10-O7-C8
36	A	410	LHG	O6-C4-C5-O7
36	a	410	LHG	O6-C4-C5-O7
38	10	319	LMG	O6-C5-C6-O5
31	11	308	CLA	C2C-C3C-CAC-CBC
31	14	315	CLA	C2C-C3C-CAC-CBC
34	A	408	SQD	C28-C29-C30-C31
42	1	314	KC1	C4B-C3B-CAB-CBB
42	9	314	KC1	C4B-C3B-CAB-CBB
42	11	314	KC1	C4B-C3B-CAB-CBB
42	13	314	KC1	C4B-C3B-CAB-CBB
42	18	313	KC1	C4B-C3B-CAB-CBB
42	19	314	KC1	C4B-C3B-CAB-CBB
45	0	310	KC2	C4B-C3B-CAB-CBB
45	2	308	KC2	C4B-C3B-CAB-CBB
45	2	310	KC2	C4C-C3C-CAC-CBC
45	3	311	KC2	C4C-C3C-CAC-CBC
45	6	310	KC2	C4B-C3B-CAB-CBB
45	6	312	KC2	C4C-C3C-CAC-CBC
45	8	310	KC2	C4C-C3C-CAC-CBC
45	9	309	KC2	C4C-C3C-CAC-CBC
45	10	310	KC2	C4B-C3B-CAB-CBB
45	10	310	KC2	C4C-C3C-CAC-CBC
45	16	310	KC2	C4B-C3B-CAB-CBB
45	16	312	KC2	C4C-C3C-CAC-CBC
45	17	309	KC2	C4B-C3B-CAB-CBB
45	18	310	KC2	C4C-C3C-CAC-CBC
45	19	309	KC2	C4C-C3C-CAC-CBC
31	7	312	CLA	CBD-CGD-O2D-CED
36	Z	103	LHG	O2-C2-C3-O3
36	8	315	LHG	O9-C7-O7-C5
43	16	302	A86	C33-C34-O4-C38
43	19	304	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	5	316	LMG	C28-C29-C30-C31
36	8	315	LHG	C14-C15-C16-C17
38	J	101	LMG	C13-C14-C15-C16
38	0	317	LMG	C2-C1-O1-C7
38	10	319	LMG	C2-C1-O1-C7
39	C	518	DGD	C2D-C1D-O3G-C3G
39	c	518	DGD	C2D-C1D-O3G-C3G
34	0	318	SQD	O47-C45-C46-O48
34	10	320	SQD	O47-C45-C46-O48
38	J	101	LMG	O7-C8-C9-O8
38	P	614	LMG	O1-C7-C8-O7
38	j	101	LMG	O7-C8-C9-O8
38	p	614	LMG	O1-C7-C8-O7
36	L	101	LHG	C34-C35-C36-C37
36	l	102	LHG	C34-C35-C36-C37
38	j	101	LMG	C13-C14-C15-C16
39	W	203	DGD	C7A-C8A-C9A-CAA
39	w	204	DGD	C7A-C8A-C9A-CAA
31	B	616	CLA	O1A-CGA-O2A-C1
31	P	602	CLA	C16-C17-C18-C19
34	l	101	SQD	C24-C25-C26-C27
38	m	101	LMG	O6-C5-C6-O5
31	C	502	CLA	C5-C6-C7-C8
31	b	608	CLA	C10-C11-C12-C13
31	c	502	CLA	C5-C6-C7-C8
31	14	309	CLA	C4-C3-C5-C6
31	6	309	CLA	C2-C3-C5-C6
31	8	309	CLA	C2-C3-C5-C6
31	14	307	CLA	C2-C3-C5-C6
31	18	307	CLA	C2-C3-C5-C6
35	A	409	PL9	C4-C3-C7-C8
35	D	406	PL9	C4-C3-C7-C8
35	a	409	PL9	C4-C3-C7-C8
35	d	406	PL9	C4-C3-C7-C8
31	C	503	CLA	C11-C10-C8-C9
31	C	503	CLA	C14-C13-C15-C16
31	C	506	CLA	C11-C12-C13-C14
31	C	513	CLA	C11-C10-C8-C9
31	P	601	CLA	C11-C10-C8-C9
31	W	202	CLA	C11-C10-C8-C9
31	a	406	CLA	C11-C10-C8-C9
31	c	503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	c	503	CLA	C14-C13-C15-C16
31	c	506	CLA	C11-C12-C13-C14
31	c	513	CLA	C11-C10-C8-C9
31	p	601	CLA	C11-C10-C8-C9
31	w	203	CLA	C11-C10-C8-C9
31	4	307	CLA	C11-C10-C8-C9
31	14	307	CLA	C11-C10-C8-C9
31	14	309	CLA	C6-C7-C8-C9
31	14	309	CLA	C11-C10-C8-C9
31	14	309	CLA	C14-C13-C15-C16
31	19	310	CLA	C11-C12-C13-C14
32	A	405	PHO	C11-C10-C8-C9
32	a	405	PHO	C11-C10-C8-C9
31	18	314	CLA	CBD-CGD-O2D-CED
38	5	315	LMG	O6-C5-C6-O5
43	9	302	A86	C35-C34-O4-C38
43	10	305	A86	C33-C34-O4-C38
31	B	616	CLA	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	12	313	CLA	C2A-CAA-CBA-CGA
31	16	313	CLA	C2A-CAA-CBA-CGA
34	0	318	SQD	C25-C26-C27-C28
39	H	102	DGD	C2B-C3B-C4B-C5B
39	h	102	DGD	C2B-C3B-C4B-C5B
33	C	515	BCR	C11-C12-C13-C35
43	2	302	A86	C7-C6-C8-C9
43	18	303	A86	C-C1-C24-C25
31	B	608	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	13	316	CLA	C15-C16-C17-C18
36	8	316	LHG	C12-C13-C14-C15
38	4	316	LMG	C11-C12-C13-C14
39	B	621	DGD	C3B-C4B-C5B-C6B
39	C	519	DGD	C7A-C8A-C9A-CAA
39	c	519	DGD	C7A-C8A-C9A-CAA
31	b	617	CLA	O1A-CGA-O2A-C1
31	A	403	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C1A-C2A-CAA-CBA
31	B	603	CLA	C1A-C2A-CAA-CBA
31	C	502	CLA	C1A-C2A-CAA-CBA
31	D	401	CLA	C1A-C2A-CAA-CBA
31	D	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	P	607	CLA	C1A-C2A-CAA-CBA
31	a	403	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	c	502	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	C1A-C2A-CAA-CBA
31	d	404	CLA	C1A-C2A-CAA-CBA
31	p	607	CLA	C1A-C2A-CAA-CBA
31	0	308	CLA	C1A-C2A-CAA-CBA
31	0	309	CLA	C1A-C2A-CAA-CBA
31	1	308	CLA	C1A-C2A-CAA-CBA
31	1	313	CLA	C1A-C2A-CAA-CBA
31	2	311	CLA	C1A-C2A-CAA-CBA
31	2	312	CLA	C1A-C2A-CAA-CBA
31	3	313	CLA	C1A-C2A-CAA-CBA
31	4	307	CLA	C1A-C2A-CAA-CBA
31	4	312	CLA	C1A-C2A-CAA-CBA
31	6	309	CLA	C1A-C2A-CAA-CBA
31	9	308	CLA	C1A-C2A-CAA-CBA
31	10	308	CLA	C1A-C2A-CAA-CBA
31	10	309	CLA	C1A-C2A-CAA-CBA
31	11	308	CLA	C1A-C2A-CAA-CBA
31	11	312	CLA	C1A-C2A-CAA-CBA
31	12	308	CLA	C1A-C2A-CAA-CBA
31	13	308	CLA	C1A-C2A-CAA-CBA
31	14	307	CLA	C1A-C2A-CAA-CBA
31	14	312	CLA	C1A-C2A-CAA-CBA
31	16	309	CLA	C1A-C2A-CAA-CBA
31	18	306	CLA	C1A-C2A-CAA-CBA
31	19	308	CLA	C1A-C2A-CAA-CBA
31	19	311	CLA	C1A-C2A-CAA-CBA
31	p	602	CLA	C16-C17-C18-C19
31	19	312	CLA	C16-C17-C18-C20
38	W	201	LMG	O9-C10-O7-C8
38	w	201	LMG	O9-C10-O7-C8
38	5	315	LMG	O9-C10-O7-C8
38	10	319	LMG	O9-C10-O7-C8
36	4	317	LHG	C15-C16-C17-C18
38	1	317	LMG	C36-C37-C38-C39
33	B	617	BCR	C9-C10-C11-C12
33	F	101	BCR	C19-C20-C21-C22
33	f	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
31	B	607	CLA	C10-C11-C12-C13
31	B	616	CLA	C8-C10-C11-C12
31	1	313	CLA	C15-C16-C17-C18
31	4	307	CLA	C8-C10-C11-C12
31	14	307	CLA	C8-C10-C11-C12
43	9	301	A86	C33-C34-O4-C38
36	B	622	LHG	C3-O3-P-O6
36	b	623	LHG	C3-O3-P-O6
36	4	317	LHG	C9-C10-C11-C12
38	m	101	LMG	C32-C33-C34-C35
36	8	315	LHG	C23-C24-C25-C26
39	1	318	DGD	O6E-C5E-C6E-O5E
31	C	502	CLA	C3-C5-C6-C7
31	c	502	CLA	C3-C5-C6-C7
38	B	620	LMG	C16-C17-C18-C19
38	b	621	LMG	C16-C17-C18-C19
39	b	622	DGD	C4B-C5B-C6B-C7B
31	8	312	CLA	C5-C6-C7-C8
31	18	307	CLA	C8-C10-C11-C12
31	2	307	CLA	CBA-CGA-O2A-C1
38	B	620	LMG	C29-C28-O8-C9
38	b	621	LMG	C29-C28-O8-C9
36	z	102	LHG	O6-C4-C5-C6
36	8	316	LHG	O6-C4-C5-C6
36	18	316	LHG	O6-C4-C5-C6
31	12	308	CLA	C2C-C3C-CAC-CBC
36	18	316	LHG	C10-C11-C12-C13
39	1	318	DGD	C5A-C6A-C7A-C8A
36	4	317	LHG	C16-C17-C18-C19
38	b	621	LMG	C33-C34-C35-C36
39	11	318	DGD	C5A-C6A-C7A-C8A
31	18	309	CLA	C3-C5-C6-C7
31	4	309	CLA	C16-C17-C18-C19
43	10	305	A86	C35-C34-O4-C38
38	K	101	LMG	C12-C13-C14-C15
39	1	318	DGD	C5B-C6B-C7B-C8B
38	K	101	LMG	C30-C31-C32-C33
38	b	621	LMG	C34-C35-C36-C37
38	k	101	LMG	C12-C13-C14-C15
38	k	101	LMG	C30-C31-C32-C33
36	D	407	LHG	C30-C31-C32-C33
39	h	102	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
31	B	614	CLA	CBA-CGA-O2A-C1
36	z	102	LHG	C1-C2-C3-O3
38	c	521	LMG	O6-C5-C6-O5
31	b	610	CLA	C2-C3-C5-C6
31	1	316	CLA	C3A-C2A-CAA-CBA
35	D	406	PL9	C33-C34-C36-C37
35	d	406	PL9	C33-C34-C36-C37
41	E	101	HEM	C2A-CAA-CBA-CGA
41	e	101	HEM	C2A-CAA-CBA-CGA
36	d	407	LHG	C30-C31-C32-C33
38	B	620	LMG	C35-C36-C37-C38
39	H	102	DGD	CAA-CBA-CCA-CDA
31	b	617	CLA	C5-C6-C7-C8
32	A	405	PHO	C13-C15-C16-C17
32	a	405	PHO	C13-C15-C16-C17
38	b	621	LMG	C17-C18-C19-C20
38	d	403	LMG	C34-C35-C36-C37
38	m	101	LMG	C12-C13-C14-C15
38	11	317	LMG	C32-C33-C34-C35
43	P	611	A86	C35-C34-O4-C38
43	0	305	A86	C35-C34-O4-C38
31	C	504	CLA	O1A-CGA-O2A-C1
31	c	504	CLA	O1A-CGA-O2A-C1
38	B	620	LMG	C17-C18-C19-C20
31	C	507	CLA	C15-C16-C17-C18
31	c	507	CLA	C15-C16-C17-C18
38	C	522	LMG	O6-C5-C6-O5
34	A	408	SQD	C32-C33-C34-C35
34	A	411	SQD	C44-C45-C46-O48
34	B	623	SQD	C44-C45-C46-O48
34	a	408	SQD	C32-C33-C34-C35
34	b	601	SQD	C44-C45-C46-O48
34	i	101	SQD	C44-C45-C46-O48
34	0	318	SQD	O6-C44-C45-C46
34	0	318	SQD	C44-C45-C46-O48
34	10	320	SQD	O6-C44-C45-C46
36	8	315	LHG	C4-C5-C6-O8
36	8	316	LHG	C4-C5-C6-O8
38	C	522	LMG	C7-C8-C9-O8
38	D	408	LMG	O1-C7-C8-C9
38	F	102	LMG	C32-C33-C34-C35
38	P	614	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
38	c	521	LMG	C7-C8-C9-O8
38	d	408	LMG	O1-C7-C8-C9
38	f	102	LMG	C32-C33-C34-C35
38	p	614	LMG	O1-C7-C8-C9
38	1	301	LMG	O1-C7-C8-C9
38	11	301	LMG	O1-C7-C8-C9
38	11	317	LMG	C7-C8-C9-O8
38	15	315	LMG	C7-C8-C9-O8
39	B	621	DGD	O1G-C1G-C2G-C3G
39	C	518	DGD	O1G-C1G-C2G-C3G
39	C	519	DGD	C1G-C2G-C3G-O3G
39	W	203	DGD	C1G-C2G-C3G-O3G
39	b	622	DGD	O1G-C1G-C2G-C3G
39	c	518	DGD	O1G-C1G-C2G-C3G
39	c	519	DGD	C1G-C2G-C3G-O3G
39	w	204	DGD	C1G-C2G-C3G-O3G
39	1	318	DGD	C1G-C2G-C3G-O3G
39	11	318	DGD	C1G-C2G-C3G-O3G
34	A	408	SQD	C11-C12-C13-C14
34	i	101	SQD	C9-C10-C11-C12
38	W	201	LMG	C29-C30-C31-C32
38	w	201	LMG	C29-C30-C31-C32
38	5	315	LMG	C17-C18-C19-C20
39	C	520	DGD	CDA-CEA-CFA-CGA
39	C	520	DGD	CDB-CEB-CFB-CGB
39	c	520	DGD	CDA-CEA-CFA-CGA
39	c	520	DGD	CDB-CEB-CFB-CGB
38	K	101	LMG	O10-C28-O8-C9
39	C	519	DGD	C5D-C6D-O5D-C1E
39	c	519	DGD	C5D-C6D-O5D-C1E
34	A	408	SQD	C35-C36-C37-C38
34	A	411	SQD	C9-C10-C11-C12
34	a	408	SQD	C11-C12-C13-C14
34	a	408	SQD	C35-C36-C37-C38
36	A	410	LHG	C32-C33-C34-C35
36	B	622	LHG	C9-C10-C11-C12
36	a	410	LHG	C32-C33-C34-C35
36	b	623	LHG	C9-C10-C11-C12
38	M	101	LMG	C15-C16-C17-C18
38	11	317	LMG	C37-C38-C39-C40
38	15	314	LMG	C31-C32-C33-C34
38	15	315	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
39	B	621	DGD	O6E-C5E-C6E-O5E
31	P	601	CLA	C15-C16-C17-C18
31	1	321	CLA	C5-C6-C7-C8
31	15	307	CLA	C8-C10-C11-C12
36	14	317	LHG	C9-C10-C11-C12
38	15	314	LMG	C17-C18-C19-C20
38	15	315	LMG	C34-C35-C36-C37
36	L	101	LHG	C23-C24-C25-C26
36	l	102	LHG	C23-C24-C25-C26
38	K	101	LMG	C28-C29-C30-C31
38	k	101	LMG	C28-C29-C30-C31
38	k	101	LMG	O10-C28-O8-C9
36	C	521	LHG	C12-C13-C14-C15
36	w	202	LHG	C12-C13-C14-C15
31	A	403	CLA	C16-C17-C18-C19
31	a	403	CLA	C16-C17-C18-C19
31	B	616	CLA	C5-C6-C7-C8
31	p	601	CLA	C15-C16-C17-C18
38	K	101	LMG	C40-C41-C42-C43
38	k	101	LMG	C40-C41-C42-C43
38	5	315	LMG	C31-C32-C33-C34
31	b	615	CLA	CBA-CGA-O2A-C1
31	10	308	CLA	CBA-CGA-O2A-C1
36	D	407	LHG	O1-C1-C2-O2
36	d	407	LHG	O1-C1-C2-O2
36	4	317	LHG	O1-C1-C2-O2
36	8	316	LHG	O1-C1-C2-O2
36	14	317	LHG	O1-C1-C2-O2
34	A	408	SQD	C33-C34-C35-C36
34	a	408	SQD	C33-C34-C35-C36
36	18	316	LHG	C15-C16-C17-C18
38	B	620	LMG	C14-C15-C16-C17
38	5	316	LMG	C34-C35-C36-C37
43	p	611	A86	C35-C34-O4-C38
43	6	302	A86	C35-C34-O4-C38
43	7	301	A86	C35-C34-O4-C38
43	13	301	A86	C35-C34-O4-C38
39	b	622	DGD	C1B-C2B-C3B-C4B
34	B	623	SQD	C34-C35-C36-C37
34	b	601	SQD	C34-C35-C36-C37
36	4	317	LHG	C10-C11-C12-C13
38	J	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
38	K	101	LMG	C35-C36-C37-C38
38	j	101	LMG	C18-C19-C20-C21
31	c	513	CLA	CBD-CGD-O2D-CED
38	B	620	LMG	C34-C35-C36-C37
38	b	621	LMG	C14-C15-C16-C17
38	k	101	LMG	C35-C36-C37-C38
39	11	318	DGD	CFB-CGB-CHB-CIB
31	9	308	CLA	C5-C6-C7-C8
33	b	618	BCR	C20-C21-C22-C37
39	b	622	DGD	O6E-C5E-C6E-O5E
31	B	609	CLA	C4-C3-C5-C6
31	C	511	CLA	C4-C3-C5-C6
31	W	202	CLA	C4-C3-C5-C6
31	b	604	CLA	C4-C3-C5-C6
31	b	610	CLA	C4-C3-C5-C6
31	c	511	CLA	C4-C3-C5-C6
31	w	203	CLA	C4-C3-C5-C6
35	A	409	PL9	C15-C14-C16-C17
35	a	409	PL9	C15-C14-C16-C17
31	4	314	CLA	C2A-CAA-CBA-CGA
38	N	101	LMG	C11-C12-C13-C14
38	0	317	LMG	C12-C13-C14-C15
31	B	609	CLA	C2-C3-C5-C6
31	W	202	CLA	C2-C3-C5-C6
31	w	203	CLA	C2-C3-C5-C6
31	A	403	CLA	C16-C17-C18-C20
31	a	403	CLA	C16-C17-C18-C20
31	6	309	CLA	CBA-CGA-O2A-C1
38	15	314	LMG	O6-C5-C6-O5
34	A	408	SQD	C11-C10-C9-C8
34	a	408	SQD	C11-C10-C9-C8
38	B	620	LMG	C36-C37-C38-C39
31	C	513	CLA	CBD-CGD-O2D-CED
31	D	405	CLA	CBD-CGD-O2D-CED
31	d	405	CLA	CBD-CGD-O2D-CED
31	D	401	CLA	C13-C15-C16-C17
31	b	617	CLA	C8-C10-C11-C12
31	d	401	CLA	C13-C15-C16-C17
43	0	305	A86	C33-C34-O4-C38
43	1	302	A86	C33-C34-O4-C38
43	10	301	A86	C35-C34-O4-C38
43	17	302	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
31	2	307	CLA	C2C-C3C-CAC-CBC
38	1	301	LMG	C34-C35-C36-C37
38	11	301	LMG	C34-C35-C36-C37
34	10	320	SQD	C44-C45-O47-C7
36	5	317	LHG	C6-C5-O7-C7
36	15	316	LHG	C6-C5-O7-C7
38	C	522	LMG	C9-C8-O7-C10
38	c	521	LMG	C9-C8-O7-C10
39	1	318	DGD	C3G-C2G-O2G-C1B
31	B	612	CLA	C15-C16-C17-C18
31	b	613	CLA	C15-C16-C17-C18
31	P	608	CLA	C2-C1-O2A-CGA
31	p	608	CLA	C2-C1-O2A-CGA
38	K	101	LMG	C31-C32-C33-C34
36	14	317	LHG	C24-C23-O8-C6
38	k	101	LMG	C31-C32-C33-C34
34	A	408	SQD	C25-C26-C27-C28
38	c	521	LMG	C22-C23-C24-C25
38	14	316	LMG	C35-C36-C37-C38
39	c	520	DGD	C4B-C5B-C6B-C7B
31	16	309	CLA	CBA-CGA-O2A-C1
31	19	307	CLA	CBA-CGA-O2A-C1
31	2	307	CLA	O1A-CGA-O2A-C1
34	a	408	SQD	C24-C25-C26-C27
34	a	408	SQD	C25-C26-C27-C28
39	C	520	DGD	C4B-C5B-C6B-C7B
34	A	408	SQD	C24-C25-C26-C27
38	d	408	LMG	C12-C13-C14-C15
36	z	102	LHG	O2-C2-C3-O3
38	D	408	LMG	C12-C13-C14-C15
36	D	407	LHG	C7-C8-C9-C10
36	d	407	LHG	C7-C8-C9-C10
31	B	604	CLA	C15-C16-C17-C18
33	Y	101	BCR	C20-C21-C22-C23
33	y	101	BCR	C20-C21-C22-C23
39	W	203	DGD	C2E-C1E-O5D-C6D
39	w	204	DGD	C2E-C1E-O5D-C6D
36	8	315	LHG	O7-C5-C6-O8
43	3	302	A86	C35-C34-O4-C38
43	9	304	A86	C35-C34-O4-C38
34	l	101	SQD	C29-C30-C31-C32
31	b	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	A	405	PHO	C10-C11-C12-C13
32	a	405	PHO	C10-C11-C12-C13
31	9	307	CLA	O1A-CGA-O2A-C1
31	10	308	CLA	O1A-CGA-O2A-C1
38	C	522	LMG	C22-C23-C24-C25
31	B	603	CLA	C4-C3-C5-C6
31	P	602	CLA	C4-C3-C5-C6
31	p	602	CLA	C4-C3-C5-C6
38	b	621	LMG	C32-C33-C34-C35
31	B	601	CLA	C11-C12-C13-C15
31	B	603	CLA	C6-C7-C8-C10
31	B	604	CLA	C11-C12-C13-C15
31	B	605	CLA	C6-C7-C8-C10
31	B	614	CLA	C11-C10-C8-C7
31	C	503	CLA	C11-C10-C8-C7
31	C	506	CLA	C6-C7-C8-C10
31	C	508	CLA	C6-C7-C8-C10
31	C	508	CLA	C12-C13-C15-C16
31	C	511	CLA	C6-C7-C8-C10
31	C	513	CLA	C11-C10-C8-C7
31	P	601	CLA	C11-C12-C13-C15
31	W	202	CLA	C11-C10-C8-C7
31	b	602	CLA	C11-C12-C13-C15
31	b	604	CLA	C6-C7-C8-C10
31	b	605	CLA	C11-C12-C13-C15
31	b	606	CLA	C6-C7-C8-C10
31	c	503	CLA	C11-C10-C8-C7
31	c	506	CLA	C6-C7-C8-C10
31	c	508	CLA	C6-C7-C8-C10
31	c	508	CLA	C12-C13-C15-C16
31	c	511	CLA	C2-C3-C5-C6
31	c	511	CLA	C6-C7-C8-C10
31	c	513	CLA	C11-C10-C8-C7
31	p	601	CLA	C11-C12-C13-C15
31	w	203	CLA	C11-C10-C8-C7
31	0	309	CLA	C6-C7-C8-C10
31	1	308	CLA	C11-C10-C8-C7
31	1	313	CLA	C11-C12-C13-C15
31	1	321	CLA	C11-C10-C8-C7
31	4	309	CLA	C11-C10-C8-C7
31	4	309	CLA	C12-C13-C15-C16
31	5	307	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	6	309	CLA	C11-C10-C8-C7
31	9	307	CLA	C11-C12-C13-C15
31	10	309	CLA	C6-C7-C8-C10
31	11	308	CLA	C11-C10-C8-C7
31	11	313	CLA	C11-C12-C13-C15
31	13	316	CLA	C11-C12-C13-C15
31	14	309	CLA	C12-C13-C15-C16
31	15	307	CLA	C12-C13-C15-C16
31	19	307	CLA	C11-C12-C13-C15
31	b	603	CLA	C3-C5-C6-C7
39	W	203	DGD	C8A-C9A-CAA-CBA
39	w	204	DGD	C8A-C9A-CAA-CBA
31	A	406	CLA	C11-C10-C8-C9
31	B	603	CLA	C6-C7-C8-C9
31	B	604	CLA	C11-C12-C13-C14
31	B	607	CLA	C14-C13-C15-C16
31	B	611	CLA	C14-C13-C15-C16
31	C	504	CLA	C6-C7-C8-C9
31	C	506	CLA	C6-C7-C8-C9
31	C	507	CLA	C11-C12-C13-C14
31	C	507	CLA	C14-C13-C15-C16
31	C	508	CLA	C6-C7-C8-C9
31	C	508	CLA	C14-C13-C15-C16
31	C	511	CLA	C6-C7-C8-C9
31	C	511	CLA	C14-C13-C15-C16
31	P	601	CLA	C11-C12-C13-C14
31	b	604	CLA	C6-C7-C8-C9
31	b	605	CLA	C11-C12-C13-C14
31	b	608	CLA	C14-C13-C15-C16
31	b	612	CLA	C14-C13-C15-C16
31	b	615	CLA	C6-C7-C8-C9
31	c	504	CLA	C6-C7-C8-C9
31	c	506	CLA	C6-C7-C8-C9
31	c	507	CLA	C11-C12-C13-C14
31	c	507	CLA	C14-C13-C15-C16
31	c	508	CLA	C6-C7-C8-C9
31	c	508	CLA	C14-C13-C15-C16
31	c	511	CLA	C6-C7-C8-C9
31	c	511	CLA	C14-C13-C15-C16
31	p	601	CLA	C11-C12-C13-C14
31	4	309	CLA	C11-C10-C8-C9
31	4	309	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	5	307	CLA	C11-C10-C8-C9
31	6	309	CLA	C14-C13-C15-C16
31	9	307	CLA	C11-C12-C13-C14
31	9	310	CLA	C14-C13-C15-C16
31	11	308	CLA	C11-C10-C8-C9
31	11	313	CLA	C11-C12-C13-C14
31	19	307	CLA	C11-C12-C13-C14
43	2	301	A86	C35-C34-O4-C38
34	A	408	SQD	C9-C10-C11-C12
34	b	601	SQD	C35-C36-C37-C38
38	P	614	LMG	C29-C30-C31-C32
38	p	614	LMG	C29-C30-C31-C32
34	B	623	SQD	C13-C14-C15-C16
34	B	623	SQD	C35-C36-C37-C38
34	a	408	SQD	C9-C10-C11-C12
34	b	601	SQD	C13-C14-C15-C16
33	B	619	BCR	C7-C8-C9-C34
33	C	516	BCR	C7-C8-C9-C34
33	b	620	BCR	C7-C8-C9-C34
33	c	516	BCR	C7-C8-C9-C34
43	7	301	A86	C7-C6-C8-C9
31	4	315	CLA	C2C-C3C-CAC-CBC
38	11	317	LMG	C34-C35-C36-C37
33	C	516	BCR	C21-C22-C23-C24
33	b	620	BCR	C7-C8-C9-C10
33	c	516	BCR	C21-C22-C23-C24
34	l	101	SQD	C31-C32-C33-C34
36	8	316	LHG	C11-C10-C9-C8
38	F	102	LMG	C18-C19-C20-C21
38	f	102	LMG	C18-C19-C20-C21
43	5	302	A86	C35-C34-O4-C38
31	W	202	CLA	C13-C15-C16-C17
31	w	203	CLA	C13-C15-C16-C17
38	b	621	LMG	C35-C36-C37-C38
38	m	101	LMG	C33-C34-C35-C36
38	10	319	LMG	C12-C13-C14-C15
31	b	615	CLA	O1A-CGA-O2A-C1
38	J	101	LMG	C37-C38-C39-C40
38	j	101	LMG	C37-C38-C39-C40
38	14	316	LMG	C30-C31-C32-C33
31	b	603	CLA	C10-C11-C12-C13
31	B	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	M	101	LMG	C13-C14-C15-C16
31	C	504	CLA	C16-C17-C18-C19
31	c	504	CLA	C16-C17-C18-C19
31	3	313	CLA	C8-C10-C11-C12
36	P	615	LHG	O6-C4-C5-C6
36	p	615	LHG	O6-C4-C5-C6
31	B	602	CLA	C3-C5-C6-C7
39	W	203	DGD	C1A-C2A-C3A-C4A
39	w	204	DGD	C1A-C2A-C3A-C4A
39	11	318	DGD	C1A-C2A-C3A-C4A
38	N	101	LMG	C29-C28-O8-C9
33	C	516	BCR	C18-C19-C20-C21
33	c	516	BCR	C18-C19-C20-C21
31	B	602	CLA	C10-C11-C12-C13
31	9	307	CLA	C4-C3-C5-C6
31	C	511	CLA	C2-C3-C5-C6
39	11	318	DGD	C9B-CAB-CBB-CCB
31	1	308	CLA	C13-C15-C16-C17
42	12	314	KC1	CAA-CBA-CGA-O1A
39	11	318	DGD	CEB-CFB-CGB-CHB
45	12	311	KC2	O1D-CGD-O2D-CED
31	b	615	CLA	C16-C17-C18-C19
31	2	309	CLA	C2A-CAA-CBA-CGA
34	10	320	SQD	C26-C27-C28-C29
38	D	408	LMG	C33-C34-C35-C36
39	H	102	DGD	C6B-C7B-C8B-C9B
39	H	102	DGD	CAB-CBB-CCB-CDB
39	h	102	DGD	C6B-C7B-C8B-C9B
31	17	312	CLA	C2A-CAA-CBA-CGA
31	C	502	CLA	CBA-CGA-O2A-C1
36	l	102	LHG	C28-C29-C30-C31
36	14	317	LHG	C10-C11-C12-C13
38	d	408	LMG	C33-C34-C35-C36
38	n	701	LMG	C11-C12-C13-C14
39	h	102	DGD	CAB-CBB-CCB-CDB
42	18	313	KC1	O1D-CGD-O2D-CED
31	2	309	CLA	C3A-C2A-CAA-CBA
31	4	315	CLA	C3A-C2A-CAA-CBA
31	8	312	CLA	C3A-C2A-CAA-CBA
31	12	310	CLA	C3A-C2A-CAA-CBA
31	14	315	CLA	C3A-C2A-CAA-CBA
36	D	407	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	L	101	LHG	C28-C29-C30-C31
36	a	410	LHG	C27-C28-C29-C30
36	d	407	LHG	C28-C29-C30-C31
36	18	315	LHG	C11-C12-C13-C14
44	P	612	DD6	C11-C10-C9-C8
36	A	410	LHG	C27-C28-C29-C30
38	4	316	LMG	C17-C18-C19-C20
43	10	303	A86	C35-C34-O4-C38
31	19	308	CLA	O1D-CGD-O2D-CED
34	b	601	SQD	C15-C16-C17-C18
39	b	622	DGD	CDB-CEB-CFB-CGB
31	9	312	CLA	C16-C17-C18-C20
31	c	502	CLA	CBA-CGA-O2A-C1
31	0	311	CLA	CBA-CGA-O2A-C1
31	10	311	CLA	CBA-CGA-O2A-C1
34	B	623	SQD	C15-C16-C17-C18
38	b	621	LMG	C29-C30-C31-C32
38	5	316	LMG	C29-C30-C31-C32
31	C	511	CLA	C13-C15-C16-C17
31	D	404	CLA	C15-C16-C17-C18
31	c	511	CLA	C13-C15-C16-C17
31	d	404	CLA	C15-C16-C17-C18
32	A	405	PHO	C15-C16-C17-C18
32	a	405	PHO	C15-C16-C17-C18
36	L	101	LHG	C4-C5-C6-O8
36	l	102	LHG	C4-C5-C6-O8
36	14	317	LHG	C4-C5-C6-O8
36	18	315	LHG	C4-C5-C6-O8
38	B	620	LMG	O1-C7-C8-C9
38	B	620	LMG	C7-C8-C9-O8
38	D	403	LMG	O1-C7-C8-C9
38	J	101	LMG	O1-C7-C8-C9
38	J	101	LMG	C7-C8-C9-O8
38	K	101	LMG	C7-C8-C9-O8
38	b	621	LMG	O1-C7-C8-C9
38	b	621	LMG	C7-C8-C9-O8
38	d	403	LMG	O1-C7-C8-C9
38	j	101	LMG	O1-C7-C8-C9
38	j	101	LMG	C7-C8-C9-O8
38	k	101	LMG	C7-C8-C9-O8
38	1	301	LMG	C7-C8-C9-O8
38	1	317	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
38	5	316	LMG	O1-C7-C8-C9
38	5	316	LMG	C7-C8-C9-O8
38	11	301	LMG	C7-C8-C9-O8
38	15	315	LMG	O1-C7-C8-C9
39	C	518	DGD	C1G-C2G-C3G-O3G
39	c	518	DGD	C1G-C2G-C3G-O3G
39	1	318	DGD	O1G-C1G-C2G-C3G
38	15	314	LMG	O9-C10-O7-C8
39	W	203	DGD	C5A-C6A-C7A-C8A
39	w	204	DGD	C5A-C6A-C7A-C8A
31	1	313	CLA	C8-C10-C11-C12
39	H	102	DGD	O2G-C1B-C2B-C3B
39	h	102	DGD	O2G-C1B-C2B-C3B
36	B	622	LHG	C26-C27-C28-C29
38	M	101	LMG	C35-C36-C37-C38
38	m	101	LMG	C15-C16-C17-C18
31	B	613	CLA	C3-C5-C6-C7
31	b	614	CLA	C3-C5-C6-C7
38	4	316	LMG	C10-C11-C12-C13
36	b	623	LHG	C26-C27-C28-C29
38	B	620	LMG	C22-C23-C24-C25
38	b	621	LMG	C22-C23-C24-C25
32	A	405	PHO	C4-C3-C5-C6
32	a	405	PHO	C4-C3-C5-C6
35	A	409	PL9	C13-C14-C16-C17
42	5	313	KC1	CAA-CBA-CGA-O2A
31	P	607	CLA	C2C-C3C-CAC-CBC
38	B	620	LMG	C18-C19-C20-C21
38	b	621	LMG	C18-C19-C20-C21
36	L	101	LHG	C4-O6-P-O3
36	l	102	LHG	C4-O6-P-O3
39	c	518	DGD	O1A-C1A-O1G-C1G
38	15	315	LMG	O6-C5-C6-O5
31	p	607	CLA	C2C-C3C-CAC-CBC
38	W	201	LMG	C14-C15-C16-C17
38	w	201	LMG	C14-C15-C16-C17
39	B	621	DGD	C9B-CAB-CBB-CCB
31	19	310	CLA	O1D-CGD-O2D-CED
32	a	405	PHO	O1D-CGD-O2D-CED
31	P	602	CLA	C2A-CAA-CBA-CGA
31	p	602	CLA	C2A-CAA-CBA-CGA
36	18	316	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
31	19	308	CLA	C5-C6-C7-C8
34	i	101	SQD	C10-C11-C12-C13
36	8	315	LHG	C11-C10-C9-C8
38	1	317	LMG	C17-C18-C19-C20
39	11	318	DGD	CCB-CDB-CEB-CFB
34	A	411	SQD	C10-C11-C12-C13
32	A	405	PHO	O1D-CGD-O2D-CED
39	C	518	DGD	O1A-C1A-O1G-C1G
45	18	310	KC2	C3A-C2A-CAA-CBA
31	14	309	CLA	C16-C17-C18-C20
38	j	101	LMG	C21-C22-C23-C24
31	6	309	CLA	O1A-CGA-O2A-C1
31	16	309	CLA	O1A-CGA-O2A-C1
38	P	614	LMG	O10-C28-O8-C9
38	p	614	LMG	O10-C28-O8-C9
38	J	101	LMG	C21-C22-C23-C24
38	1	317	LMG	C37-C38-C39-C40
34	L	102	SQD	O47-C45-C46-O48
34	0	318	SQD	O6-C44-C45-O47
36	L	101	LHG	O7-C5-C6-O8
36	l	102	LHG	O7-C5-C6-O8
36	8	316	LHG	O7-C5-C6-O8
38	B	620	LMG	O1-C7-C8-O7
38	D	403	LMG	O1-C7-C8-O7
38	D	408	LMG	O7-C8-C9-O8
38	J	101	LMG	O1-C7-C8-O7
38	b	621	LMG	O1-C7-C8-O7
38	d	408	LMG	O7-C8-C9-O8
38	j	101	LMG	O1-C7-C8-O7
38	11	317	LMG	O1-C7-C8-O7
38	11	317	LMG	O7-C8-C9-O8
39	C	518	DGD	O1G-C1G-C2G-O2G
39	C	518	DGD	O2G-C2G-C3G-O3G
39	C	519	DGD	O2G-C2G-C3G-O3G
39	C	520	DGD	O1G-C1G-C2G-O2G
39	W	203	DGD	O1G-C1G-C2G-O2G
39	c	518	DGD	O1G-C1G-C2G-O2G
39	c	518	DGD	O2G-C2G-C3G-O3G
39	c	519	DGD	O2G-C2G-C3G-O3G
39	c	520	DGD	O1G-C1G-C2G-O2G
39	w	204	DGD	O1G-C1G-C2G-O2G
31	b	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C19-C20-C21-C22
43	3	305	A86	C33-C34-O4-C38
43	19	301	A86	C33-C34-O4-C38
31	B	614	CLA	C16-C17-C18-C19
31	18	312	CLA	C6-C7-C8-C9
34	L	102	SQD	C29-C30-C31-C32
36	L	101	LHG	C19-C20-C21-C22
38	K	101	LMG	O6-C1-O1-C7
38	k	101	LMG	O6-C1-O1-C7
31	C	503	CLA	C5-C6-C7-C8
31	c	503	CLA	C5-C6-C7-C8
31	B	610	CLA	CBD-CGD-O2D-CED
43	P	613	A86	C10-C11-C13-C14
43	p	613	A86	C10-C11-C13-C14
43	0	302	A86	C10-C11-C13-C14
43	0	303	A86	C10-C11-C13-C14
43	0	304	A86	C10-C11-C13-C14
43	0	305	A86	C10-C11-C13-C14
43	0	306	A86	C10-C11-C13-C14
43	1	303	A86	C10-C11-C13-C14
43	1	306	A86	C10-C11-C13-C14
43	1	319	A86	C10-C11-C13-C14
43	1	320	A86	C10-C11-C13-C14
43	2	301	A86	C10-C11-C13-C14
43	2	302	A86	C10-C11-C13-C14
43	2	303	A86	C10-C11-C13-C14
43	2	304	A86	C10-C11-C13-C14
43	3	302	A86	C10-C11-C13-C14
43	3	303	A86	C10-C11-C13-C14
43	3	305	A86	C10-C11-C13-C14
43	4	301	A86	C10-C11-C13-C14
43	4	302	A86	C10-C11-C13-C14
43	4	304	A86	C10-C11-C13-C14
43	4	305	A86	C10-C11-C13-C14
43	5	301	A86	C10-C11-C13-C14
43	5	302	A86	C10-C11-C13-C14
43	5	318	A86	C10-C11-C13-C14
43	6	302	A86	C10-C11-C13-C14
43	6	304	A86	C10-C11-C13-C14
43	6	307	A86	C10-C11-C13-C14
43	7	301	A86	C10-C11-C13-C14
43	7	302	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
43	7	303	A86	C10-C11-C13-C14
43	7	306	A86	C10-C11-C13-C14
43	8	301	A86	C10-C11-C13-C14
43	8	303	A86	C10-C11-C13-C14
43	9	301	A86	C10-C11-C13-C14
43	9	304	A86	C10-C11-C13-C14
43	9	305	A86	C10-C11-C13-C14
43	9	306	A86	C10-C11-C13-C14
43	10	302	A86	C10-C11-C13-C14
43	10	303	A86	C10-C11-C13-C14
43	10	304	A86	C10-C11-C13-C14
43	10	305	A86	C10-C11-C13-C14
43	10	306	A86	C10-C11-C13-C14
43	11	302	A86	C10-C11-C13-C14
43	11	303	A86	C10-C11-C13-C14
43	11	305	A86	C10-C11-C13-C14
43	12	301	A86	C10-C11-C13-C14
43	12	302	A86	C10-C11-C13-C14
43	12	303	A86	C10-C11-C13-C14
43	12	304	A86	C10-C11-C13-C14
43	12	305	A86	C10-C11-C13-C14
43	13	301	A86	C10-C11-C13-C14
43	13	302	A86	C10-C11-C13-C14
43	13	304	A86	C10-C11-C13-C14
43	13	305	A86	C10-C11-C13-C14
43	13	306	A86	C10-C11-C13-C14
43	14	303	A86	C10-C11-C13-C14
43	14	304	A86	C10-C11-C13-C14
43	15	301	A86	C10-C11-C13-C14
43	15	302	A86	C10-C11-C13-C14
43	16	302	A86	C10-C11-C13-C14
43	16	303	A86	C10-C11-C13-C14
43	16	304	A86	C10-C11-C13-C14
43	16	305	A86	C10-C11-C13-C14
43	17	301	A86	C10-C11-C13-C14
43	17	302	A86	C10-C11-C13-C14
43	17	303	A86	C10-C11-C13-C14
43	17	304	A86	C10-C11-C13-C14
43	17	316	A86	C10-C11-C13-C14
43	18	305	A86	C10-C11-C13-C14
43	19	304	A86	C10-C11-C13-C14
43	19	305	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
36	C	521	LHG	C24-C25-C26-C27
36	w	202	LHG	C24-C25-C26-C27
38	14	316	LMG	C33-C34-C35-C36
39	H	102	DGD	CDA-CEA-CFA-CGA
39	h	102	DGD	CDA-CEA-CFA-CGA
42	5	313	KC1	CAA-CBA-CGA-O1A
42	12	314	KC1	CAA-CBA-CGA-O2A
31	B	602	CLA	C2-C1-O2A-CGA
31	C	513	CLA	C2-C1-O2A-CGA
31	b	603	CLA	C2-C1-O2A-CGA
31	c	513	CLA	C2-C1-O2A-CGA
31	17	313	CLA	C2-C1-O2A-CGA
35	d	406	PL9	C47-C48-C49-C50
35	a	409	PL9	C13-C14-C16-C17
36	L	101	LHG	C11-C12-C13-C14
36	l	102	LHG	C11-C12-C13-C14
31	B	601	CLA	C11-C12-C13-C14
31	B	608	CLA	C11-C12-C13-C14
31	B	609	CLA	C6-C7-C8-C9
31	B	609	CLA	C14-C13-C15-C16
31	B	614	CLA	C6-C7-C8-C9
31	C	513	CLA	C14-C13-C15-C16
31	b	602	CLA	C11-C12-C13-C14
31	b	609	CLA	C11-C12-C13-C14
31	b	610	CLA	C6-C7-C8-C9
31	b	610	CLA	C14-C13-C15-C16
31	c	513	CLA	C14-C13-C15-C16
31	2	307	CLA	C6-C7-C8-C9
31	3	313	CLA	C11-C12-C13-C14
31	4	307	CLA	C14-C13-C15-C16
31	9	313	CLA	C11-C12-C13-C14
31	13	313	CLA	C11-C12-C13-C14
31	14	307	CLA	C14-C13-C15-C16
31	15	307	CLA	C11-C10-C8-C9
31	16	309	CLA	C14-C13-C15-C16
31	19	310	CLA	C14-C13-C15-C16
31	19	312	CLA	C6-C7-C8-C9
31	19	313	CLA	C11-C12-C13-C14
39	W	203	DGD	C4B-C5B-C6B-C7B
39	w	204	DGD	C4B-C5B-C6B-C7B
39	11	318	DGD	C3A-C4A-C5A-C6A
31	B	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b	617	CLA	C10-C11-C12-C13
31	19	310	CLA	C15-C16-C17-C18
36	C	521	LHG	C2-C3-O3-P
36	w	202	LHG	C2-C3-O3-P
36	18	316	LHG	C2-C3-O3-P
34	A	411	SQD	C25-C26-C27-C28
34	i	101	SQD	C25-C26-C27-C28
39	C	520	DGD	CAA-CBA-CCA-CDA
39	c	518	DGD	C3B-C4B-C5B-C6B
39	c	520	DGD	CAA-CBA-CCA-CDA
33	B	618	BCR	C5-C6-C7-C8
33	B	618	BCR	C23-C24-C25-C26
33	B	618	BCR	C23-C24-C25-C30
33	C	515	BCR	C1-C6-C7-C8
33	C	515	BCR	C23-C24-C25-C30
33	C	517	BCR	C23-C24-C25-C26
33	H	101	BCR	C23-C24-C25-C26
33	Y	101	BCR	C5-C6-C7-C8
33	b	619	BCR	C5-C6-C7-C8
33	b	619	BCR	C23-C24-C25-C26
33	b	619	BCR	C23-C24-C25-C30
33	c	515	BCR	C1-C6-C7-C8
33	c	515	BCR	C23-C24-C25-C30
33	c	517	BCR	C23-C24-C25-C26
33	h	101	BCR	C23-C24-C25-C26
33	y	101	BCR	C1-C6-C7-C8
33	y	101	BCR	C5-C6-C7-C8
31	B	616	CLA	C10-C11-C12-C13
31	C	503	CLA	C15-C16-C17-C18
31	c	503	CLA	C15-C16-C17-C18
31	3	313	CLA	C13-C15-C16-C17
38	11	317	LMG	C13-C14-C15-C16
39	C	518	DGD	C3B-C4B-C5B-C6B
43	13	303	A86	C7-C6-C8-C9
35	D	406	PL9	C47-C48-C49-C50
39	c	519	DGD	O6E-C5E-C6E-O5E
31	3	307	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	C1A-C2A-CAA-CBA
31	13	307	CLA	C1A-C2A-CAA-CBA
31	16	308	CLA	C1A-C2A-CAA-CBA
33	B	617	BCR	C21-C22-C23-C24
33	B	619	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	C	515	BCR	C21-C22-C23-C24
33	C	517	BCR	C7-C8-C9-C10
33	F	101	BCR	C21-C22-C23-C24
33	b	618	BCR	C21-C22-C23-C24
33	c	515	BCR	C21-C22-C23-C24
33	c	517	BCR	C7-C8-C9-C10
33	f	101	BCR	C21-C22-C23-C24
43	0	301	A86	C35-C34-O4-C38
43	7	306	A86	C35-C34-O4-C38
31	A	406	CLA	C8-C10-C11-C12
31	a	406	CLA	C8-C10-C11-C12
38	11	317	LMG	C17-C18-C19-C20
31	18	314	CLA	O1D-CGD-O2D-CED
39	C	519	DGD	O6E-C5E-C6E-O5E
36	D	407	LHG	C10-C11-C12-C13
36	d	407	LHG	C10-C11-C12-C13
31	b	615	CLA	C16-C17-C18-C20
31	1	321	CLA	C14-C13-C15-C16
31	14	306	CLA	C14-C13-C15-C16
34	A	411	SQD	C30-C31-C32-C33
36	8	316	LHG	C15-C16-C17-C18
43	3	301	A86	C33-C34-O4-C38
34	i	101	SQD	C30-C31-C32-C33
38	1	317	LMG	C35-C36-C37-C38
31	19	307	CLA	O1A-CGA-O2A-C1
34	L	102	SQD	C31-C32-C33-C34
38	M	101	LMG	C30-C31-C32-C33
36	D	407	LHG	O6-C4-C5-C6
36	d	407	LHG	O6-C4-C5-C6
31	B	606	CLA	C11-C12-C13-C15
31	B	608	CLA	C6-C7-C8-C10
31	B	612	CLA	C11-C10-C8-C7
31	B	614	CLA	C6-C7-C8-C10
31	C	504	CLA	C11-C12-C13-C15
31	C	507	CLA	C11-C12-C13-C15
31	C	507	CLA	C12-C13-C15-C16
31	C	511	CLA	C12-C13-C15-C16
31	C	513	CLA	C12-C13-C15-C16
31	P	601	CLA	C11-C10-C8-C7
31	P	601	CLA	C12-C13-C15-C16
31	P	602	CLA	C2-C3-C5-C6
31	P	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	b	607	CLA	C11-C12-C13-C15
31	b	609	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C10-C8-C7
31	b	615	CLA	C6-C7-C8-C10
31	c	504	CLA	C11-C12-C13-C15
31	c	507	CLA	C11-C12-C13-C15
31	c	507	CLA	C12-C13-C15-C16
31	c	511	CLA	C12-C13-C15-C16
31	c	513	CLA	C12-C13-C15-C16
31	p	601	CLA	C11-C10-C8-C7
31	p	601	CLA	C12-C13-C15-C16
31	p	602	CLA	C2-C3-C5-C6
31	p	602	CLA	C11-C10-C8-C7
31	2	307	CLA	C11-C10-C8-C7
31	2	307	CLA	C12-C13-C15-C16
31	4	307	CLA	C12-C13-C15-C16
31	5	307	CLA	C11-C10-C8-C7
31	6	309	CLA	C12-C13-C15-C16
31	9	313	CLA	C11-C12-C13-C15
31	11	308	CLA	C12-C13-C15-C16
31	12	308	CLA	C11-C10-C8-C7
31	12	308	CLA	C12-C13-C15-C16
31	13	313	CLA	C11-C12-C13-C15
31	14	307	CLA	C12-C13-C15-C16
31	15	307	CLA	C11-C10-C8-C7
31	16	309	CLA	C11-C10-C8-C7
31	16	309	CLA	C12-C13-C15-C16
31	19	313	CLA	C11-C12-C13-C15
32	A	405	PHO	C2-C3-C5-C6
32	D	402	PHO	C6-C7-C8-C10
32	a	405	PHO	C2-C3-C5-C6
32	d	402	PHO	C6-C7-C8-C10
43	18	305	A86	C24-C25-C26-C27
31	D	404	CLA	C16-C17-C18-C19
31	d	404	CLA	C16-C17-C18-C19
31	z	103	CLA	CBA-CGA-O2A-C1
36	18	316	LHG	C11-C10-C9-C8
31	Z	101	CLA	C2A-CAA-CBA-CGA
31	6	313	CLA	C2A-CAA-CBA-CGA
31	13	313	CLA	C2A-CAA-CBA-CGA
31	9	310	CLA	CBD-CGD-O2D-CED
45	2	310	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	B	617	BCR	C20-C21-C22-C37
34	a	408	SQD	C19-C20-C21-C22
43	3	303	A86	C35-C34-O4-C38
43	4	301	A86	C35-C34-O4-C38
34	A	408	SQD	C19-C20-C21-C22
31	B	614	CLA	C16-C17-C18-C20
38	D	403	LMG	C34-C35-C36-C37
31	1	321	CLA	C12-C13-C15-C16
31	14	306	CLA	C12-C13-C15-C16
38	D	403	LMG	C13-C14-C15-C16
38	m	101	LMG	C11-C12-C13-C14
39	B	621	DGD	C4A-C5A-C6A-C7A
31	B	607	CLA	C8-C10-C11-C12
31	C	504	CLA	C8-C10-C11-C12
31	b	608	CLA	C8-C10-C11-C12
31	c	504	CLA	C8-C10-C11-C12
36	L	101	LHG	C32-C33-C34-C35
36	l	102	LHG	C32-C33-C34-C35
31	B	601	CLA	CAD-CBD-CGD-O2D
31	B	603	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	CAD-CBD-CGD-O2D
31	B	614	CLA	CAD-CBD-CGD-O2D
31	C	506	CLA	CAD-CBD-CGD-O2D
31	C	513	CLA	CAD-CBD-CGD-O2D
31	C	514	CLA	CAD-CBD-CGD-O2D
31	P	606	CLA	CAD-CBD-CGD-O2D
31	b	602	CLA	CAD-CBD-CGD-O2D
31	b	604	CLA	CAD-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O2D
31	b	615	CLA	CAD-CBD-CGD-O2D
31	b	617	CLA	CAD-CBD-CGD-O2D
31	c	506	CLA	CAD-CBD-CGD-O2D
31	c	513	CLA	CAD-CBD-CGD-O2D
31	c	514	CLA	CAD-CBD-CGD-O2D
31	p	606	CLA	CAD-CBD-CGD-O2D
31	1	316	CLA	CAD-CBD-CGD-O2D
31	2	309	CLA	CAD-CBD-CGD-O2D
31	2	312	CLA	CAD-CBD-CGD-O2D
31	3	307	CLA	CAD-CBD-CGD-O2D
31	4	309	CLA	CAD-CBD-CGD-O2D
31	4	315	CLA	CAD-CBD-CGD-O2D
31	6	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	6	313	CLA	CAD-CBD-CGD-O2D
31	7	310	CLA	CAD-CBD-CGD-O2D
31	8	306	CLA	CAD-CBD-CGD-O2D
31	8	309	CLA	CAD-CBD-CGD-O2D
31	9	310	CLA	CAD-CBD-CGD-O2D
31	11	307	CLA	CAD-CBD-CGD-O2D
31	11	312	CLA	CAD-CBD-CGD-O2D
31	12	310	CLA	CAD-CBD-CGD-O2D
31	12	313	CLA	CAD-CBD-CGD-O2D
31	12	316	CLA	CAD-CBD-CGD-O2D
31	14	309	CLA	CAD-CBD-CGD-O2D
31	15	307	CLA	CAD-CBD-CGD-O2D
31	16	308	CLA	CAD-CBD-CGD-O2D
31	16	311	CLA	CAD-CBD-CGD-O2D
31	18	309	CLA	CAD-CBD-CGD-O2D
32	A	405	PHO	CAD-CBD-CGD-O2D
32	a	405	PHO	CAD-CBD-CGD-O2D
34	L	102	SQD	C46-C45-O47-C7
34	l	101	SQD	C46-C45-O47-C7
36	Z	103	LHG	C6-C5-O7-C7
36	z	102	LHG	C6-C5-O7-C7
38	d	403	LMG	C9-C8-O7-C10
39	B	621	DGD	C3G-C2G-O2G-C1B
39	11	318	DGD	C3G-C2G-O2G-C1B
42	12	314	KC1	CAD-CBD-CGD-O2D
43	17	305	A86	C28-C27-C29-C30
43	19	302	A86	C28-C27-C29-C30
45	1	309	KC2	C2B-C3B-CAB-CBB
45	4	310	KC2	C2B-C3B-CAB-CBB
45	5	308	KC2	CAD-CBD-CGD-O2D
45	14	308	KC2	CAD-CBD-CGD-O2D
45	14	310	KC2	C2B-C3B-CAB-CBB
45	15	308	KC2	CAD-CBD-CGD-O2D
43	0	303	A86	C35-C34-O4-C38
31	14	309	CLA	C15-C16-C17-C18
33	B	617	BCR	C22-C23-C24-C25
31	3	313	CLA	C4-C3-C5-C6
38	0	317	LMG	O6-C1-O1-C7
38	c	522	LMG	C30-C31-C32-C33
34	L	102	SQD	C44-C45-C46-O48
34	l	101	SQD	C44-C45-C46-O48
36	C	521	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
36	P	615	LHG	C2-C3-O3-P
36	p	615	LHG	C2-C3-O3-P
36	w	202	LHG	C5-C4-O6-P
36	18	316	LHG	C4-C5-C6-O8
38	C	522	LMG	O1-C7-C8-C9
38	c	521	LMG	O1-C7-C8-C9
38	m	101	LMG	O1-C7-C8-C9
38	15	314	LMG	O1-C7-C8-C9
39	11	318	DGD	O1G-C1G-C2G-C3G
43	0	301	A86	C12-C11-C13-O
43	0	305	A86	C12-C11-C13-O
43	0	306	A86	C12-C11-C13-O
43	1	303	A86	C12-C11-C13-O
43	1	304	A86	C12-C11-C13-O
43	1	305	A86	C12-C11-C13-O
43	1	319	A86	C12-C11-C13-O
43	1	320	A86	C12-C11-C13-O
43	2	301	A86	C12-C11-C13-O
43	2	304	A86	C12-C11-C13-O
43	2	305	A86	C12-C11-C13-O
43	3	301	A86	C12-C11-C13-O
43	3	303	A86	C12-C11-C13-O
43	3	304	A86	C12-C11-C13-O
43	3	306	A86	C12-C11-C13-O
43	4	301	A86	C12-C11-C13-O
43	4	303	A86	C12-C11-C13-O
43	4	304	A86	C12-C11-C13-O
43	4	305	A86	C12-C11-C13-O
43	5	302	A86	C12-C11-C13-O
43	5	303	A86	C12-C11-C13-O
43	5	304	A86	C12-C11-C13-O
43	5	305	A86	C12-C11-C13-O
43	6	304	A86	C12-C11-C13-O
43	6	305	A86	C12-C11-C13-O
43	6	307	A86	C12-C11-C13-O
43	7	302	A86	C12-C11-C13-O
43	7	303	A86	C12-C11-C13-O
43	7	305	A86	C12-C11-C13-O
43	8	301	A86	C12-C11-C13-O
43	8	302	A86	C12-C11-C13-O
43	8	303	A86	C12-C11-C13-O
43	8	304	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	8	305	A86	C12-C11-C13-O
43	9	301	A86	C12-C11-C13-O
43	9	302	A86	C12-C11-C13-O
43	9	303	A86	C12-C11-C13-O
43	9	305	A86	C12-C11-C13-O
43	9	306	A86	C12-C11-C13-O
43	10	301	A86	C12-C11-C13-O
43	10	304	A86	C12-C11-C13-O
43	10	305	A86	C12-C11-C13-O
43	10	306	A86	C12-C11-C13-O
43	10	318	A86	C12-C11-C13-O
43	11	303	A86	C12-C11-C13-O
43	11	304	A86	C12-C11-C13-O
43	11	319	A86	C12-C11-C13-O
43	11	320	A86	C12-C11-C13-O
43	12	302	A86	C12-C11-C13-O
43	12	304	A86	C12-C11-C13-O
43	12	306	A86	C12-C11-C13-O
43	13	302	A86	C12-C11-C13-O
43	13	303	A86	C12-C11-C13-O
43	13	305	A86	C12-C11-C13-O
43	14	303	A86	C12-C11-C13-O
43	14	304	A86	C12-C11-C13-O
43	15	302	A86	C12-C11-C13-O
43	15	303	A86	C12-C11-C13-O
43	15	304	A86	C12-C11-C13-O
43	15	305	A86	C12-C11-C13-O
43	16	304	A86	C12-C11-C13-O
43	16	305	A86	C12-C11-C13-O
43	16	306	A86	C12-C11-C13-O
43	17	303	A86	C12-C11-C13-O
43	17	304	A86	C12-C11-C13-O
43	17	306	A86	C12-C11-C13-O
43	17	316	A86	C12-C11-C13-O
43	18	304	A86	C12-C11-C13-O
43	19	301	A86	C12-C11-C13-O
43	19	302	A86	C12-C11-C13-O
43	19	303	A86	C12-C11-C13-O
43	19	304	A86	C12-C11-C13-O
43	19	305	A86	C12-C11-C13-O
43	19	306	A86	C12-C11-C13-O
38	d	403	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
38	0	317	LMG	O6-C5-C6-O5
31	12	313	CLA	C2C-C3C-CAC-CBC
39	W	203	DGD	C4A-C5A-C6A-C7A
42	2	313	KC1	C4B-C3B-CAB-CBB
42	3	314	KC1	C4B-C3B-CAB-CBB
42	4	313	KC1	C4B-C3B-CAB-CBB
42	6	315	KC1	C4B-C3B-CAB-CBB
42	14	313	KC1	C4B-C3B-CAB-CBB
42	16	315	KC1	C4B-C3B-CAB-CBB
45	1	309	KC2	C4B-C3B-CAB-CBB
45	1	309	KC2	C4C-C3C-CAC-CBC
45	11	309	KC2	C4B-C3B-CAB-CBB
45	12	311	KC2	C4C-C3C-CAC-CBC
45	15	310	KC2	C4B-C3B-CAB-CBB
31	z	101	CLA	C2A-CAA-CBA-CGA
34	10	320	SQD	C11-C10-C9-C8
39	w	204	DGD	C4A-C5A-C6A-C7A
31	5	309	CLA	C6-C7-C8-C10
31	8	312	CLA	C6-C7-C8-C9
31	14	309	CLA	C16-C17-C18-C19
38	D	408	LMG	C30-C31-C32-C33
38	Z	102	LMG	C30-C31-C32-C33
38	d	408	LMG	C30-C31-C32-C33
38	1	317	LMG	C19-C20-C21-C22
31	B	604	CLA	CHA-CBD-CGD-O1D
31	B	604	CLA	CHA-CBD-CGD-O2D
31	B	612	CLA	CHA-CBD-CGD-O1D
31	C	504	CLA	CHA-CBD-CGD-O1D
31	C	504	CLA	CHA-CBD-CGD-O2D
31	P	603	CLA	CHA-CBD-CGD-O2D
31	b	605	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CHA-CBD-CGD-O2D
31	b	613	CLA	CHA-CBD-CGD-O1D
31	c	504	CLA	CHA-CBD-CGD-O1D
31	c	504	CLA	CHA-CBD-CGD-O2D
31	p	603	CLA	CHA-CBD-CGD-O2D
31	0	309	CLA	CHA-CBD-CGD-O2D
31	2	314	CLA	CHA-CBD-CGD-O1D
31	4	314	CLA	CHA-CBD-CGD-O1D
31	4	314	CLA	CHA-CBD-CGD-O2D
31	5	309	CLA	CHA-CBD-CGD-O2D
31	6	316	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	6	316	CLA	CHA-CBD-CGD-O2D
31	7	315	CLA	CHA-CBD-CGD-O1D
31	7	315	CLA	CHA-CBD-CGD-O2D
31	10	308	CLA	CHA-CBD-CGD-O1D
31	10	309	CLA	CHA-CBD-CGD-O1D
31	14	314	CLA	CHA-CBD-CGD-O1D
31	14	314	CLA	CHA-CBD-CGD-O2D
42	4	313	KC1	CHA-CBD-CGD-O1D
42	4	313	KC1	CHA-CBD-CGD-O2D
42	14	313	KC1	CHA-CBD-CGD-O1D
42	14	313	KC1	CHA-CBD-CGD-O2D
43	15	303	A86	C35-C34-O4-C38
43	17	316	A86	C33-C34-O4-C38
31	C	502	CLA	O1A-CGA-O2A-C1
31	c	502	CLA	O1A-CGA-O2A-C1
38	15	315	LMG	O10-C28-O8-C9
39	C	518	DGD	C5A-C6A-C7A-C8A
31	12	313	CLA	O2A-C1-C2-C3
33	C	517	BCR	C11-C10-C9-C8
33	c	517	BCR	C11-C10-C9-C8
38	B	620	LMG	C29-C30-C31-C32
38	11	317	LMG	C19-C20-C21-C22
39	c	518	DGD	C5A-C6A-C7A-C8A
34	10	320	SQD	O6-C44-C45-O47
36	14	317	LHG	O7-C5-C6-O8
36	18	316	LHG	O7-C5-C6-O8
38	C	522	LMG	O7-C8-C9-O8
38	D	408	LMG	O1-C7-C8-O7
38	c	521	LMG	O1-C7-C8-O7
38	c	521	LMG	O7-C8-C9-O8
38	d	403	LMG	O1-C7-C8-O7
38	d	408	LMG	O1-C7-C8-O7
38	1	317	LMG	O7-C8-C9-O8
38	5	316	LMG	O1-C7-C8-O7
38	15	314	LMG	O1-C7-C8-O7
38	15	315	LMG	O1-C7-C8-O7
39	B	621	DGD	O2G-C2G-C3G-O3G
39	b	622	DGD	O2G-C2G-C3G-O3G
39	1	318	DGD	O2G-C2G-C3G-O3G
38	14	316	LMG	C11-C12-C13-C14
43	P	611	A86	C10-C11-C13-O
43	p	611	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	0	301	A86	C10-C11-C13-O
43	0	302	A86	C10-C11-C13-O
43	0	303	A86	C10-C11-C13-O
43	0	304	A86	C10-C11-C13-O
43	0	305	A86	C10-C11-C13-O
43	0	306	A86	C10-C11-C13-O
43	1	303	A86	C10-C11-C13-O
43	1	304	A86	C10-C11-C13-O
43	1	305	A86	C10-C11-C13-O
43	1	306	A86	C10-C11-C13-O
43	1	319	A86	C10-C11-C13-O
43	1	320	A86	C10-C11-C13-O
43	2	301	A86	C10-C11-C13-O
43	2	302	A86	C10-C11-C13-O
43	2	303	A86	C10-C11-C13-O
43	2	304	A86	C10-C11-C13-O
43	2	305	A86	C10-C11-C13-O
43	3	301	A86	C10-C11-C13-O
43	3	302	A86	C10-C11-C13-O
43	3	303	A86	C10-C11-C13-O
43	3	304	A86	C10-C11-C13-O
43	3	305	A86	C10-C11-C13-O
43	3	306	A86	C10-C11-C13-O
43	4	301	A86	C10-C11-C13-O
43	4	301	A86	C13-C14-C15-O1
43	4	303	A86	C10-C11-C13-O
43	4	304	A86	C10-C11-C13-O
43	4	305	A86	C10-C11-C13-O
43	4	306	A86	C10-C11-C13-O
43	5	301	A86	C10-C11-C13-O
43	5	302	A86	C10-C11-C13-O
43	5	303	A86	C10-C11-C13-O
43	5	304	A86	C10-C11-C13-O
43	5	305	A86	C10-C11-C13-O
43	6	301	A86	C10-C11-C13-O
43	6	302	A86	C10-C11-C13-O
43	6	304	A86	C10-C11-C13-O
43	6	305	A86	C10-C11-C13-O
43	6	306	A86	C10-C11-C13-O
43	7	302	A86	C10-C11-C13-O
43	7	303	A86	C10-C11-C13-O
43	7	304	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	7	305	A86	C10-C11-C13-O
43	7	306	A86	C10-C11-C13-O
43	8	302	A86	C10-C11-C13-O
43	8	303	A86	C10-C11-C13-O
43	8	304	A86	C10-C11-C13-O
43	8	305	A86	C10-C11-C13-O
43	9	301	A86	C10-C11-C13-O
43	9	302	A86	C10-C11-C13-O
43	9	303	A86	C10-C11-C13-O
43	9	304	A86	C10-C11-C13-O
43	9	305	A86	C10-C11-C13-O
43	9	306	A86	C10-C11-C13-O
43	10	301	A86	C10-C11-C13-O
43	10	302	A86	C10-C11-C13-O
43	10	303	A86	C10-C11-C13-O
43	10	304	A86	C10-C11-C13-O
43	10	305	A86	C10-C11-C13-O
43	10	318	A86	C10-C11-C13-O
43	11	303	A86	C10-C11-C13-O
43	11	304	A86	C10-C11-C13-O
43	11	305	A86	C10-C11-C13-O
43	11	306	A86	C10-C11-C13-O
43	11	319	A86	C10-C11-C13-O
43	11	320	A86	C10-C11-C13-O
43	12	301	A86	C10-C11-C13-O
43	12	302	A86	C10-C11-C13-O
43	12	303	A86	C10-C11-C13-O
43	12	304	A86	C10-C11-C13-O
43	12	305	A86	C10-C11-C13-O
43	12	306	A86	C10-C11-C13-O
43	13	301	A86	C10-C11-C13-O
43	13	302	A86	C10-C11-C13-O
43	13	303	A86	C10-C11-C13-O
43	13	305	A86	C10-C11-C13-O
43	13	306	A86	C10-C11-C13-O
43	14	303	A86	C10-C11-C13-O
43	14	304	A86	C10-C11-C13-O
43	14	305	A86	C10-C11-C13-O
43	15	301	A86	C10-C11-C13-O
43	15	302	A86	C10-C11-C13-O
43	15	303	A86	C10-C11-C13-O
43	15	304	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	16	303	A86	C10-C11-C13-O
43	16	304	A86	C10-C11-C13-O
43	16	305	A86	C10-C11-C13-O
43	16	306	A86	C10-C11-C13-O
43	16	307	A86	C10-C11-C13-O
43	17	301	A86	C10-C11-C13-O
43	17	303	A86	C10-C11-C13-O
43	17	304	A86	C10-C11-C13-O
43	17	306	A86	C10-C11-C13-O
43	17	316	A86	C10-C11-C13-O
43	18	301	A86	C10-C11-C13-O
43	18	304	A86	C10-C11-C13-O
43	18	305	A86	C10-C11-C13-O
43	19	301	A86	C10-C11-C13-O
43	19	302	A86	C10-C11-C13-O
43	19	303	A86	C10-C11-C13-O
43	19	304	A86	C10-C11-C13-O
43	19	305	A86	C10-C11-C13-O
43	19	306	A86	C10-C11-C13-O
38	W	201	LMG	C39-C40-C41-C42
38	w	201	LMG	C39-C40-C41-C42
31	9	310	CLA	C3-C5-C6-C7
31	11	308	CLA	C3-C5-C6-C7
31	9	308	CLA	CBD-CGD-O2D-CED
31	10	311	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	C2-C3-C5-C6
31	7	312	CLA	O1D-CGD-O2D-CED
31	9	310	CLA	O1D-CGD-O2D-CED
44	P	612	DD6	C27-C29-C30-C31
39	b	622	DGD	C4A-C5A-C6A-C7A
31	B	612	CLA	C11-C10-C8-C9
31	C	511	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C10-C8-C9
31	c	511	CLA	C11-C10-C8-C9
31	1	313	CLA	C11-C12-C13-C14
31	19	310	CLA	C11-C10-C8-C9
43	11	302	A86	C35-C34-O4-C38
31	z	103	CLA	O1A-CGA-O2A-C1
31	0	311	CLA	O1A-CGA-O2A-C1
38	Z	102	LMG	C29-C30-C31-C32
31	b	613	CLA	C3-C5-C6-C7
39	b	622	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
33	B	619	BCR	C37-C22-C23-C24
33	C	515	BCR	C7-C8-C9-C34
33	Y	101	BCR	C7-C8-C9-C34
33	b	620	BCR	C37-C22-C23-C24
33	c	515	BCR	C7-C8-C9-C34
33	y	101	BCR	C7-C8-C9-C34
38	w	201	LMG	C12-C13-C14-C15
43	19	302	A86	C35-C34-O4-C38
38	W	201	LMG	C12-C13-C14-C15
31	B	612	CLA	C3-C5-C6-C7
31	A	404	CLA	C1A-C2A-CAA-CBA
31	a	404	CLA	C1A-C2A-CAA-CBA
31	10	307	CLA	C1A-C2A-CAA-CBA
31	13	313	CLA	C1A-C2A-CAA-CBA
38	15	315	LMG	C10-C11-C12-C13
39	B	621	DGD	C1B-C2B-C3B-C4B
31	C	509	CLA	C16-C17-C18-C19
31	c	509	CLA	C16-C17-C18-C19
31	B	615	CLA	C15-C16-C17-C18
31	b	616	CLA	C15-C16-C17-C18
31	B	612	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
34	A	408	SQD	C17-C18-C19-C20
34	a	408	SQD	C17-C18-C19-C20
34	0	318	SQD	C11-C10-C9-C8
31	D	405	CLA	O1D-CGD-O2D-CED
31	d	405	CLA	O1D-CGD-O2D-CED
43	3	303	A86	C33-C34-O4-C38
43	10	302	A86	C33-C34-O4-C38
36	8	316	LHG	O10-C23-O8-C6
36	A	410	LHG	C4-O6-P-O3
36	a	410	LHG	C4-O6-P-O3
36	4	317	LHG	C3-O3-P-O6
36	14	317	LHG	C3-O3-P-O6
31	B	614	CLA	O1D-CGD-O2D-CED
38	m	101	LMG	C34-C35-C36-C37
31	D	405	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
36	Z	103	LHG	C2-C3-O3-P
36	z	102	LHG	C2-C3-O3-P
39	c	519	DGD	C5B-C6B-C7B-C8B
39	1	318	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
36	A	410	LHG	C3-O3-P-O5
36	A	410	LHG	C4-O6-P-O4
36	D	407	LHG	C4-O6-P-O5
36	L	101	LHG	C4-O6-P-O5
36	P	615	LHG	C4-O6-P-O4
36	Z	103	LHG	C4-O6-P-O4
36	a	410	LHG	C3-O3-P-O5
36	a	410	LHG	C4-O6-P-O4
36	d	407	LHG	C4-O6-P-O5
36	l	102	LHG	C4-O6-P-O5
36	p	615	LHG	C4-O6-P-O4
36	z	102	LHG	C4-O6-P-O4
36	4	317	LHG	C3-O3-P-O4
36	5	317	LHG	C4-O6-P-O4
36	8	316	LHG	C4-O6-P-O5
36	14	317	LHG	C3-O3-P-O4
36	15	316	LHG	C4-O6-P-O4
36	18	316	LHG	C4-O6-P-O5
39	c	520	DGD	C1B-C2B-C3B-C4B
39	C	519	DGD	C5B-C6B-C7B-C8B
31	B	614	CLA	C5-C6-C7-C8
31	C	512	CLA	C13-C15-C16-C17
31	b	606	CLA	C13-C15-C16-C17
31	c	512	CLA	C13-C15-C16-C17
36	A	410	LHG	O6-C4-C5-C6
36	a	410	LHG	O6-C4-C5-C6
45	2	310	KC2	CAA-CBA-CGA-O1A
38	W	201	LMG	C4-C5-C6-O5
38	w	201	LMG	C4-C5-C6-O5
39	C	520	DGD	C3B-C4B-C5B-C6B
31	B	605	CLA	C13-C15-C16-C17
39	C	520	DGD	C1B-C2B-C3B-C4B
39	c	520	DGD	C3B-C4B-C5B-C6B
38	Z	102	LMG	C11-C10-O7-C8
43	14	305	A86	C33-C34-O4-C38
31	B	604	CLA	CAD-CBD-CGD-O1D
31	C	502	CLA	CAD-CBD-CGD-O1D
31	P	608	CLA	C2-C3-C5-C6
31	b	605	CLA	CAD-CBD-CGD-O1D
31	c	502	CLA	CAD-CBD-CGD-O1D
31	p	608	CLA	C2-C3-C5-C6
31	1	315	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	3	316	CLA	CAD-CBD-CGD-O1D
31	4	312	CLA	C2-C3-C5-C6
31	5	309	CLA	CAD-CBD-CGD-O1D
31	13	316	CLA	CAD-CBD-CGD-O1D
31	15	309	CLA	CAD-CBD-CGD-O1D
34	A	411	SQD	C5-C6-S-O9
34	i	101	SQD	C5-C6-S-O9
31	2	314	CLA	CBD-CGD-O2D-CED
31	4	311	CLA	CAA-CBA-CGA-O2A
31	14	311	CLA	CAA-CBA-CGA-O2A
38	5	316	LMG	O10-C28-O8-C9
38	14	316	LMG	C37-C38-C39-C40
31	9	308	CLA	O1D-CGD-O2D-CED
38	1	301	LMG	C31-C32-C33-C34
38	11	301	LMG	C31-C32-C33-C34
31	C	502	CLA	C16-C17-C18-C20
31	c	502	CLA	C16-C17-C18-C20
31	4	307	CLA	C4-C3-C5-C6
31	9	310	CLA	C4-C3-C5-C6
31	B	603	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C10-C8-C7
31	B	611	CLA	C6-C7-C8-C10
31	C	505	CLA	C11-C12-C13-C15
31	C	510	CLA	C11-C10-C8-C7
31	C	511	CLA	C11-C10-C8-C7
31	C	513	CLA	C6-C7-C8-C10
31	b	602	CLA	C11-C10-C8-C7
31	b	604	CLA	C11-C10-C8-C7
31	b	611	CLA	C11-C10-C8-C7
31	b	612	CLA	C6-C7-C8-C10
31	c	505	CLA	C11-C12-C13-C15
31	c	510	CLA	C11-C10-C8-C7
31	c	511	CLA	C11-C10-C8-C7
31	c	513	CLA	C6-C7-C8-C10
31	1	308	CLA	C12-C13-C15-C16
31	3	313	CLA	C11-C12-C13-C15
31	11	308	CLA	C11-C12-C13-C15
36	D	407	LHG	O6-C4-C5-O7
36	d	407	LHG	O6-C4-C5-O7
36	z	102	LHG	O6-C4-C5-O7
34	L	102	SQD	C33-C34-C35-C36
32	D	402	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	d	402	PHO	C8-C10-C11-C12
38	F	102	LMG	C17-C18-C19-C20
38	F	102	LMG	C29-C30-C31-C32
38	f	102	LMG	C29-C30-C31-C32
31	10	307	CLA	CBD-CGD-O2D-CED
38	f	102	LMG	C17-C18-C19-C20
38	1	317	LMG	C32-C33-C34-C35
38	14	316	LMG	C17-C18-C19-C20
39	c	519	DGD	CCA-CDA-CEA-CFA
38	c	522	LMG	C11-C10-O7-C8
38	1	301	LMG	C11-C10-O7-C8
38	11	301	LMG	C11-C10-O7-C8
36	l	102	LHG	C15-C16-C17-C18
38	W	201	LMG	C36-C37-C38-C39
38	w	201	LMG	C36-C37-C38-C39
39	C	519	DGD	CCA-CDA-CEA-CFA
39	c	518	DGD	C7B-C8B-C9B-CAB
38	f	102	LMG	O10-C28-O8-C9
36	L	101	LHG	C15-C16-C17-C18
38	c	522	LMG	C29-C30-C31-C32
39	C	518	DGD	C7B-C8B-C9B-CAB
31	b	615	CLA	C8-C10-C11-C12
31	C	513	CLA	C2A-CAA-CBA-CGA
31	P	604	CLA	C2A-CAA-CBA-CGA
31	c	513	CLA	C2A-CAA-CBA-CGA
31	p	604	CLA	C2A-CAA-CBA-CGA
31	15	311	CLA	C2A-CAA-CBA-CGA
31	1	308	CLA	C5-C6-C7-C8
38	1	317	LMG	O1-C7-C8-C9
38	10	319	LMG	C29-C30-C31-C32
39	B	621	DGD	C1G-C2G-C3G-O3G
39	b	622	DGD	C1G-C2G-C3G-O3G
38	F	102	LMG	O10-C28-O8-C9
34	A	411	SQD	O47-C45-C46-O48
34	B	623	SQD	O47-C45-C46-O48
34	b	601	SQD	O47-C45-C46-O48
34	i	101	SQD	O47-C45-C46-O48
34	l	101	SQD	O47-C45-C46-O48
36	18	315	LHG	O7-C5-C6-O8
38	C	522	LMG	O1-C7-C8-O7
38	m	101	LMG	O1-C7-C8-O7
38	1	301	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
38	1	317	LMG	O1-C7-C8-O7
38	5	315	LMG	O1-C7-C8-O7
38	11	301	LMG	O1-C7-C8-O7
39	B	621	DGD	O1G-C1G-C2G-O2G
39	W	203	DGD	O2G-C2G-C3G-O3G
39	b	622	DGD	O1G-C1G-C2G-O2G
39	w	204	DGD	O2G-C2G-C3G-O3G
39	11	318	DGD	O2G-C2G-C3G-O3G
38	b	621	LMG	C36-C37-C38-C39
39	C	520	DGD	C7A-C8A-C9A-CAA
34	l	101	SQD	C33-C34-C35-C36
38	11	317	LMG	C36-C37-C38-C39
39	c	520	DGD	C7A-C8A-C9A-CAA
38	C	522	LMG	C11-C12-C13-C14
38	4	316	LMG	C37-C38-C39-C40
43	13	306	A86	C35-C34-O4-C38
36	8	316	LHG	C2-C3-O3-P
31	19	310	CLA	C4-C3-C5-C6
43	0	302	A86	C13-C14-C15-C20
43	0	303	A86	C13-C14-C15-C20
43	0	304	A86	C13-C14-C15-C20
43	1	305	A86	C13-C14-C15-C20
43	1	306	A86	C13-C14-C15-C20
43	2	302	A86	C13-C14-C15-C20
43	2	303	A86	C13-C14-C15-C20
43	4	305	A86	C13-C14-C15-C20
43	5	303	A86	C13-C14-C15-C20
43	5	318	A86	C13-C14-C15-C20
43	7	303	A86	C13-C14-C15-C20
43	8	303	A86	C13-C14-C15-C20
43	9	303	A86	C13-C14-C15-C20
43	9	304	A86	C13-C14-C15-C20
43	9	306	A86	C13-C14-C15-C20
43	10	302	A86	C13-C14-C15-C20
43	10	303	A86	C13-C14-C15-C20
43	10	304	A86	C13-C14-C15-C20
43	11	320	A86	C13-C14-C15-C20
43	12	301	A86	C13-C14-C15-C20
43	12	305	A86	C13-C14-C15-C20
43	13	305	A86	C13-C14-C15-C20
43	14	301	A86	C13-C14-C15-C20
43	14	304	A86	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
43	15	303	A86	C13-C14-C15-C20
43	17	303	A86	C13-C14-C15-C20
43	17	304	A86	C13-C14-C15-C20
43	19	303	A86	C13-C14-C15-C20
43	19	304	A86	C13-C14-C15-C20
43	19	306	A86	C13-C14-C15-C20
34	B	623	SQD	C28-C29-C30-C31
34	b	601	SQD	C28-C29-C30-C31
38	F	102	LMG	C12-C13-C14-C15
38	f	102	LMG	C12-C13-C14-C15
39	H	102	DGD	C8B-C9B-CAB-CBB
39	h	102	DGD	C8B-C9B-CAB-CBB
31	B	602	CLA	C8-C10-C11-C12
31	b	603	CLA	C8-C10-C11-C12
31	B	606	CLA	C11-C12-C13-C14
31	B	607	CLA	C6-C7-C8-C9
31	B	608	CLA	C6-C7-C8-C9
31	B	612	CLA	C6-C7-C8-C9
31	C	504	CLA	C11-C10-C8-C9
31	P	601	CLA	C14-C13-C15-C16
31	P	602	CLA	C11-C10-C8-C9
31	b	607	CLA	C11-C12-C13-C14
31	b	608	CLA	C6-C7-C8-C9
31	b	609	CLA	C6-C7-C8-C9
31	b	613	CLA	C6-C7-C8-C9
31	c	504	CLA	C11-C10-C8-C9
31	p	601	CLA	C14-C13-C15-C16
31	p	602	CLA	C11-C10-C8-C9
31	1	308	CLA	C11-C10-C8-C9
31	2	307	CLA	C14-C13-C15-C16
31	6	309	CLA	C11-C10-C8-C9
31	9	308	CLA	C11-C10-C8-C9
31	12	308	CLA	C11-C10-C8-C9
31	12	308	CLA	C14-C13-C15-C16
31	16	309	CLA	C11-C10-C8-C9
32	D	402	PHO	C6-C7-C8-C9
32	d	402	PHO	C6-C7-C8-C9
33	C	515	BCR	C6-C7-C8-C9
33	b	618	BCR	C22-C23-C24-C25
33	c	515	BCR	C6-C7-C8-C9
38	b	621	LMG	C19-C20-C21-C22
31	2	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	4	312	CLA	CAA-CBA-CGA-O2A
31	11	307	CLA	C2C-C3C-CAC-CBC
38	D	403	LMG	C33-C34-C35-C36
39	b	622	DGD	C6A-C7A-C8A-C9A
43	14	301	A86	C6-C8-C9-C10
43	18	302	A86	C1-C24-C25-C26
33	b	618	BCR	C11-C12-C13-C35
43	3	304	A86	C7-C6-C8-C9
43	4	302	A86	C7-C6-C8-C9
31	16	309	CLA	C5-C6-C7-C8
38	B	620	LMG	C19-C20-C21-C22
38	F	102	LMG	C31-C32-C33-C34
34	A	408	SQD	C23-C24-C25-C26
34	a	408	SQD	C23-C24-C25-C26
38	c	521	LMG	C15-C16-C17-C18
38	d	403	LMG	C33-C34-C35-C36
38	f	102	LMG	C31-C32-C33-C34
45	13	309	KC2	O1D-CGD-O2D-CED
31	b	615	CLA	C5-C6-C7-C8
38	W	201	LMG	C19-C20-C21-C22
38	w	201	LMG	C19-C20-C21-C22
43	8	301	A86	C35-C34-O4-C38
43	16	303	A86	C35-C34-O4-C38
36	D	407	LHG	C33-C34-C35-C36
38	C	522	LMG	C29-C30-C31-C32
38	W	201	LMG	C13-C14-C15-C16
38	w	201	LMG	C13-C14-C15-C16
31	B	603	CLA	C2-C3-C5-C6
31	b	604	CLA	C2-C3-C5-C6
36	d	407	LHG	C33-C34-C35-C36
38	15	314	LMG	C11-C12-C13-C14
39	H	102	DGD	C2A-C3A-C4A-C5A
38	P	614	LMG	C29-C28-O8-C9
36	a	410	LHG	C30-C31-C32-C33
39	h	102	DGD	C2A-C3A-C4A-C5A
31	6	309	CLA	C5-C6-C7-C8
31	12	308	CLA	C5-C6-C7-C8
31	A	404	CLA	C1-C2-C3-C4
31	C	514	CLA	C1-C2-C3-C4
31	a	404	CLA	C1-C2-C3-C4
31	c	514	CLA	C1-C2-C3-C4
43	10	306	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
43	11	319	A86	C35-C34-O4-C38
36	A	410	LHG	C30-C31-C32-C33
36	18	315	LHG	C11-C10-C9-C8
38	J	101	LMG	C12-C13-C14-C15
38	j	101	LMG	C12-C13-C14-C15
38	j	101	LMG	C36-C37-C38-C39
38	4	316	LMG	C35-C36-C37-C38
39	1	318	DGD	C9A-CAA-CBA-CCA
34	0	318	SQD	C44-C45-O47-C7
38	M	101	LMG	C9-C8-O7-C10
38	m	101	LMG	C9-C8-O7-C10
39	b	622	DGD	C3G-C2G-O2G-C1B
31	4	311	CLA	C2A-CAA-CBA-CGA
31	14	311	CLA	C2A-CAA-CBA-CGA
38	J	101	LMG	C36-C37-C38-C39
38	p	614	LMG	C29-C28-O8-C9
31	0	308	CLA	C2-C1-O2A-CGA
31	7	313	CLA	C2-C1-O2A-CGA
31	9	313	CLA	C2-C1-O2A-CGA
31	13	316	CLA	C2-C1-O2A-CGA
31	18	306	CLA	C2-C1-O2A-CGA
31	19	313	CLA	C2-C1-O2A-CGA
38	M	101	LMG	C29-C30-C31-C32
31	19	312	CLA	C5-C6-C7-C8
31	12	308	CLA	C3-C5-C6-C7
35	A	409	PL9	C2-C3-C7-C8
35	a	409	PL9	C2-C3-C7-C8
36	8	316	LHG	C11-C12-C13-C14
43	0	301	A86	C12-C11-C13-C14
43	1	305	A86	C12-C11-C13-C14
43	1	306	A86	C12-C11-C13-C14
43	1	320	A86	C12-C11-C13-C14
43	2	301	A86	C12-C11-C13-C14
43	2	302	A86	C12-C11-C13-C14
43	2	304	A86	C12-C11-C13-C14
43	2	305	A86	C12-C11-C13-C14
43	3	301	A86	C12-C11-C13-C14
43	3	305	A86	C12-C11-C13-C14
43	3	306	A86	C12-C11-C13-C14
43	4	304	A86	C12-C11-C13-C14
43	4	305	A86	C12-C11-C13-C14
43	5	301	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
43	5	302	A86	C12-C11-C13-C14
43	5	303	A86	C12-C11-C13-C14
43	5	304	A86	C12-C11-C13-C14
43	6	301	A86	C12-C11-C13-C14
43	6	302	A86	C12-C11-C13-C14
43	6	304	A86	C12-C11-C13-C14
43	6	305	A86	C12-C11-C13-C14
43	7	302	A86	C12-C11-C13-C14
43	7	303	A86	C12-C11-C13-C14
43	7	305	A86	C12-C11-C13-C14
43	8	301	A86	C12-C11-C13-C14
43	8	302	A86	C12-C11-C13-C14
43	8	303	A86	C12-C11-C13-C14
43	8	305	A86	C12-C11-C13-C14
43	9	301	A86	C12-C11-C13-C14
43	9	303	A86	C12-C11-C13-C14
43	9	305	A86	C12-C11-C13-C14
43	9	306	A86	C12-C11-C13-C14
43	10	301	A86	C12-C11-C13-C14
43	10	318	A86	C12-C11-C13-C14
43	11	304	A86	C12-C11-C13-C14
43	11	305	A86	C12-C11-C13-C14
43	11	306	A86	C12-C11-C13-C14
43	11	320	A86	C12-C11-C13-C14
43	12	304	A86	C12-C11-C13-C14
43	12	305	A86	C12-C11-C13-C14
43	12	306	A86	C12-C11-C13-C14
43	13	304	A86	C12-C11-C13-C14
43	13	306	A86	C12-C11-C13-C14
43	14	303	A86	C12-C11-C13-C14
43	14	304	A86	C12-C11-C13-C14
43	15	301	A86	C12-C11-C13-C14
43	15	302	A86	C12-C11-C13-C14
43	15	303	A86	C12-C11-C13-C14
43	15	304	A86	C12-C11-C13-C14
43	16	302	A86	C12-C11-C13-C14
43	16	303	A86	C12-C11-C13-C14
43	16	304	A86	C12-C11-C13-C14
43	16	305	A86	C12-C11-C13-C14
43	16	306	A86	C12-C11-C13-C14
43	17	301	A86	C12-C11-C13-C14
43	17	303	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
43	17	304	A86	C12-C11-C13-C14
43	17	306	A86	C12-C11-C13-C14
43	18	303	A86	C12-C11-C13-C14
43	18	305	A86	C12-C11-C13-C14
43	19	301	A86	C12-C11-C13-C14
43	19	303	A86	C12-C11-C13-C14
43	19	305	A86	C12-C11-C13-C14
43	19	306	A86	C12-C11-C13-C14
31	0	309	CLA	C10-C11-C12-C13
31	2	312	CLA	C2C-C3C-CAC-CBC
38	c	521	LMG	C11-C12-C13-C14
36	Z	103	LHG	O6-C4-C5-O7
36	8	316	LHG	O6-C4-C5-O7
36	18	316	LHG	O6-C4-C5-O7
36	4	317	LHG	C13-C14-C15-C16
31	c	511	CLA	C15-C16-C17-C18
31	18	307	CLA	C5-C6-C7-C8
31	9	311	CLA	O1D-CGD-O2D-CED
33	B	617	BCR	C23-C24-C25-C26
33	B	618	BCR	C1-C6-C7-C8
33	C	515	BCR	C5-C6-C7-C8
33	C	515	BCR	C23-C24-C25-C26
33	C	517	BCR	C23-C24-C25-C30
33	H	101	BCR	C23-C24-C25-C30
33	Y	101	BCR	C1-C6-C7-C8
33	b	618	BCR	C23-C24-C25-C26
33	b	619	BCR	C1-C6-C7-C8
33	c	515	BCR	C5-C6-C7-C8
33	c	515	BCR	C23-C24-C25-C26
33	c	517	BCR	C23-C24-C25-C30
33	h	101	BCR	C23-C24-C25-C30
35	D	406	PL9	C43-C44-C46-C47
35	d	406	PL9	C43-C44-C46-C47
31	2	314	CLA	O1D-CGD-O2D-CED
38	C	522	LMG	C30-C31-C32-C33
39	c	518	DGD	C4B-C5B-C6B-C7B
43	2	301	A86	C33-C34-O4-C38
38	c	521	LMG	C30-C31-C32-C33
39	C	518	DGD	C4B-C5B-C6B-C7B
31	18	312	CLA	C6-C7-C8-C10
38	15	315	LMG	C11-C10-O7-C8
31	C	511	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	B	610	CLA	O1D-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
33	C	515	BCR	C16-C17-C18-C19
33	c	515	BCR	C16-C17-C18-C19
36	P	615	LHG	O7-C5-C6-O8
36	p	615	LHG	O7-C5-C6-O8
36	C	521	LHG	C4-O6-P-O3
36	P	615	LHG	C4-O6-P-O3
36	p	615	LHG	C4-O6-P-O3
36	w	202	LHG	C4-O6-P-O3
36	5	317	LHG	C3-O3-P-O6
36	15	316	LHG	C3-O3-P-O6
34	A	411	SQD	C24-C25-C26-C27
34	i	101	SQD	C24-C25-C26-C27
38	b	621	LMG	C20-C21-C22-C23
39	c	519	DGD	C4E-C5E-C6E-O5E
31	2	307	CLA	C5-C6-C7-C8
38	c	521	LMG	C17-C18-C19-C20
31	c	513	CLA	O1D-CGD-O2D-CED
36	P	615	LHG	C4-C5-C6-O8
36	p	615	LHG	C4-C5-C6-O8
38	M	101	LMG	O1-C7-C8-C9
38	11	317	LMG	O1-C7-C8-C9
31	p	605	CLA	C2C-C3C-CAC-CBC
38	B	620	LMG	C20-C21-C22-C23
31	A	406	CLA	C11-C10-C8-C7
31	a	406	CLA	C11-C10-C8-C7
31	9	307	CLA	C2-C3-C5-C6
31	9	310	CLA	C2-C3-C5-C6
31	P	605	CLA	C2C-C3C-CAC-CBC
39	B	621	DGD	C4E-C5E-C6E-O5E
31	B	603	CLA	C11-C10-C8-C9
31	C	510	CLA	C11-C10-C8-C9
31	b	604	CLA	C11-C10-C8-C9
31	c	510	CLA	C11-C10-C8-C9
31	2	307	CLA	C11-C10-C8-C9
31	5	307	CLA	C14-C13-C15-C16
31	15	307	CLA	C14-C13-C15-C16
36	P	615	LHG	O8-C23-C24-C25
36	p	615	LHG	O8-C23-C24-C25
38	14	316	LMG	C31-C32-C33-C34
43	13	302	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
39	C	519	DGD	C4E-C5E-C6E-O5E
31	7	308	CLA	C2C-C3C-CAC-CBC
36	14	317	LHG	C16-C17-C18-C19
31	B	612	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
36	b	623	LHG	C32-C33-C34-C35
42	13	314	KC1	O1D-CGD-O2D-CED
31	11	307	CLA	C4C-C3C-CAC-CBC
38	W	201	LMG	C15-C16-C17-C18
33	B	617	BCR	C11-C12-C13-C35
33	F	101	BCR	C36-C18-C19-C20
33	f	101	BCR	C36-C18-C19-C20
36	B	622	LHG	C32-C33-C34-C35
38	w	201	LMG	C15-C16-C17-C18
36	5	317	LHG	C2-C3-O3-P
38	5	316	LMG	C11-C12-C13-C14
31	C	513	CLA	O1D-CGD-O2D-CED
43	18	303	A86	C2-C1-C24-C25
38	c	521	LMG	C29-C30-C31-C32
39	C	520	DGD	O1B-C1B-O2G-C2G
39	c	520	DGD	O1B-C1B-O2G-C2G
31	B	606	CLA	C8-C10-C11-C12
31	b	607	CLA	C8-C10-C11-C12
35	A	409	PL9	C16-C17-C18-C19
35	a	409	PL9	C16-C17-C18-C19
31	19	310	CLA	C2-C3-C5-C6
38	15	315	LMG	C11-C12-C13-C14
31	10	317	CLA	CBA-CGA-O2A-C1
31	14	309	CLA	CBA-CGA-O2A-C1
38	1	301	LMG	C29-C30-C31-C32
38	11	301	LMG	C29-C30-C31-C32
39	c	520	DGD	CBB-CCB-CDB-CEB
39	W	203	DGD	O6D-C5D-C6D-O5D
39	w	204	DGD	O6D-C5D-C6D-O5D
31	2	312	CLA	O2A-C1-C2-C3
34	A	408	SQD	C7-C8-C9-C10
38	4	316	LMG	C40-C41-C42-C43
39	C	520	DGD	CBB-CCB-CDB-CEB
31	B	603	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
38	B	620	LMG	O10-C28-C29-C30
33	C	517	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	C	517	BCR	C19-C20-C21-C22
33	H	101	BCR	C9-C10-C11-C12
33	c	517	BCR	C9-C10-C11-C12
33	c	517	BCR	C19-C20-C21-C22
33	h	101	BCR	C9-C10-C11-C12
43	14	302	A86	C11-C10-C9-C8
43	18	303	A86	C1-C2-C3-C4
43	18	303	A86	C3-C4-C5-C6
34	a	408	SQD	C7-C8-C9-C10
33	F	101	BCR	C18-C19-C20-C21
33	f	101	BCR	C18-C19-C20-C21
31	b	607	CLA	C16-C17-C18-C19
45	4	310	KC2	C4B-C3B-CAB-CBB
45	5	310	KC2	C4B-C3B-CAB-CBB
43	0	302	A86	C33-C34-O4-C38
31	5	311	CLA	CAA-CBA-CGA-O1A
31	12	312	CLA	CAA-CBA-CGA-O1A
31	D	405	CLA	C13-C15-C16-C17
31	d	405	CLA	C13-C15-C16-C17
31	11	308	CLA	C8-C10-C11-C12
38	M	101	LMG	C11-C12-C13-C14
31	C	511	CLA	C2-C1-O2A-CGA
31	P	601	CLA	C2-C1-O2A-CGA
31	c	511	CLA	C2-C1-O2A-CGA
31	p	601	CLA	C2-C1-O2A-CGA
31	4	307	CLA	C2-C1-O2A-CGA
31	11	313	CLA	C2-C1-O2A-CGA
31	14	307	CLA	C2-C1-O2A-CGA
43	9	303	A86	C33-C34-O4-C38
31	B	607	CLA	C5-C6-C7-C8
31	10	317	CLA	O1A-CGA-O2A-C1
31	1	321	CLA	C2A-CAA-CBA-CGA
38	M	101	LMG	O1-C7-C8-O7
38	Z	102	LMG	O7-C8-C9-O8
38	c	522	LMG	O7-C8-C9-O8
31	9	310	CLA	C15-C16-C17-C18
36	8	316	LHG	C14-C15-C16-C17
43	4	305	A86	C35-C34-O4-C38
36	15	316	LHG	C2-C3-O3-P
31	B	608	CLA	C3A-C2A-CAA-CBA
31	B	616	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	b	617	CLA	C3A-C2A-CAA-CBA
31	8	307	CLA	C3A-C2A-CAA-CBA
31	9	313	CLA	C3A-C2A-CAA-CBA
31	18	312	CLA	C3A-C2A-CAA-CBA
31	19	313	CLA	C3A-C2A-CAA-CBA
31	c	510	CLA	O1D-CGD-O2D-CED
42	5	313	KC1	O1D-CGD-O2D-CED
36	A	410	LHG	C10-C11-C12-C13
38	D	403	LMG	C12-C13-C14-C15
36	a	410	LHG	C10-C11-C12-C13
43	5	318	A86	O-C13-C14-C15
43	15	304	A86	O-C13-C14-C15
38	1	317	LMG	C13-C14-C15-C16
43	18	301	A86	C35-C34-O4-C38
31	15	311	CLA	CAA-CBA-CGA-O2A
34	B	623	SQD	C16-C17-C18-C19
34	b	601	SQD	C16-C17-C18-C19
44	p	612	DD6	C27-C29-C30-C31
34	A	408	SQD	C26-C27-C28-C29
34	a	408	SQD	C26-C27-C28-C29
36	14	317	LHG	C13-C14-C15-C16
38	b	621	LMG	O8-C28-C29-C30
31	B	602	CLA	C6-C7-C8-C9
31	B	611	CLA	C6-C7-C8-C9
31	D	401	CLA	C14-C13-C15-C16
31	b	603	CLA	C6-C7-C8-C9
31	b	612	CLA	C6-C7-C8-C9
31	d	401	CLA	C14-C13-C15-C16
31	6	309	CLA	C6-C7-C8-C9
31	9	310	CLA	C11-C10-C8-C9
31	9	312	CLA	C6-C7-C8-C9
31	19	313	CLA	C11-C10-C8-C9
34	B	623	SQD	C10-C11-C12-C13
34	b	601	SQD	C10-C11-C12-C13
38	j	101	LMG	C20-C21-C22-C23
31	10	309	CLA	C10-C11-C12-C13
31	17	308	CLA	C2C-C3C-CAC-CBC
38	J	101	LMG	C20-C21-C22-C23
31	C	510	CLA	O1D-CGD-O2D-CED
34	10	320	SQD	C8-C7-O47-C45
38	D	403	LMG	C7-C8-C9-O8
39	H	102	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
39	h	102	DGD	O1G-C1G-C2G-C3G
44	p	612	DD6	C9-C10-C11-C12
39	b	622	DGD	C4E-C5E-C6E-O5E
31	13	312	CLA	CAA-CBA-CGA-O2A
31	10	307	CLA	O1D-CGD-O2D-CED
31	C	514	CLA	C2A-CAA-CBA-CGA
31	c	514	CLA	C2A-CAA-CBA-CGA
31	7	312	CLA	C2A-CAA-CBA-CGA
38	d	403	LMG	C35-C36-C37-C38
38	Z	102	LMG	O10-C28-O8-C9
38	b	621	LMG	O10-C28-C29-C30
31	B	606	CLA	C16-C17-C18-C19
31	15	309	CLA	C6-C7-C8-C10
31	0	309	CLA	O2A-C1-C2-C3
31	3	313	CLA	O2A-C1-C2-C3
31	10	309	CLA	O2A-C1-C2-C3
31	5	311	CLA	CAA-CBA-CGA-O2A
31	12	312	CLA	CAA-CBA-CGA-O2A
43	6	302	A86	C7-C6-C8-C9
35	D	406	PL9	C2-C3-C7-C8
35	d	406	PL9	C2-C3-C7-C8
36	14	317	LHG	C19-C20-C21-C22
38	w	201	LMG	C40-C41-C42-C43
39	C	520	DGD	C4D-C5D-C6D-O5D
39	c	520	DGD	C4D-C5D-C6D-O5D
33	F	101	BCR	C7-C8-C9-C10
34	l	101	SQD	C11-C12-C13-C14
31	13	312	CLA	CAA-CBA-CGA-O1A
31	15	311	CLA	CAA-CBA-CGA-O1A
36	18	316	LHG	C6-C5-O7-C7
38	D	403	LMG	C9-C8-O7-C10
39	C	519	DGD	C1G-C2G-O2G-C1B
39	C	519	DGD	C3G-C2G-O2G-C1B
39	c	519	DGD	C1G-C2G-O2G-C1B
39	c	519	DGD	C3G-C2G-O2G-C1B
31	B	608	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	C1A-C2A-CAA-CBA
31	c	504	CLA	C1A-C2A-CAA-CBA
31	0	307	CLA	C1A-C2A-CAA-CBA
31	12	313	CLA	C1A-C2A-CAA-CBA
31	18	311	CLA	C1A-C2A-CAA-CBA
38	W	201	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C11-C10-C8-C7
31	B	616	CLA	C6-C7-C8-C10
31	b	617	CLA	C6-C7-C8-C10
31	9	308	CLA	C6-C7-C8-C10
36	8	315	LHG	C28-C29-C30-C31
31	3	312	CLA	CAA-CBA-CGA-O2A
31	4	309	CLA	C13-C15-C16-C17
31	11	308	CLA	C15-C16-C17-C18
34	i	101	SQD	C7-C8-C9-C10
36	18	316	LHG	C7-C8-C9-C10
43	15	302	A86	C33-C34-O4-C38
38	B	620	LMG	O8-C28-C29-C30
38	w	201	LMG	C38-C39-C40-C41
38	4	316	LMG	C38-C39-C40-C41
38	W	201	LMG	C38-C39-C40-C41
42	2	313	KC1	C3A-C2A-CAA-CBA
42	10	315	KC1	C3A-C2A-CAA-CBA
35	A	409	PL9	C26-C27-C28-C29
35	a	409	PL9	C26-C27-C28-C29
31	8	307	CLA	C8-C10-C11-C12
31	2	311	CLA	CAA-CBA-CGA-O2A
39	C	518	DGD	C4D-C5D-C6D-O5D
39	c	518	DGD	C4D-C5D-C6D-O5D
31	11	313	CLA	C4-C3-C5-C6
31	13	313	CLA	C4-C3-C5-C6
31	b	608	CLA	C5-C6-C7-C8
31	16	309	CLA	C10-C11-C12-C13
34	A	411	SQD	C7-C8-C9-C10
34	l	101	SQD	C27-C28-C29-C30
38	4	316	LMG	C39-C40-C41-C42
38	c	522	LMG	O10-C28-O8-C9
43	7	304	A86	C35-C34-O4-C38
43	7	305	A86	C35-C34-O4-C38
33	C	515	BCR	C12-C13-C14-C15
33	c	515	BCR	C12-C13-C14-C15
43	1	320	A86	C13-C14-C15-C16
43	3	301	A86	C13-C14-C15-C16
43	4	304	A86	C13-C14-C15-C16
43	5	318	A86	C13-C14-C15-C16
43	8	304	A86	C13-C14-C15-C16
43	13	306	A86	C13-C14-C15-C16
43	14	303	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
43	16	302	A86	C13-C14-C15-C16
43	17	301	A86	C13-C14-C15-C16
44	p	612	DD6	C9-C10-C11-C13
31	B	601	CLA	C10-C11-C12-C13
34	0	318	SQD	C13-C14-C15-C16
39	11	318	DGD	CAB-CBB-CCB-CDB
34	b	601	SQD	C31-C32-C33-C34
34	B	623	SQD	C31-C32-C33-C34
33	F	101	BCR	C6-C7-C8-C9
33	f	101	BCR	C6-C7-C8-C9
43	4	303	A86	C33-C34-O4-C38
43	17	306	A86	C35-C34-O4-C38
34	L	102	SQD	C11-C12-C13-C14
38	11	317	LMG	C16-C17-C18-C19
31	d	401	CLA	O1D-CGD-O2D-CED
43	0	301	A86	C10-C11-C13-C14
43	1	305	A86	C10-C11-C13-C14
43	2	305	A86	C10-C11-C13-C14
43	3	301	A86	C10-C11-C13-C14
43	3	306	A86	C10-C11-C13-C14
43	5	303	A86	C10-C11-C13-C14
43	5	304	A86	C10-C11-C13-C14
43	5	305	A86	C10-C11-C13-C14
43	6	301	A86	C10-C11-C13-C14
43	6	303	A86	C10-C11-C13-C14
43	6	305	A86	C10-C11-C13-C14
43	6	306	A86	C10-C11-C13-C14
43	7	304	A86	C10-C11-C13-C14
43	7	305	A86	C10-C11-C13-C14
43	8	302	A86	C10-C11-C13-C14
43	8	304	A86	C10-C11-C13-C14
43	8	305	A86	C10-C11-C13-C14
43	9	302	A86	C10-C11-C13-C14
43	9	303	A86	C10-C11-C13-C14
43	10	301	A86	C10-C11-C13-C14
43	10	318	A86	C10-C11-C13-C14
43	11	304	A86	C10-C11-C13-C14
43	11	306	A86	C10-C11-C13-C14
43	11	320	A86	C10-C11-C13-C14
43	12	306	A86	C10-C11-C13-C14
43	15	303	A86	C10-C11-C13-C14
43	15	304	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
43	16	306	A86	C10-C11-C13-C14
43	16	307	A86	C10-C11-C13-C14
43	17	306	A86	C10-C11-C13-C14
43	19	301	A86	C10-C11-C13-C14
43	19	302	A86	C10-C11-C13-C14
43	19	303	A86	C10-C11-C13-C14
43	19	306	A86	C10-C11-C13-C14
31	3	312	CLA	CAA-CBA-CGA-O1A
31	D	401	CLA	O1D-CGD-O2D-CED
31	0	311	CLA	C4-C3-C5-C6
35	D	406	PL9	C15-C14-C16-C17
35	d	406	PL9	C15-C14-C16-C17
31	3	316	CLA	C2-C1-O2A-CGA
31	10	308	CLA	C2-C1-O2A-CGA
31	13	313	CLA	C2-C1-O2A-CGA
31	14	309	CLA	O1A-CGA-O2A-C1
31	b	616	CLA	C13-C15-C16-C17
33	C	515	BCR	C10-C11-C12-C13
33	Y	101	BCR	C18-C19-C20-C21
33	c	515	BCR	C10-C11-C12-C13
33	y	101	BCR	C18-C19-C20-C21
31	2	311	CLA	CAA-CBA-CGA-O1A
41	E	101	HEM	CAD-CBD-CGD-O2D
41	e	101	HEM	CAD-CBD-CGD-O2D
31	4	309	CLA	C6-C7-C8-C9
39	c	520	DGD	O6D-C5D-C6D-O5D
38	f	102	LMG	C35-C36-C37-C38
43	7	302	A86	C35-C34-O4-C38
31	16	309	CLA	C3-C5-C6-C7
34	10	320	SQD	C13-C14-C15-C16
31	P	608	CLA	C4-C3-C5-C6
31	p	608	CLA	C4-C3-C5-C6
36	z	102	LHG	C5-C4-O6-P
39	W	203	DGD	C2B-C1B-O2G-C2G
39	w	204	DGD	C2B-C1B-O2G-C2G
42	14	313	KC1	C1A-C2A-CAA-CBA
45	9	309	KC2	C1A-C2A-CAA-CBA
38	C	522	LMG	C17-C18-C19-C20
38	F	102	LMG	C35-C36-C37-C38
31	15	312	CLA	C2A-CAA-CBA-CGA
33	B	617	BCR	C23-C24-C25-C30
33	B	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
33	Y	101	BCR	C23-C24-C25-C26
33	Y	101	BCR	C23-C24-C25-C30
33	b	618	BCR	C23-C24-C25-C30
33	b	620	BCR	C23-C24-C25-C30
33	y	101	BCR	C23-C24-C25-C26
33	y	101	BCR	C23-C24-C25-C30
31	B	604	CLA	C8-C10-C11-C12
31	14	312	CLA	CAA-CBA-CGA-O2A
31	b	602	CLA	C10-C11-C12-C13
31	b	605	CLA	C8-C10-C11-C12
36	18	316	LHG	O1-C1-C2-C3
33	A	407	BCR	C13-C14-C15-C16
33	a	407	BCR	C13-C14-C15-C16
43	18	305	A86	C1-C2-C3-C4
31	B	614	CLA	C4-C3-C5-C6
31	C	512	CLA	C4-C3-C5-C6
31	b	615	CLA	C4-C3-C5-C6
31	c	512	CLA	C4-C3-C5-C6
31	1	313	CLA	C4-C3-C5-C6
31	10	311	CLA	C4-C3-C5-C6
33	f	101	BCR	C7-C8-C9-C10
43	11	303	A86	C35-C34-O4-C38
39	C	520	DGD	O6D-C5D-C6D-O5D
38	D	408	LMG	C8-C7-O1-C1
38	d	408	LMG	C8-C7-O1-C1
38	m	101	LMG	C8-C7-O1-C1
38	C	522	LMG	C15-C16-C17-C18
38	C	522	LMG	C33-C34-C35-C36
31	4	309	CLA	CBA-CGA-O2A-C1
41	V	201	HEM	CAD-CBD-CGD-O2D
41	v	201	HEM	CAD-CBD-CGD-O2D
38	1	317	LMG	O8-C28-C29-C30
34	l	101	SQD	C26-C27-C28-C29
38	D	403	LMG	C35-C36-C37-C38
31	r	101	CLA	C2-C1-O2A-CGA
39	W	203	DGD	CBB-CCB-CDB-CEB
39	w	204	DGD	CBB-CCB-CDB-CEB
31	c	512	CLA	C8-C10-C11-C12
31	13	308	CLA	C2A-CAA-CBA-CGA
31	C	509	CLA	C5-C6-C7-C8
31	C	512	CLA	C8-C10-C11-C12
31	c	509	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	8	315	LHG	O6-C4-C5-C6
31	B	603	CLA	C11-C12-C13-C15
31	B	605	CLA	C12-C13-C15-C16
31	B	607	CLA	C6-C7-C8-C10
31	C	512	CLA	C2-C3-C5-C6
31	b	604	CLA	C11-C12-C13-C15
31	b	606	CLA	C12-C13-C15-C16
31	b	608	CLA	C6-C7-C8-C10
31	b	615	CLA	C2-C3-C5-C6
31	c	512	CLA	C2-C3-C5-C6
31	0	311	CLA	C2-C3-C5-C6
31	4	307	CLA	C2-C3-C5-C6
35	D	406	PL9	C13-C14-C16-C17
35	d	406	PL9	C13-C14-C16-C17
31	R	101	CLA	C2-C1-O2A-CGA
34	L	102	SQD	O47-C7-C8-C9
38	1	301	LMG	O8-C28-C29-C30
38	11	301	LMG	O8-C28-C29-C30
36	Z	103	LHG	C5-C4-O6-P
39	H	102	DGD	O1G-C1G-C2G-O2G
39	h	102	DGD	O1G-C1G-C2G-O2G
38	10	319	LMG	C4-C5-C6-O5
39	11	318	DGD	C8B-C9B-CAB-CBB
38	j	101	LMG	O8-C28-C29-C30
31	15	312	CLA	C2-C1-O2A-CGA
31	B	615	CLA	C13-C15-C16-C17
39	1	318	DGD	C8B-C9B-CAB-CBB
31	3	316	CLA	C16-C17-C18-C20
38	W	201	LMG	C16-C17-C18-C19
39	C	519	DGD	CCB-CDB-CEB-CFB
32	D	402	PHO	C4C-C3C-CAC-CBC
32	d	402	PHO	C4C-C3C-CAC-CBC
33	B	618	BCR	C16-C17-C18-C36
33	H	101	BCR	C20-C21-C22-C37
33	b	619	BCR	C16-C17-C18-C36
33	h	101	BCR	C20-C21-C22-C37
39	c	519	DGD	CCB-CDB-CEB-CFB
31	b	603	CLA	CAA-CBA-CGA-O2A
38	J	101	LMG	O8-C28-C29-C30
39	B	621	DGD	C2G-C1G-O1G-C1A
38	w	201	LMG	C16-C17-C18-C19
35	D	406	PL9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
35	d	406	PL9	C40-C39-C41-C42
31	5	307	CLA	C5-C6-C7-C8
43	10	318	A86	C35-C34-O4-C38
31	B	614	CLA	C2-C3-C5-C6
31	10	311	CLA	C2-C3-C5-C6
31	11	313	CLA	C2-C3-C5-C6
31	13	313	CLA	C2-C3-C5-C6
35	A	409	PL9	C23-C24-C26-C27
35	a	409	PL9	C23-C24-C26-C27
31	B	602	CLA	CAA-CBA-CGA-O2A
31	8	311	CLA	CAA-CBA-CGA-O2A
31	13	313	CLA	CAA-CBA-CGA-O2A
34	l	101	SQD	O47-C7-C8-C9
31	B	608	CLA	C14-C13-C15-C16
31	B	610	CLA	C11-C12-C13-C14
31	b	609	CLA	C14-C13-C15-C16
31	b	611	CLA	C11-C12-C13-C14
43	16	307	A86	C35-C34-O4-C38
31	B	607	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	0	307	CLA	C3A-C2A-CAA-CBA
31	18	307	CLA	C3A-C2A-CAA-CBA
31	D	404	CLA	C4C-C3C-CAC-CBC
31	d	404	CLA	C4C-C3C-CAC-CBC
31	C	510	CLA	CBD-CGD-O2D-CED
31	c	510	CLA	CBD-CGD-O2D-CED
31	17	310	CLA	CAA-CBA-CGA-O2A
31	A	404	CLA	CAD-CBD-CGD-O2D
31	B	607	CLA	CAD-CBD-CGD-O2D
31	B	613	CLA	CAD-CBD-CGD-O2D
31	C	509	CLA	CAD-CBD-CGD-O2D
31	C	511	CLA	CAD-CBD-CGD-O2D
31	D	405	CLA	CAD-CBD-CGD-O2D
31	a	404	CLA	CAD-CBD-CGD-O2D
31	b	608	CLA	CAD-CBD-CGD-O2D
31	b	614	CLA	CAD-CBD-CGD-O2D
31	c	509	CLA	CAD-CBD-CGD-O2D
31	c	511	CLA	CAD-CBD-CGD-O2D
31	d	405	CLA	CAD-CBD-CGD-O2D
31	0	312	CLA	CAD-CBD-CGD-O2D
31	1	307	CLA	CAD-CBD-CGD-O2D
31	2	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	2	315	CLA	CAD-CBD-CGD-O2D
31	3	310	CLA	CAD-CBD-CGD-O2D
31	4	307	CLA	CAD-CBD-CGD-O2D
31	5	314	CLA	CAD-CBD-CGD-O2D
31	10	312	CLA	CAD-CBD-CGD-O2D
31	11	310	CLA	CAD-CBD-CGD-O2D
31	12	307	CLA	CAD-CBD-CGD-O2D
31	12	308	CLA	CAD-CBD-CGD-O2D
31	13	308	CLA	CAD-CBD-CGD-O2D
31	14	307	CLA	CAD-CBD-CGD-O2D
31	14	315	CLA	CAD-CBD-CGD-O2D
31	16	313	CLA	CAD-CBD-CGD-O2D
31	17	310	CLA	CAD-CBD-CGD-O2D
31	18	311	CLA	CAD-CBD-CGD-O2D
31	19	310	CLA	CAD-CBD-CGD-O2D
36	8	316	LHG	C6-C5-O7-C7
36	18	316	LHG	C4-C5-O7-C7
45	4	308	KC2	CAD-CBD-CGD-O2D
31	12	310	CLA	C2A-CAA-CBA-CGA
31	D	404	CLA	C10-C11-C12-C13
31	c	507	CLA	C13-C15-C16-C17
31	4	309	CLA	C2A-CAA-CBA-CGA
31	12	316	CLA	C2A-CAA-CBA-CGA
31	14	309	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C15-C16-C17-C18
31	b	611	CLA	C15-C16-C17-C18
31	d	404	CLA	C10-C11-C12-C13
31	14	306	CLA	C2-C1-O2A-CGA
31	6	313	CLA	CAA-CBA-CGA-O2A
31	17	312	CLA	CAA-CBA-CGA-O2A
31	C	507	CLA	C13-C15-C16-C17
38	c	521	LMG	C33-C34-C35-C36
35	D	406	PL9	C45-C44-C46-C47
35	d	406	PL9	C45-C44-C46-C47
31	D	404	CLA	C16-C17-C18-C20
31	d	404	CLA	C16-C17-C18-C20
31	7	310	CLA	CAA-CBA-CGA-O2A
31	2	315	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A
31	16	313	CLA	CAA-CBA-CGA-O2A
36	8	315	LHG	O8-C23-C24-C25
38	1	301	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	C	516	BCR	C7-C8-C9-C10
33	Y	101	BCR	C11-C12-C13-C14
33	c	516	BCR	C7-C8-C9-C10
33	y	101	BCR	C11-C12-C13-C14
31	18	314	CLA	C2A-CAA-CBA-CGA
32	D	402	PHO	C2C-C3C-CAC-CBC
32	d	402	PHO	C2C-C3C-CAC-CBC
36	4	317	LHG	C4-C5-C6-O8
39	C	520	DGD	C1G-C2G-C3G-O3G
39	c	520	DGD	C1G-C2G-C3G-O3G
43	P	611	A86	C12-C11-C13-O
43	p	611	A86	C12-C11-C13-O
43	0	302	A86	C12-C11-C13-O
43	0	303	A86	C12-C11-C13-O
43	0	304	A86	C12-C11-C13-O
43	2	302	A86	C12-C11-C13-O
43	2	303	A86	C12-C11-C13-O
43	3	305	A86	C12-C11-C13-O
43	4	306	A86	C12-C11-C13-O
43	5	301	A86	C12-C11-C13-O
43	6	302	A86	C12-C11-C13-O
43	7	304	A86	C12-C11-C13-O
43	7	306	A86	C12-C11-C13-O
43	9	304	A86	C12-C11-C13-O
43	10	303	A86	C12-C11-C13-O
43	11	306	A86	C12-C11-C13-O
43	12	301	A86	C12-C11-C13-O
43	12	305	A86	C12-C11-C13-O
43	13	301	A86	C12-C11-C13-O
43	13	304	A86	C12-C11-C13-O
43	14	302	A86	C12-C11-C13-O
43	14	305	A86	C12-C11-C13-O
43	15	301	A86	C12-C11-C13-O
43	16	303	A86	C12-C11-C13-O
43	18	303	A86	C12-C11-C13-O
31	3	308	CLA	C2C-C3C-CAC-CBC
31	4	309	CLA	O1A-CGA-O2A-C1
31	8	306	CLA	O1A-CGA-O2A-C1
38	11	301	LMG	O7-C10-C11-C12
31	C	509	CLA	C16-C17-C18-C20
31	c	509	CLA	C16-C17-C18-C20
33	C	515	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	c	515	BCR	C18-C19-C20-C21
36	18	316	LHG	O10-C23-O8-C6
39	H	102	DGD	O1B-C1B-C2B-C3B
39	h	102	DGD	O1B-C1B-C2B-C3B
41	E	101	HEM	CAD-CBD-CGD-O1D
41	V	201	HEM	CAD-CBD-CGD-O1D
41	e	101	HEM	CAD-CBD-CGD-O1D
41	v	201	HEM	CAD-CBD-CGD-O1D
31	B	602	CLA	O2A-C1-C2-C3
31	b	603	CLA	O2A-C1-C2-C3
31	1	313	CLA	O2A-C1-C2-C3
31	10	308	CLA	O2A-C1-C2-C3
45	13	311	KC2	C4B-C3B-CAB-CBB
45	14	310	KC2	C4B-C3B-CAB-CBB
31	0	314	CLA	C2A-CAA-CBA-CGA
31	5	309	CLA	C2A-CAA-CBA-CGA
31	11	310	CLA	C2A-CAA-CBA-CGA
31	15	309	CLA	C2A-CAA-CBA-CGA
36	18	316	LHG	C13-C14-C15-C16
39	C	520	DGD	C8A-C9A-CAA-CBA
31	C	502	CLA	CAA-CBA-CGA-O2A
39	C	518	DGD	O2G-C1B-C2B-C3B
39	c	518	DGD	O2G-C1B-C2B-C3B
31	19	310	CLA	C3-C5-C6-C7
39	c	520	DGD	C8A-C9A-CAA-CBA
31	B	602	CLA	CHA-CBD-CGD-O1D
31	B	602	CLA	CHA-CBD-CGD-O2D
31	B	610	CLA	CHA-CBD-CGD-O2D
31	B	615	CLA	CHA-CBD-CGD-O1D
31	B	615	CLA	CHA-CBD-CGD-O2D
31	C	508	CLA	CHA-CBD-CGD-O1D
31	C	508	CLA	CHA-CBD-CGD-O2D
31	C	511	CLA	CHA-CBD-CGD-O2D
31	P	601	CLA	CHA-CBD-CGD-O2D
31	P	604	CLA	CHA-CBD-CGD-O1D
31	b	603	CLA	CHA-CBD-CGD-O1D
31	b	603	CLA	CHA-CBD-CGD-O2D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	b	616	CLA	CHA-CBD-CGD-O1D
31	b	616	CLA	CHA-CBD-CGD-O2D
31	c	508	CLA	CHA-CBD-CGD-O1D
31	c	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	c	511	CLA	CHA-CBD-CGD-O2D
31	p	601	CLA	CHA-CBD-CGD-O2D
31	p	604	CLA	CHA-CBD-CGD-O1D
31	1	307	CLA	CHA-CBD-CGD-O1D
31	1	308	CLA	CHA-CBD-CGD-O1D
31	1	308	CLA	CHA-CBD-CGD-O2D
31	9	307	CLA	CHA-CBD-CGD-O1D
31	9	307	CLA	CHA-CBD-CGD-O2D
31	10	309	CLA	CHA-CBD-CGD-O2D
31	11	308	CLA	CHA-CBD-CGD-O1D
31	11	308	CLA	CHA-CBD-CGD-O2D
31	19	307	CLA	CHA-CBD-CGD-O1D
31	19	307	CLA	CHA-CBD-CGD-O2D
45	0	310	KC2	CHA-CBD-CGD-O1D
45	0	310	KC2	CHA-CBD-CGD-O2D
31	7	310	CLA	CAA-CBA-CGA-O1A
31	17	310	CLA	CAA-CBA-CGA-O1A
31	c	502	CLA	CAA-CBA-CGA-O2A
36	18	315	LHG	C29-C30-C31-C32
39	C	519	DGD	C8B-C9B-CAB-CBB
39	c	519	DGD	C8B-C9B-CAB-CBB
34	l	101	SQD	C34-C35-C36-C37
38	11	301	LMG	C33-C34-C35-C36
38	14	316	LMG	C38-C39-C40-C41
31	B	608	CLA	CAA-CBA-CGA-O2A
31	0	309	CLA	CAA-CBA-CGA-O2A
36	18	315	LHG	O8-C23-C24-C25
38	1	301	LMG	C33-C34-C35-C36
34	A	408	SQD	O6-C44-C45-O47
34	a	408	SQD	O6-C44-C45-O47
38	14	316	LMG	O1-C7-C8-O7
39	C	520	DGD	O2G-C2G-C3G-O3G
39	c	520	DGD	O2G-C2G-C3G-O3G
43	P	613	A86	C33-C34-O4-C38
43	p	613	A86	C33-C34-O4-C38
43	5	303	A86	C33-C34-O4-C38
36	8	315	LHG	C24-C25-C26-C27
36	8	315	LHG	C25-C26-C27-C28
38	W	201	LMG	C34-C35-C36-C37
38	w	201	LMG	C34-C35-C36-C37
38	5	316	LMG	O9-C10-O7-C8
31	b	609	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	12	316	CLA	CAA-CBA-CGA-O2A
36	B	622	LHG	O8-C23-C24-C25
38	D	403	LMG	O8-C28-C29-C30
39	1	318	DGD	O1G-C1A-C2A-C3A
39	C	518	DGD	C5B-C6B-C7B-C8B
39	c	518	DGD	C5B-C6B-C7B-C8B
43	1	302	A86	C10-C11-C13-O
43	1	320	A86	C13-C14-C15-O1
43	3	301	A86	C13-C14-C15-O1
43	4	302	A86	C10-C11-C13-O
43	6	307	A86	C13-C14-C15-O1
43	7	301	A86	C10-C11-C13-O
43	9	305	A86	C13-C14-C15-O1
43	11	302	A86	C10-C11-C13-O
43	13	304	A86	C10-C11-C13-O
43	14	302	A86	C10-C11-C13-O
43	15	305	A86	C10-C11-C13-O
43	17	302	A86	C10-C11-C13-O
43	17	303	A86	C13-C14-C15-O1
43	17	305	A86	C10-C11-C13-O
43	18	301	A86	C13-C14-C15-O1
43	18	303	A86	C10-C11-C13-O
43	18	303	A86	C13-C14-C15-O1
43	19	305	A86	C13-C14-C15-O1
31	C	511	CLA	C10-C11-C12-C13
31	c	511	CLA	C10-C11-C12-C13
31	18	307	CLA	C10-C11-C12-C13
38	D	403	LMG	C15-C16-C17-C18
38	n	701	LMG	C28-C29-C30-C31
31	10	309	CLA	CAA-CBA-CGA-O2A
34	A	411	SQD	O47-C7-C8-C9
34	b	601	SQD	O47-C7-C8-C9
34	i	101	SQD	O47-C7-C8-C9
36	b	623	LHG	O8-C23-C24-C25
31	19	312	CLA	C4-C3-C5-C6
31	16	309	CLA	C2C-C3C-CAC-CBC
34	A	408	SQD	O10-C23-C24-C25
34	a	408	SQD	O10-C23-C24-C25
43	13	305	A86	C33-C34-O4-C38
31	B	601	CLA	C12-C13-C15-C16
31	b	602	CLA	C12-C13-C15-C16
31	9	308	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	8	312	CLA	C6-C7-C8-C10
38	B	620	LMG	O9-C10-O7-C8
38	b	621	LMG	O9-C10-O7-C8
31	W	202	CLA	C11-C12-C13-C14
31	w	203	CLA	C11-C12-C13-C14
31	b	603	CLA	CAA-CBA-CGA-O1A
31	8	311	CLA	CAA-CBA-CGA-O1A
43	6	307	A86	C33-C34-O4-C38
43	8	303	A86	C35-C34-O4-C38
31	B	606	CLA	CBA-CGA-O2A-C1
31	P	603	CLA	CAA-CBA-CGA-O2A
34	B	623	SQD	O47-C7-C8-C9
34	A	411	SQD	C4-C5-C6-S
34	0	318	SQD	C5-C6-S-O8
34	10	320	SQD	C5-C6-S-O8
36	w	202	LHG	C10-C11-C12-C13
36	Z	103	LHG	C8-C7-O7-C5
36	z	102	LHG	C8-C7-O7-C5
39	C	520	DGD	C2B-C1B-O2G-C2G
39	c	520	DGD	C2B-C1B-O2G-C2G
31	C	505	CLA	C2A-CAA-CBA-CGA
31	c	505	CLA	C2A-CAA-CBA-CGA
31	1	310	CLA	C2A-CAA-CBA-CGA
31	10	307	CLA	C2A-CAA-CBA-CGA
31	10	311	CLA	C2A-CAA-CBA-CGA
31	17	310	CLA	C2A-CAA-CBA-CGA
31	p	606	CLA	C2C-C3C-CAC-CBC
31	p	603	CLA	CAA-CBA-CGA-O2A
31	5	312	CLA	C2-C1-O2A-CGA
36	C	521	LHG	C10-C11-C12-C13
36	14	317	LHG	C17-C18-C19-C20
41	E	101	HEM	CAA-CBA-CGA-O1A
31	17	312	CLA	CAA-CBA-CGA-O1A
39	C	518	DGD	O1B-C1B-C2B-C3B
39	c	518	DGD	O1B-C1B-C2B-C3B
31	3	313	CLA	C16-C17-C18-C19
31	b	608	CLA	C4-C3-C5-C6
39	11	318	DGD	O2G-C1B-C2B-C3B
31	P	606	CLA	C2C-C3C-CAC-CBC
41	e	101	HEM	CAA-CBA-CGA-O1A
38	4	316	LMG	O10-C28-C29-C30
31	8	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	D	405	CLA	C8-C10-C11-C12
31	d	405	CLA	C8-C10-C11-C12
31	B	607	CLA	C1A-C2A-CAA-CBA
31	B	611	CLA	C1A-C2A-CAA-CBA
31	C	503	CLA	C1A-C2A-CAA-CBA
31	C	504	CLA	C1A-C2A-CAA-CBA
31	C	509	CLA	C1A-C2A-CAA-CBA
31	D	405	CLA	C1A-C2A-CAA-CBA
31	Z	101	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	612	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	C1A-C2A-CAA-CBA
31	c	503	CLA	C1A-C2A-CAA-CBA
31	c	509	CLA	C1A-C2A-CAA-CBA
31	d	405	CLA	C1A-C2A-CAA-CBA
31	z	101	CLA	C1A-C2A-CAA-CBA
31	0	312	CLA	C1A-C2A-CAA-CBA
31	7	313	CLA	C1A-C2A-CAA-CBA
31	8	307	CLA	C1A-C2A-CAA-CBA
31	12	316	CLA	C1A-C2A-CAA-CBA
31	14	306	CLA	C1A-C2A-CAA-CBA
31	18	307	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	CAA-CBA-CGA-O1A
31	6	313	CLA	CAA-CBA-CGA-O1A
39	C	518	DGD	C4E-C5E-C6E-O5E
39	11	318	DGD	C4D-C5D-C6D-O5D
42	13	314	KC1	CAA-CBA-CGA-O1A
38	B	620	LMG	C32-C33-C34-C35
38	14	316	LMG	C14-C15-C16-C17
31	b	607	CLA	CBA-CGA-O2A-C1
31	7	312	CLA	CBA-CGA-O2A-C1
31	2	315	CLA	CAA-CBA-CGA-O1A
31	7	312	CLA	CAA-CBA-CGA-O1A
34	0	318	SQD	O10-C23-C24-C25
36	C	521	LHG	O10-C23-C24-C25
36	w	202	LHG	O10-C23-C24-C25
38	m	101	LMG	C30-C31-C32-C33
41	V	201	HEM	CAA-CBA-CGA-O1A
41	v	201	HEM	CAA-CBA-CGA-O1A
39	C	520	DGD	O1G-C1G-C2G-C3G
39	c	520	DGD	O1G-C1G-C2G-C3G
31	P	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	p	602	CLA	C8-C10-C11-C12
31	0	311	CLA	C2A-CAA-CBA-CGA
31	7	310	CLA	C2A-CAA-CBA-CGA
31	9	310	CLA	C2A-CAA-CBA-CGA
31	19	310	CLA	C2A-CAA-CBA-CGA
31	D	401	CLA	CBD-CGD-O2D-CED
31	d	401	CLA	CBD-CGD-O2D-CED
31	9	311	CLA	CBD-CGD-O2D-CED
39	H	102	DGD	CDB-CEB-CFB-CGB
39	h	102	DGD	CDB-CEB-CFB-CGB
31	C	508	CLA	C16-C17-C18-C20
31	c	508	CLA	C16-C17-C18-C20
38	c	522	LMG	O9-C10-C11-C12
31	C	506	CLA	C13-C15-C16-C17
31	c	506	CLA	C13-C15-C16-C17
39	c	518	DGD	C4E-C5E-C6E-O5E
38	P	614	LMG	C8-C9-O8-C28
31	C	513	CLA	CAA-CBA-CGA-O2A
31	c	513	CLA	CAA-CBA-CGA-O2A
31	C	508	CLA	C13-C15-C16-C17
31	c	508	CLA	C13-C15-C16-C17
34	B	623	SQD	C17-C18-C19-C20
34	L	102	SQD	C12-C13-C14-C15
36	8	315	LHG	O10-C23-C24-C25
36	18	315	LHG	O10-C23-C24-C25
38	5	316	LMG	O10-C28-C29-C30
39	1	318	DGD	O1B-C1B-C2B-C3B
34	b	601	SQD	C17-C18-C19-C20
36	B	622	LHG	C3-O3-P-O5
36	b	623	LHG	C3-O3-P-O5
36	15	316	LHG	C3-O3-P-O5
31	12	316	CLA	CAA-CBA-CGA-O1A
31	13	313	CLA	CAA-CBA-CGA-O1A
36	4	317	LHG	O9-C7-C8-C9
36	5	317	LHG	O9-C7-C8-C9
38	p	614	LMG	C8-C9-O8-C28
39	B	621	DGD	O1B-C1B-C2B-C3B
39	b	622	DGD	O1B-C1B-C2B-C3B
31	B	616	CLA	CAA-CBA-CGA-O2A
31	5	312	CLA	CAA-CBA-CGA-O2A
34	A	408	SQD	O48-C23-C24-C25
34	a	408	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
39	C	519	DGD	CDB-CEB-CFB-CGB
39	W	203	DGD	C8B-C9B-CAB-CBB
31	6	309	CLA	C10-C11-C12-C13
31	C	502	CLA	CAA-CBA-CGA-O1A
31	c	502	CLA	CAA-CBA-CGA-O1A
36	14	317	LHG	O9-C7-C8-C9
36	15	316	LHG	O9-C7-C8-C9
38	Z	102	LMG	O9-C10-C11-C12
31	p	604	CLA	CAA-CBA-CGA-O2A
31	8	311	CLA	C2A-CAA-CBA-CGA
31	11	308	CLA	C2A-CAA-CBA-CGA
31	8	312	CLA	O1A-CGA-O2A-C1
39	c	519	DGD	CDB-CEB-CFB-CGB
31	15	307	CLA	C13-C15-C16-C17
39	w	204	DGD	C8B-C9B-CAB-CBB
34	i	101	SQD	O49-C7-C8-C9
31	B	612	CLA	CAD-CBD-CGD-O1D
31	C	510	CLA	CAD-CBD-CGD-O1D
31	b	613	CLA	CAD-CBD-CGD-O1D
31	c	510	CLA	CAD-CBD-CGD-O1D
31	2	306	CLA	CAD-CBD-CGD-O1D
31	3	307	CLA	CAD-CBD-CGD-O1D
31	3	315	CLA	CAD-CBD-CGD-O1D
31	7	307	CLA	CAD-CBD-CGD-O1D
31	8	306	CLA	CAD-CBD-CGD-O1D
31	11	308	CLA	CAD-CBD-CGD-O1D
31	11	315	CLA	CAD-CBD-CGD-O1D
31	12	315	CLA	CAD-CBD-CGD-O1D
31	17	307	CLA	CAD-CBD-CGD-O1D
31	18	306	CLA	CAD-CBD-CGD-O1D
34	A	411	SQD	O5-C5-C6-S
34	i	101	SQD	O5-C5-C6-S
36	14	317	LHG	C6-C5-O7-C7
38	D	403	LMG	C7-C8-O7-C10
42	8	313	KC1	CAD-CBD-CGD-O1D
43	17	305	A86	C26-C27-C29-C30
31	16	313	CLA	CAA-CBA-CGA-O1A
34	A	411	SQD	O49-C7-C8-C9
34	L	102	SQD	C13-C14-C15-C16
34	l	101	SQD	C12-C13-C14-C15
39	11	318	DGD	C5B-C6B-C7B-C8B
31	B	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	P	604	CLA	CAA-CBA-CGA-O2A
31	C	509	CLA	C11-C12-C13-C14
31	c	509	CLA	C11-C12-C13-C14
31	1	321	CLA	C6-C7-C8-C9
31	9	313	CLA	C11-C10-C8-C9
39	c	519	DGD	C4B-C5B-C6B-C7B
39	C	519	DGD	C4B-C5B-C6B-C7B
31	B	608	CLA	CAA-CBA-CGA-O1A
31	b	609	CLA	CAA-CBA-CGA-O1A
31	0	309	CLA	CAA-CBA-CGA-O1A
43	1	303	A86	C33-C34-O4-C38
43	6	306	A86	C35-C34-O4-C38
38	N	101	LMG	C28-C29-C30-C31
31	C	511	CLA	CAA-CBA-CGA-O2A
31	b	614	CLA	CAA-CBA-CGA-O2A
31	c	511	CLA	CAA-CBA-CGA-O2A
31	z	103	CLA	CAA-CBA-CGA-O2A
31	4	309	CLA	CAA-CBA-CGA-O2A
31	18	309	CLA	CAA-CBA-CGA-O2A
34	10	320	SQD	O48-C23-C24-C25
36	C	521	LHG	O8-C23-C24-C25
39	B	621	DGD	O1A-C1A-C2A-C3A
31	b	609	CLA	C13-C15-C16-C17
31	0	316	CLA	C2A-CAA-CBA-CGA
39	B	621	DGD	C6A-C7A-C8A-C9A
43	3	306	A86	C35-C34-O4-C38
31	5	309	CLA	CAA-CBA-CGA-O2A
31	8	309	CLA	CAA-CBA-CGA-O2A
31	9	310	CLA	CAA-CBA-CGA-O2A
31	10	317	CLA	CAA-CBA-CGA-O2A
31	15	309	CLA	CAA-CBA-CGA-O2A
31	19	310	CLA	CAA-CBA-CGA-O2A
36	w	202	LHG	O8-C23-C24-C25
38	N	101	LMG	O8-C28-C29-C30
38	n	701	LMG	O8-C28-C29-C30
31	W	202	CLA	C5-C6-C7-C8
31	w	203	CLA	C5-C6-C7-C8
34	l	101	SQD	C13-C14-C15-C16
38	W	201	LMG	C10-C11-C12-C13
38	w	201	LMG	C10-C11-C12-C13
31	D	404	CLA	C3-C5-C6-C7
31	d	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	3	313	CLA	C3-C5-C6-C7
38	J	101	LMG	O10-C28-C29-C30
38	15	315	LMG	O10-C28-C29-C30
42	1	314	KC1	O1D-CGD-O2D-CED
31	10	309	CLA	C4-C3-C5-C6
31	b	604	CLA	C8-C10-C11-C12
38	P	614	LMG	C12-C13-C14-C15
31	B	604	CLA	C12-C13-C15-C16
31	B	614	CLA	C3A-C2A-CAA-CBA
31	C	509	CLA	C11-C12-C13-C15
31	P	601	CLA	C6-C7-C8-C10
31	W	202	CLA	C11-C12-C13-C15
31	b	605	CLA	C12-C13-C15-C16
31	b	615	CLA	C3A-C2A-CAA-CBA
31	c	509	CLA	C11-C12-C13-C15
31	p	601	CLA	C6-C7-C8-C10
31	w	203	CLA	C11-C12-C13-C15
31	1	308	CLA	C11-C12-C13-C15
31	1	321	CLA	C3A-C2A-CAA-CBA
31	1	321	CLA	C6-C7-C8-C10
31	2	307	CLA	C3A-C2A-CAA-CBA
31	5	307	CLA	C3A-C2A-CAA-CBA
31	14	306	CLA	C3A-C2A-CAA-CBA
31	15	306	CLA	C3A-C2A-CAA-CBA
31	15	307	CLA	C3A-C2A-CAA-CBA
31	19	310	CLA	C6-C7-C8-C10
31	B	601	CLA	CAA-CBA-CGA-O1A
31	B	613	CLA	CAA-CBA-CGA-O1A
31	b	602	CLA	CAA-CBA-CGA-O1A
38	j	101	LMG	O10-C28-C29-C30
38	14	316	LMG	O10-C28-C29-C30
38	k	101	LMG	C37-C38-C39-C40
38	p	614	LMG	C12-C13-C14-C15
43	6	303	A86	C35-C34-O4-C38
43	8	305	A86	C35-C34-O4-C38
43	12	301	A86	C33-C34-O4-C38
31	B	601	CLA	CAA-CBA-CGA-O2A
31	P	602	CLA	CAA-CBA-CGA-O2A
31	b	602	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
31	p	602	CLA	CAA-CBA-CGA-O2A
31	1	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	11	310	CLA	CAA-CBA-CGA-O2A
31	15	312	CLA	CAA-CBA-CGA-O2A
31	19	308	CLA	CAA-CBA-CGA-O2A
38	c	521	LMG	O8-C28-C29-C30
38	5	315	LMG	O7-C10-C11-C12
39	11	318	DGD	O1G-C1A-C2A-C3A
38	K	101	LMG	C37-C38-C39-C40
39	11	318	DGD	C2A-C3A-C4A-C5A
31	5	309	CLA	CAA-CBA-CGA-O1A
31	15	312	CLA	CAA-CBA-CGA-O1A
41	v	201	HEM	CAA-CBA-CGA-O2A
43	14	301	A86	C3-C4-C5-C6
43	1	319	A86	O-C13-C14-C15
43	14	301	A86	O-C13-C14-C15
31	1	313	CLA	CAA-CBA-CGA-O2A
31	3	316	CLA	CAA-CBA-CGA-O2A
31	9	308	CLA	CAA-CBA-CGA-O2A
31	10	314	CLA	CAA-CBA-CGA-O2A
31	13	316	CLA	CAA-CBA-CGA-O2A
34	0	318	SQD	O48-C23-C24-C25
31	B	603	CLA	C8-C10-C11-C12
31	B	608	CLA	C13-C15-C16-C17
31	6	309	CLA	C2C-C3C-CAC-CBC
31	P	603	CLA	CAA-CBA-CGA-O1A
31	c	513	CLA	CAA-CBA-CGA-O1A
31	p	603	CLA	CAA-CBA-CGA-O1A
34	10	320	SQD	O49-C7-C8-C9
34	A	411	SQD	C24-C23-O48-C46
34	i	101	SQD	C24-C23-O48-C46
41	E	101	HEM	CAA-CBA-CGA-O2A
41	V	201	HEM	CAA-CBA-CGA-O2A
31	C	510	CLA	C13-C15-C16-C17
31	c	510	CLA	C13-C15-C16-C17
31	15	307	CLA	C5-C6-C7-C8
31	14	309	CLA	CAA-CBA-CGA-O2A
38	C	522	LMG	O8-C28-C29-C30
31	C	513	CLA	CAA-CBA-CGA-O1A
31	b	614	CLA	CAA-CBA-CGA-O1A
31	p	602	CLA	CAA-CBA-CGA-O1A
31	9	310	CLA	CAA-CBA-CGA-O1A
31	10	309	CLA	CAA-CBA-CGA-O1A
34	B	623	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	b	601	SQD	O49-C7-C8-C9
34	10	320	SQD	O10-C23-C24-C25
39	11	318	DGD	O1B-C1B-C2B-C3B
31	10	314	CLA	C2A-CAA-CBA-CGA
43	2	302	A86	C33-C34-O4-C38
41	e	101	HEM	CAA-CBA-CGA-O2A
36	18	315	LHG	C13-C14-C15-C16
31	B	603	CLA	C13-C15-C16-C17
31	B	606	CLA	C10-C11-C12-C13
31	b	607	CLA	C10-C11-C12-C13
31	15	309	CLA	CAA-CBA-CGA-O1A
35	A	409	PL9	C12-C11-C9-C10

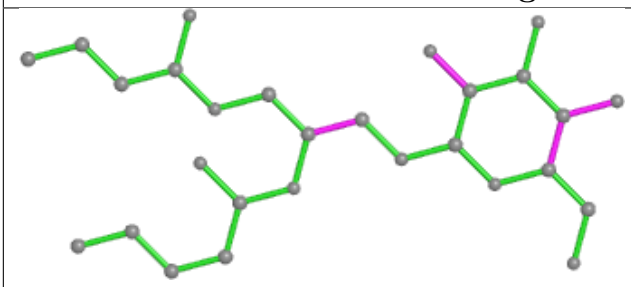
All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	14	305	A86	C31-C32-C33-C34-C35-C36
43	p	613	A86	C31-C32-C33-C34-C35-C36
43	P	613	A86	C31-C32-C33-C34-C35-C36
43	2	304	A86	C31-C32-C33-C34-C35-C36
43	4	306	A86	C31-C32-C33-C34-C35-C36
43	15	302	A86	C31-C32-C33-C34-C35-C36
43	P	611	A86	C31-C32-C33-C34-C35-C36
43	p	611	A86	C31-C32-C33-C34-C35-C36
43	15	304	A86	C31-C32-C33-C34-C35-C36

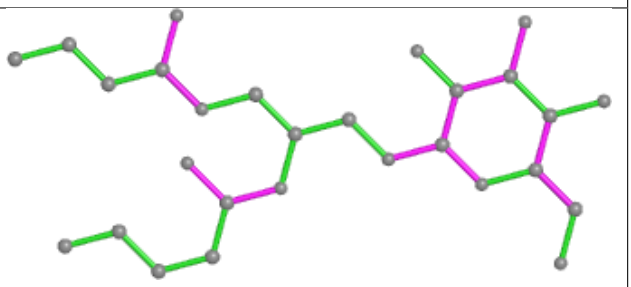
No monomer is involved in short contacts.

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

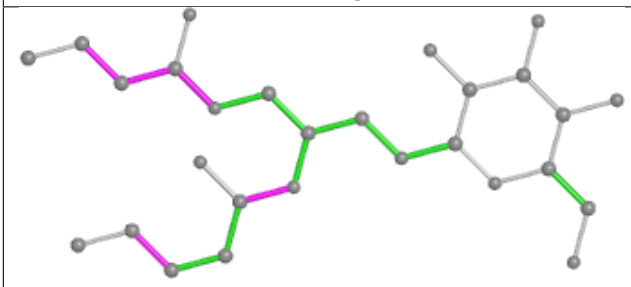
Ligand LMG N 101



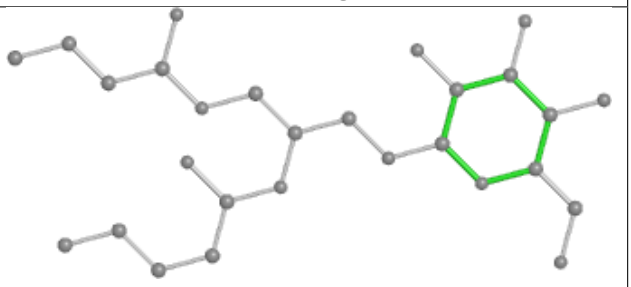
Bond lengths



Bond angles

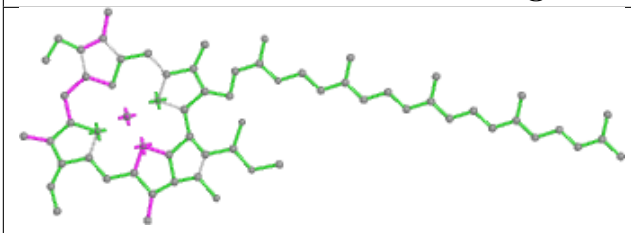


Torsions



Rings

Ligand CLA b 617



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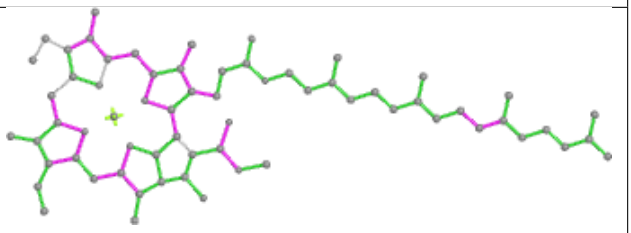

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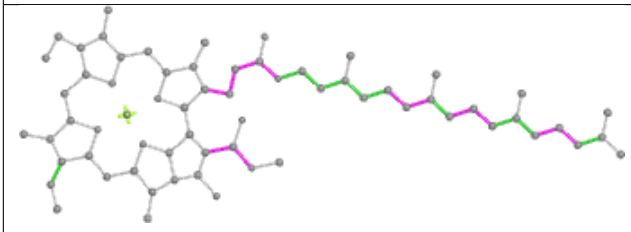

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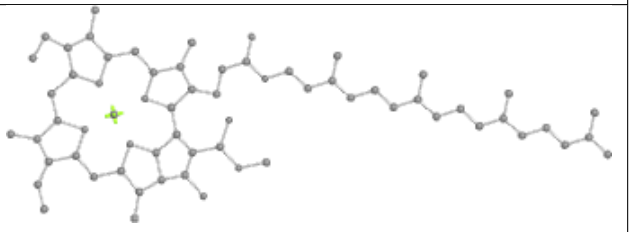
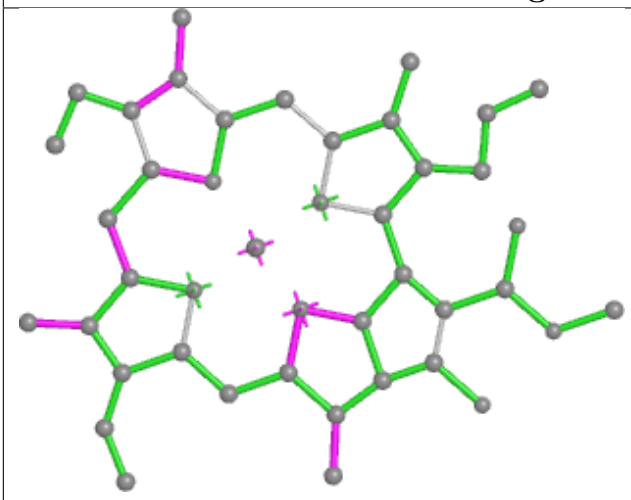


Rings

Ligand CLA 8 314



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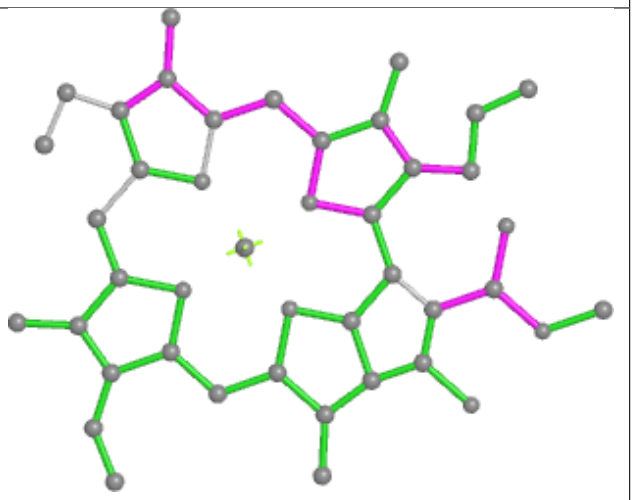

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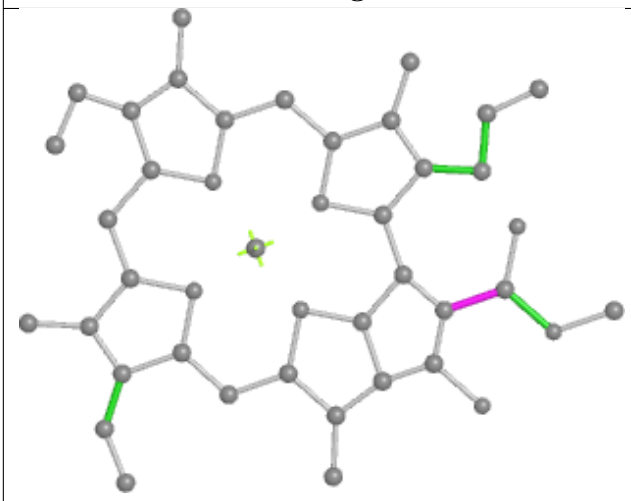

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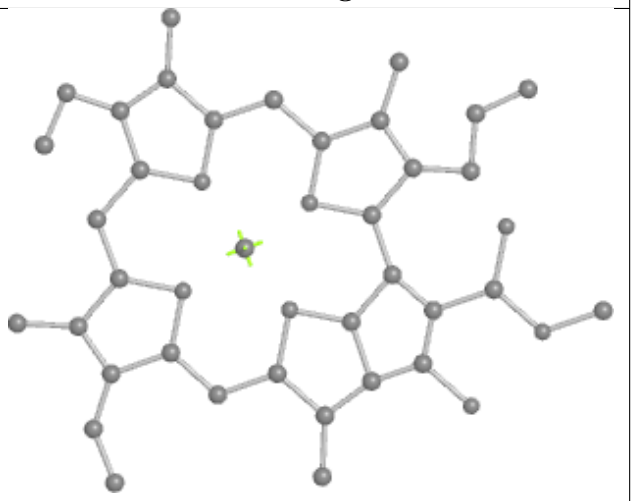
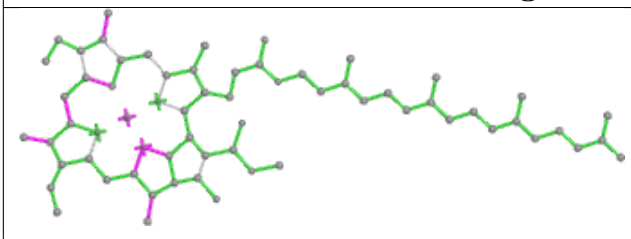


Rings

Ligand CLA 15 307



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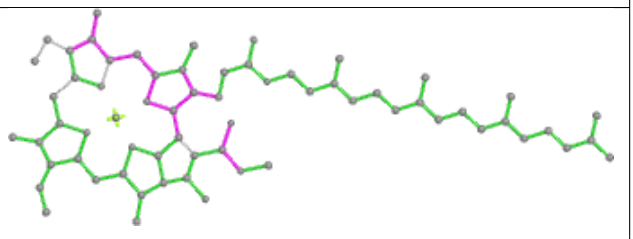

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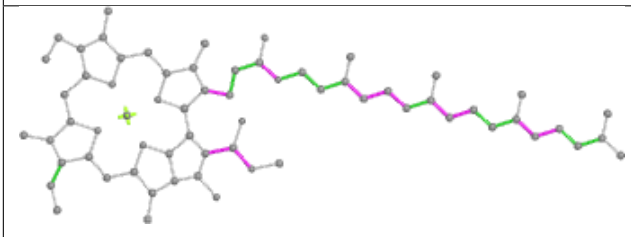

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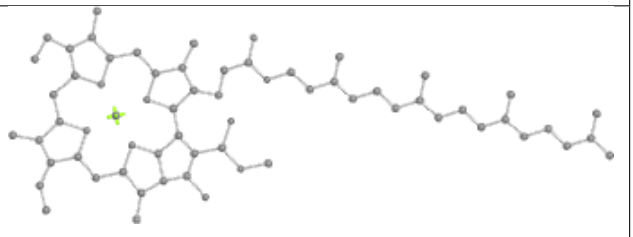
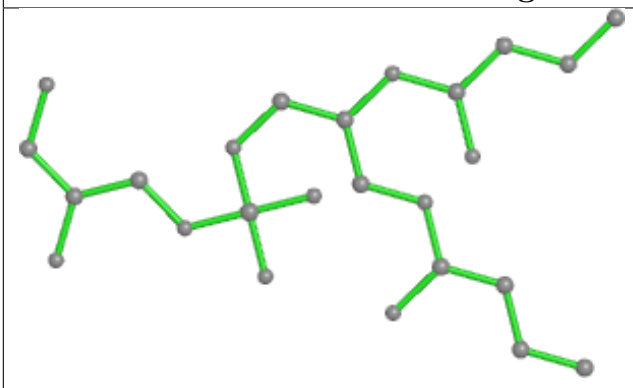


Rings

Ligand LHG 15 316



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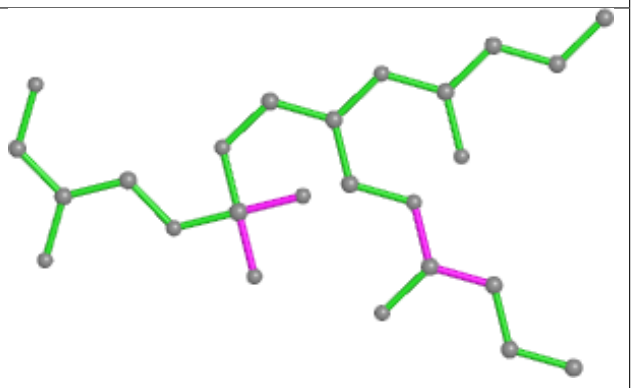

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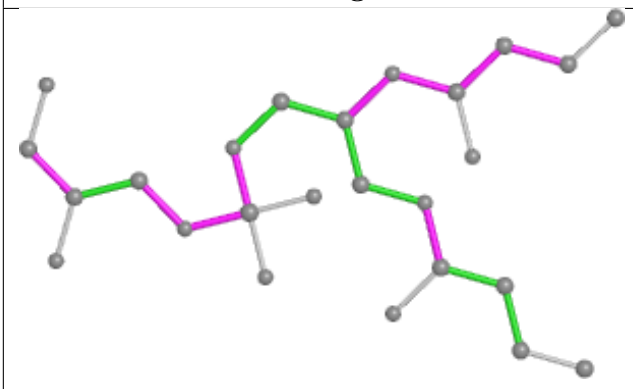

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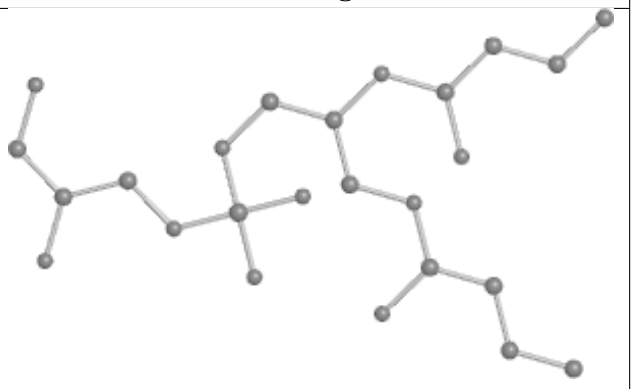
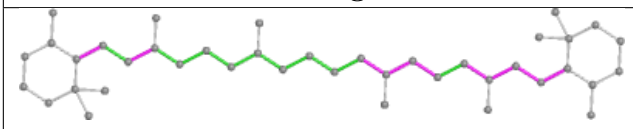


Rings

Ligand BCR b 620

Bond lengths

Bond angles



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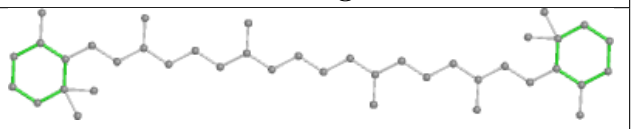
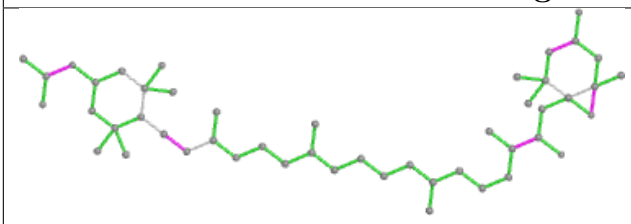
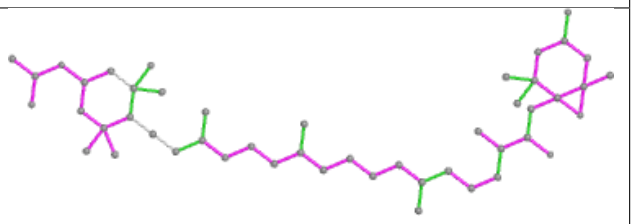


Rings

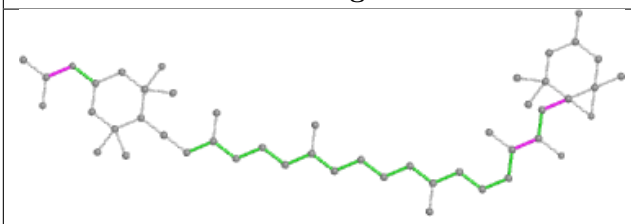
Ligand A86 8 302



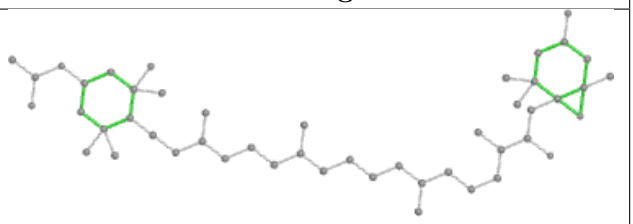
Bond lengths



Bond angles

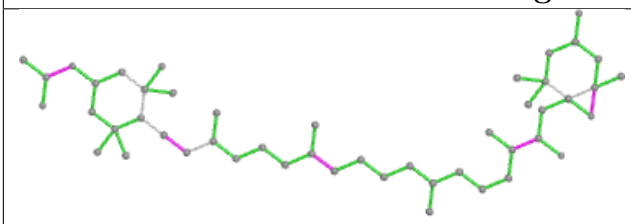


Torsions



Rings

Ligand A86 2 301



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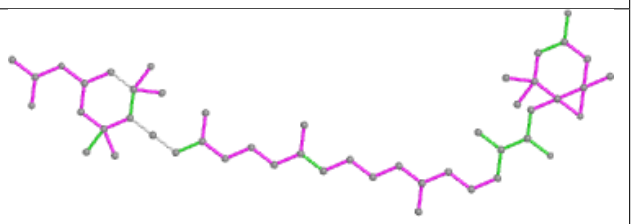

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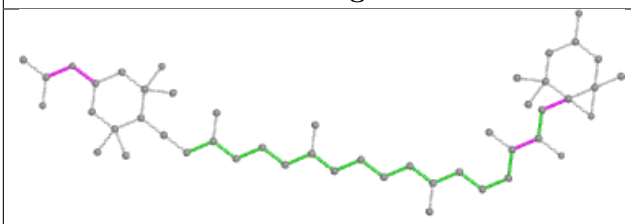

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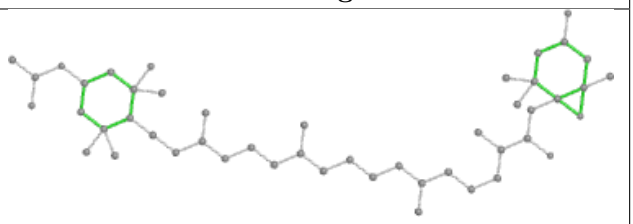
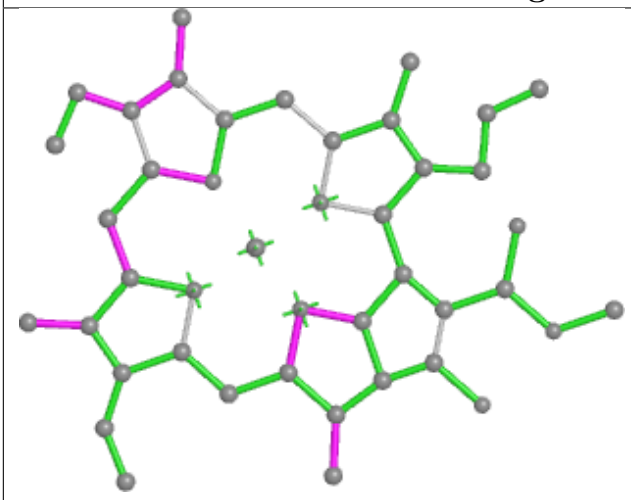


Rings

Ligand CLA 4 314



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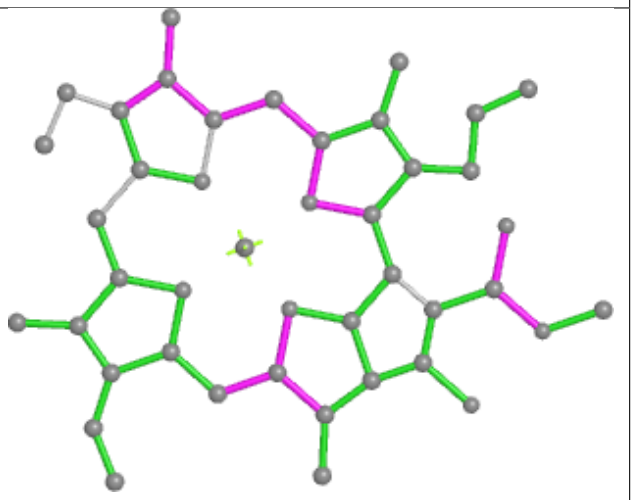

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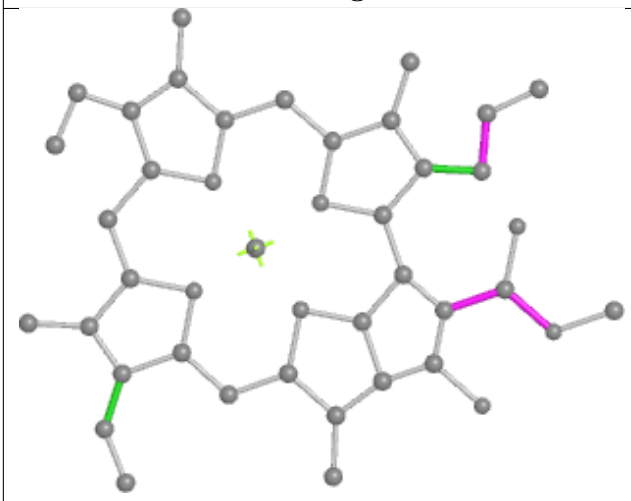

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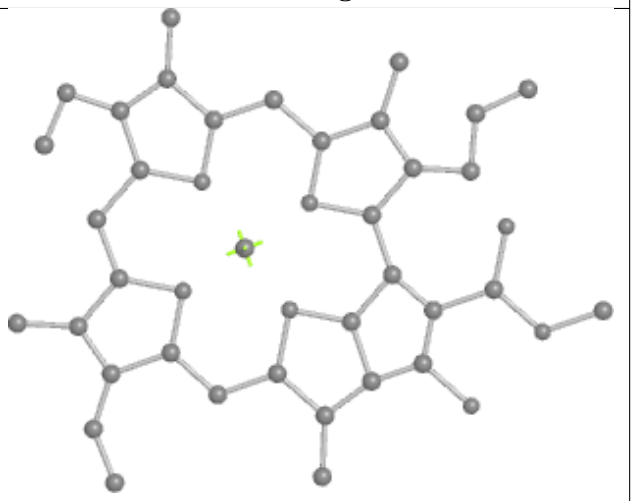
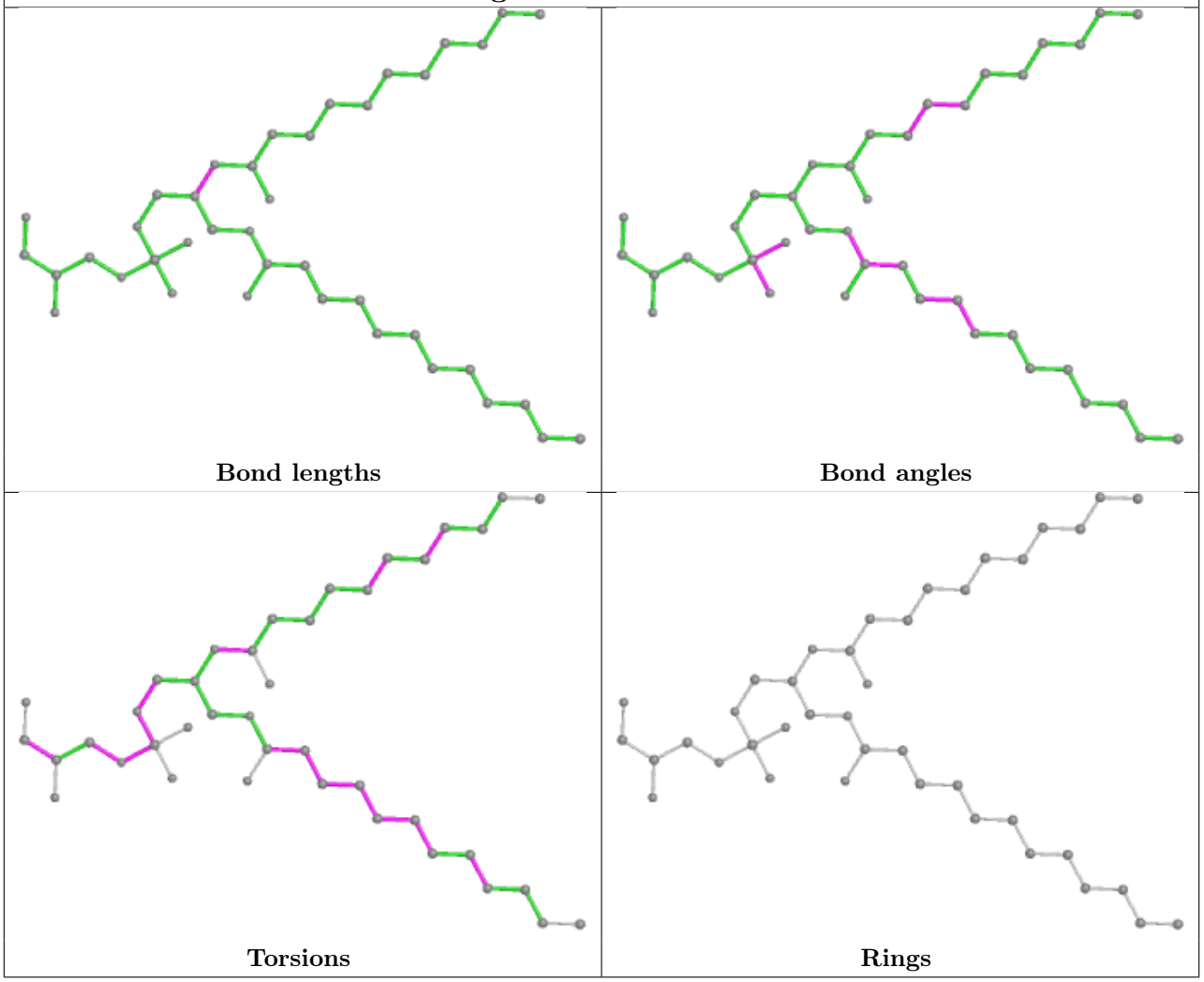
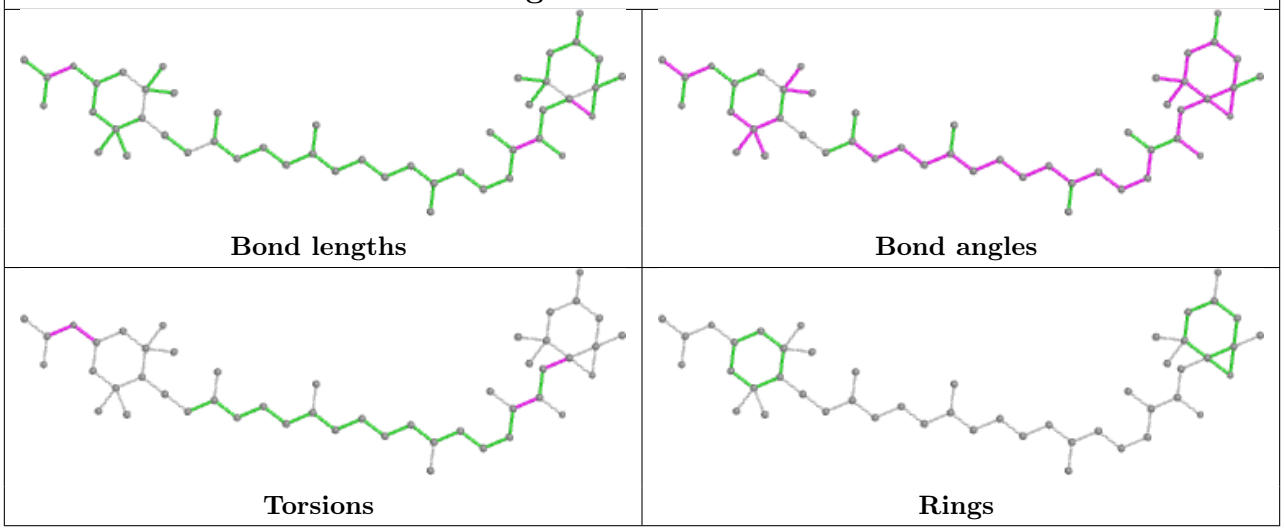


Rings

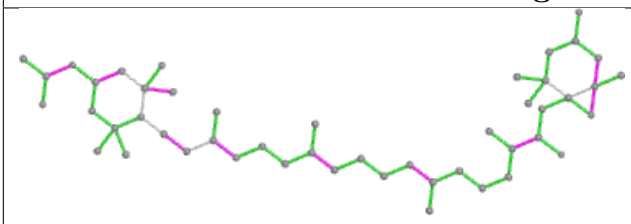
Ligand LHG w 202



Ligand A86 13 306



Ligand A86 p 611



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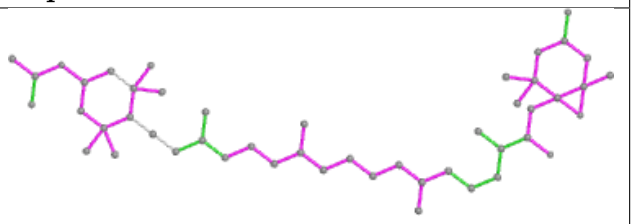

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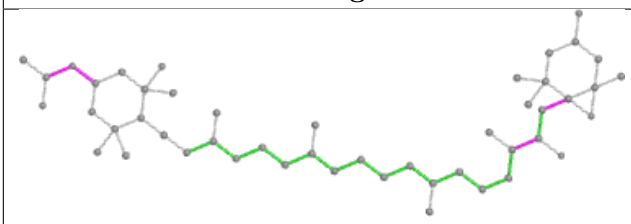

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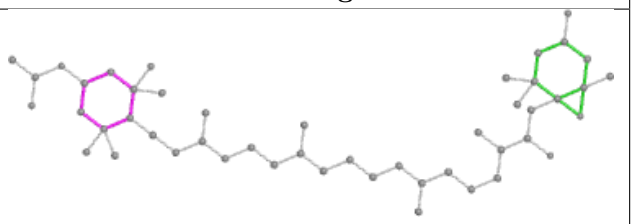
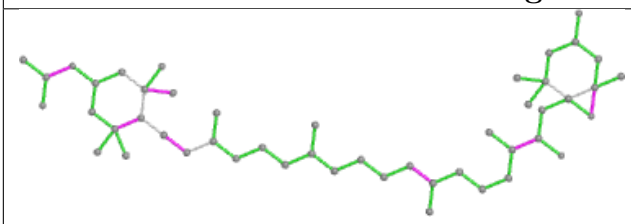


Rings

Ligand A86 10 303



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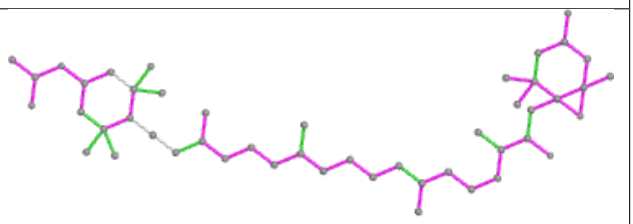

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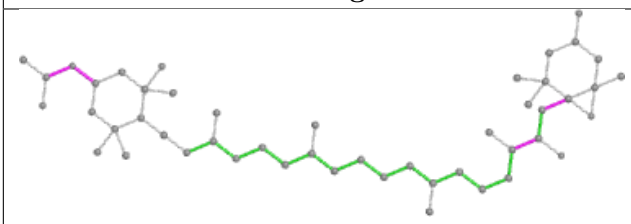

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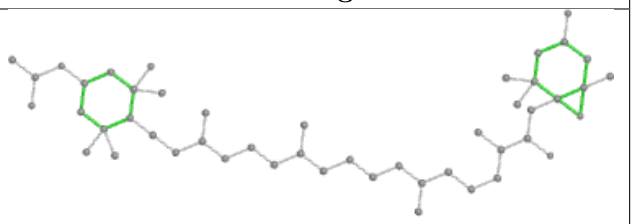
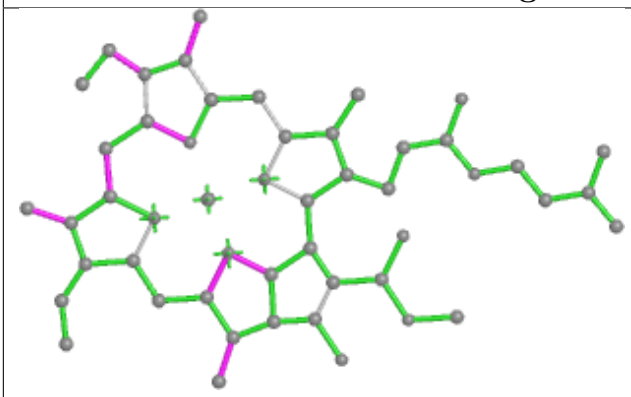


Rings

Ligand CLA 11 310



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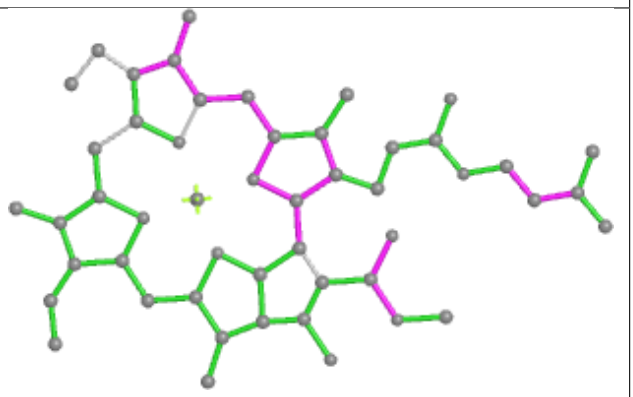

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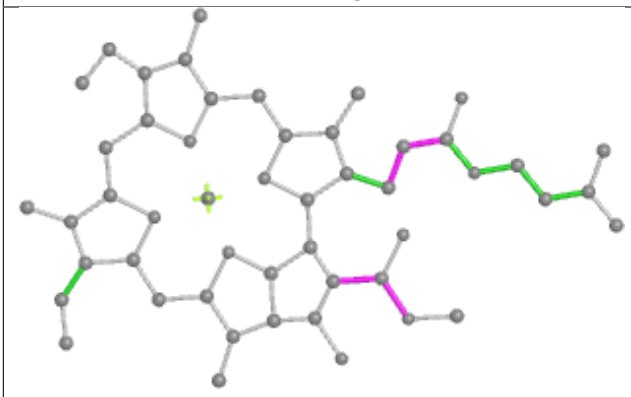

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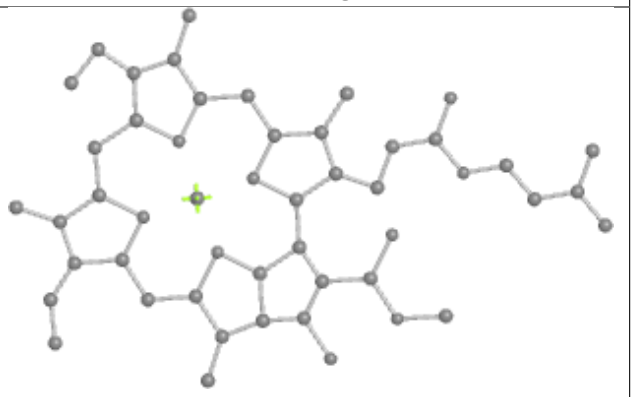
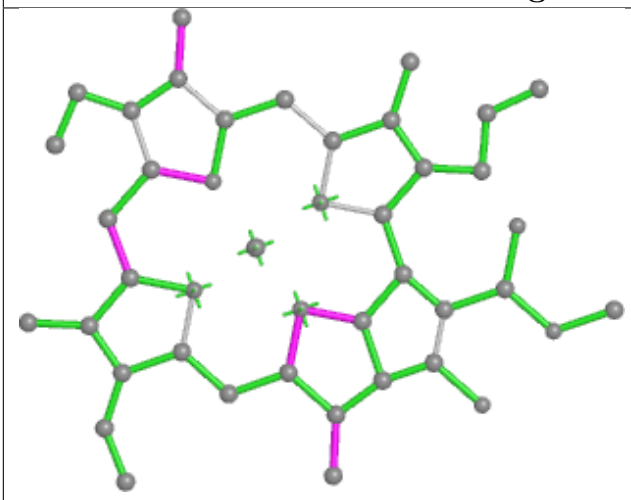


Rings

Ligand CLA 6 316



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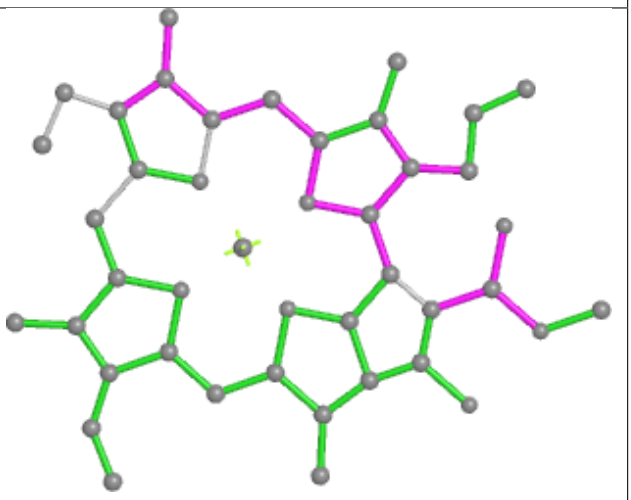

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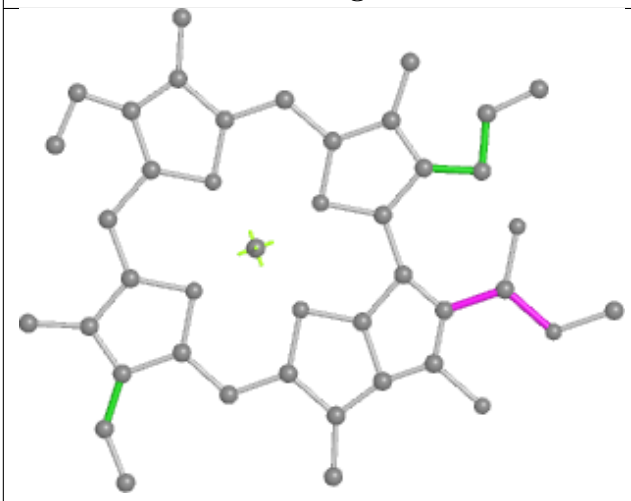

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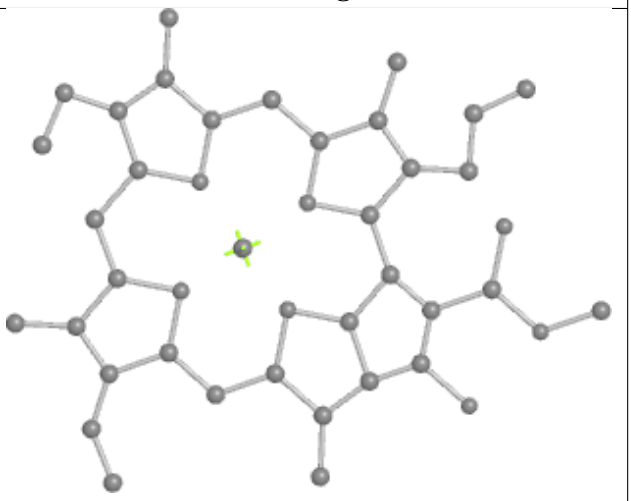
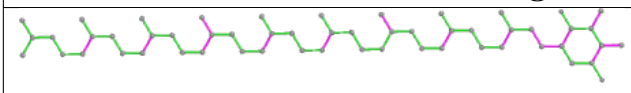


Rings

Ligand PL9 D 406



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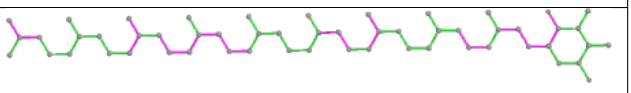

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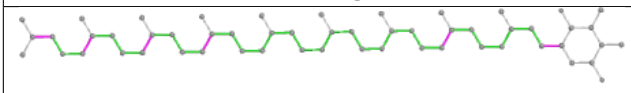

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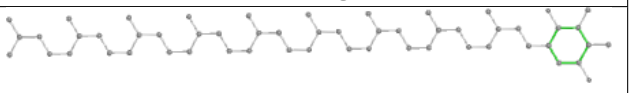
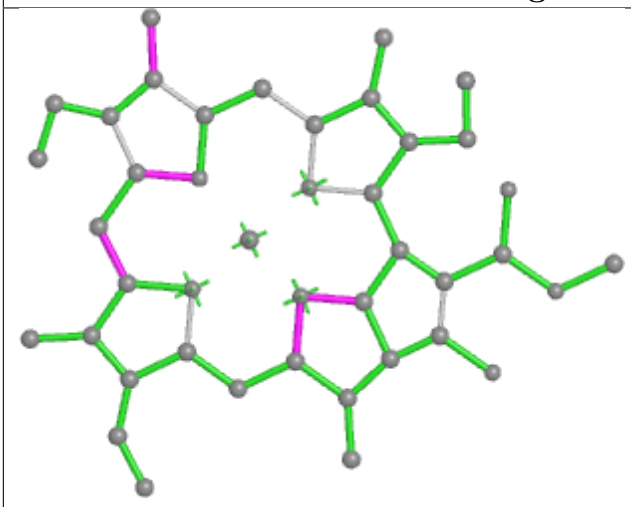


Rings

Ligand CLA 2 306



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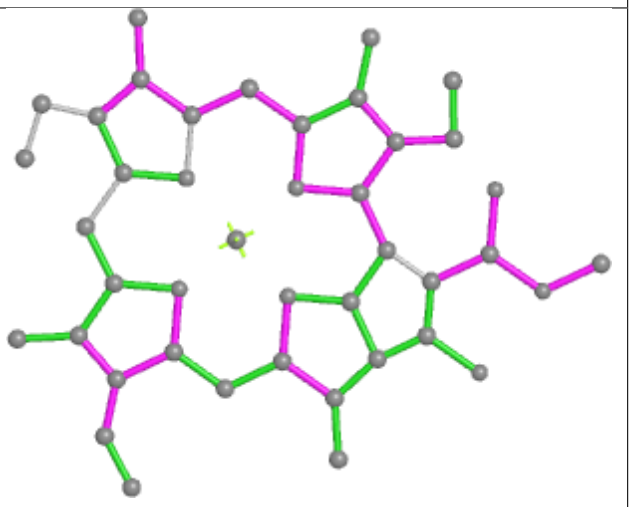
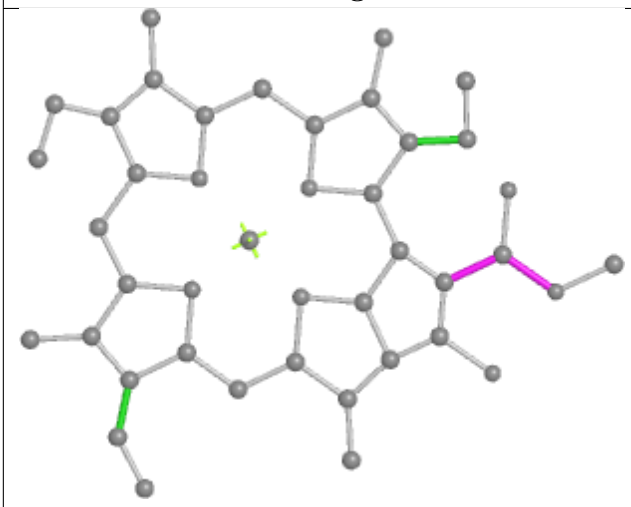


Bond angles



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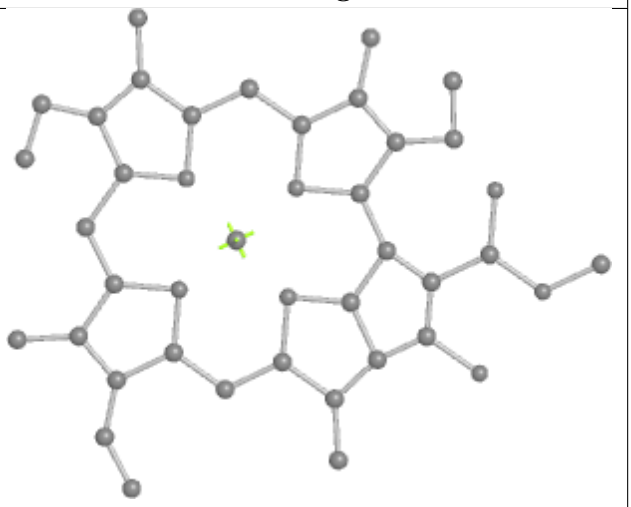
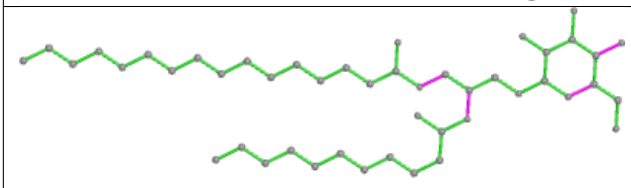


Rings

Ligand LMG k 101



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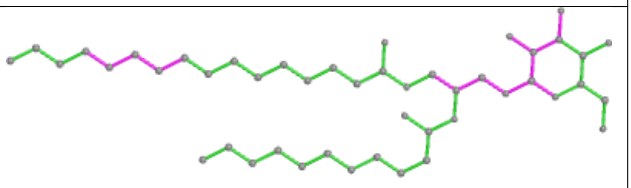

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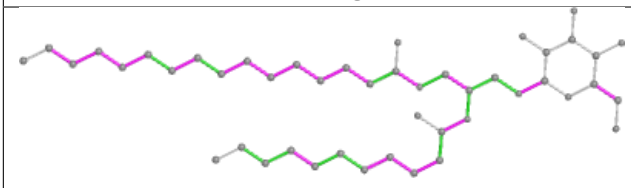

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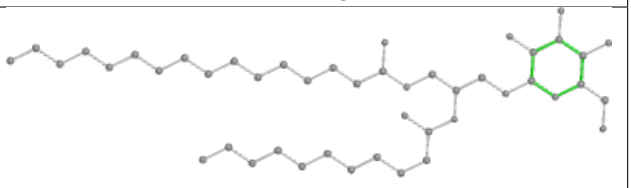
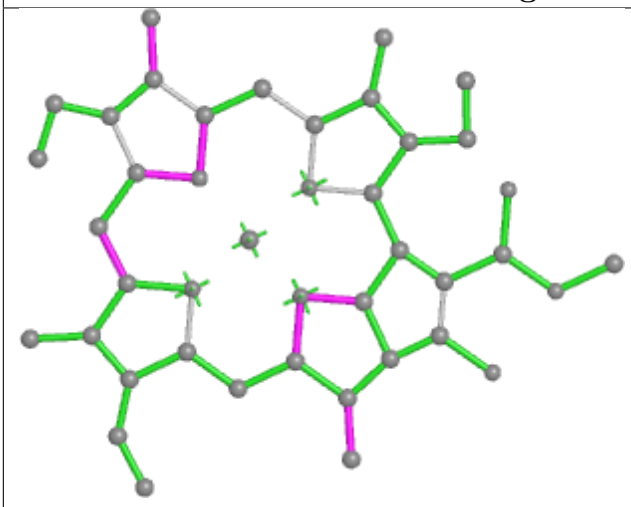


Rings

Ligand CLA 15 306



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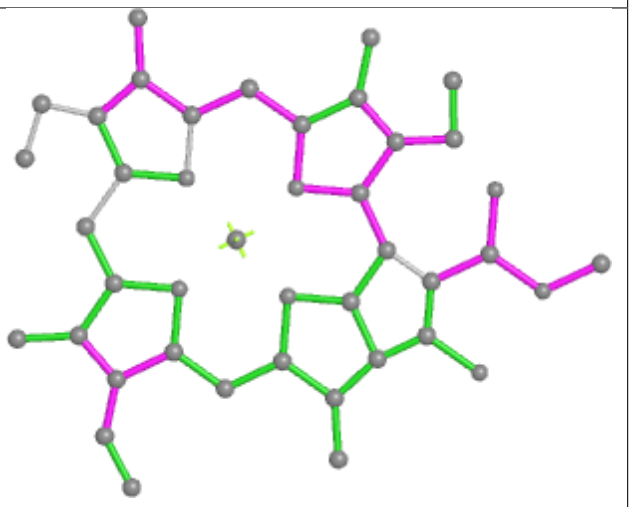

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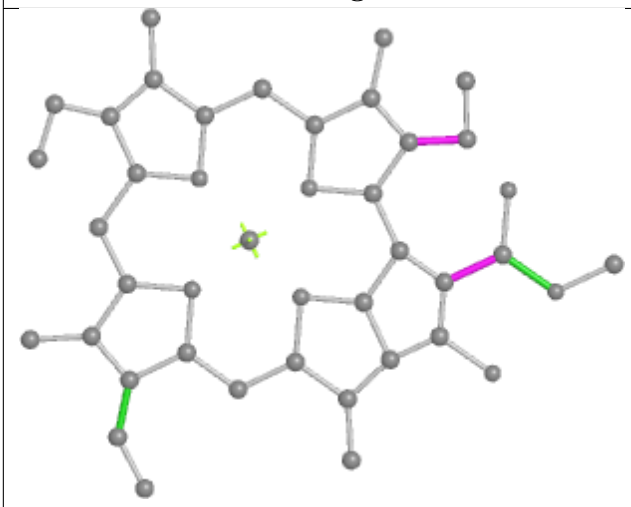

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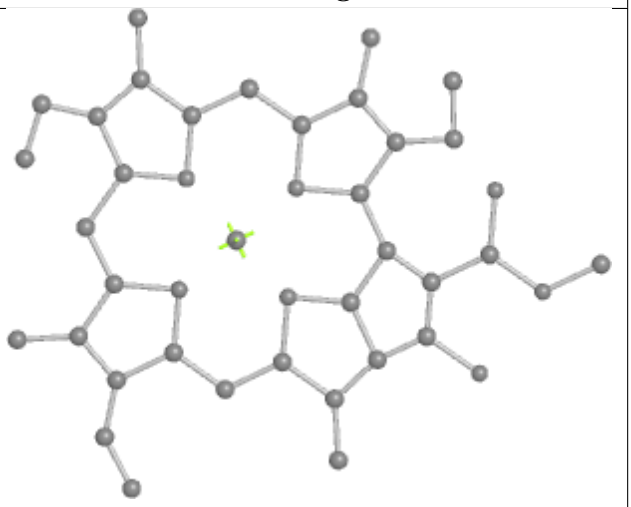
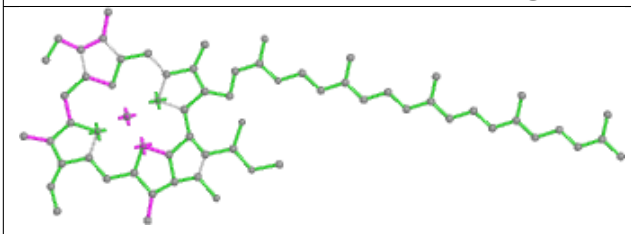


Rings

Ligand CLA C 512



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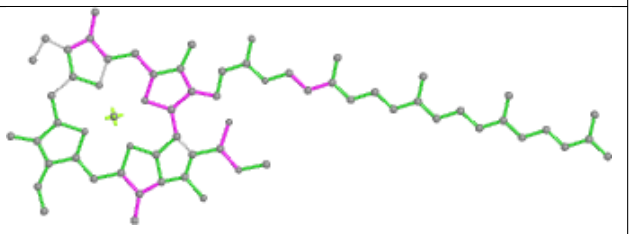
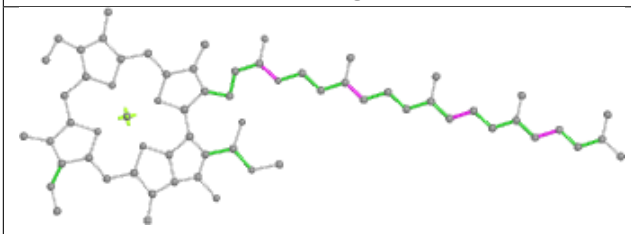


Bond angles



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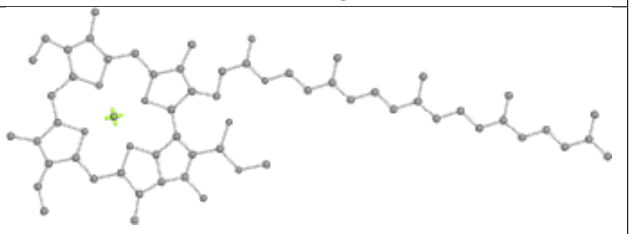
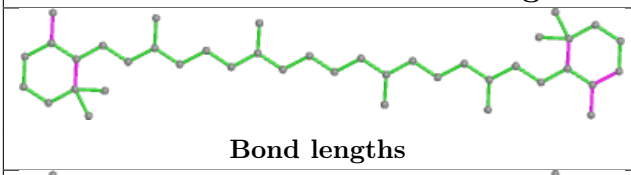


Rings

Ligand BCR C 516



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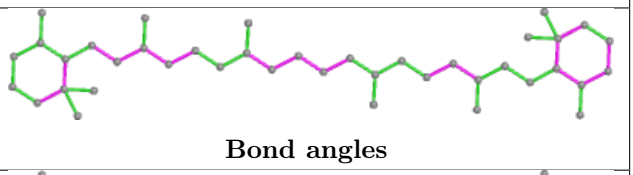
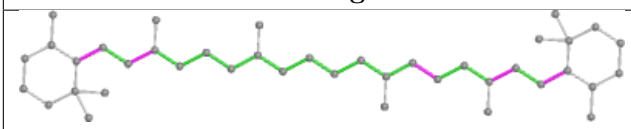


Bond angles



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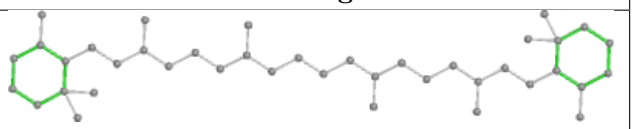
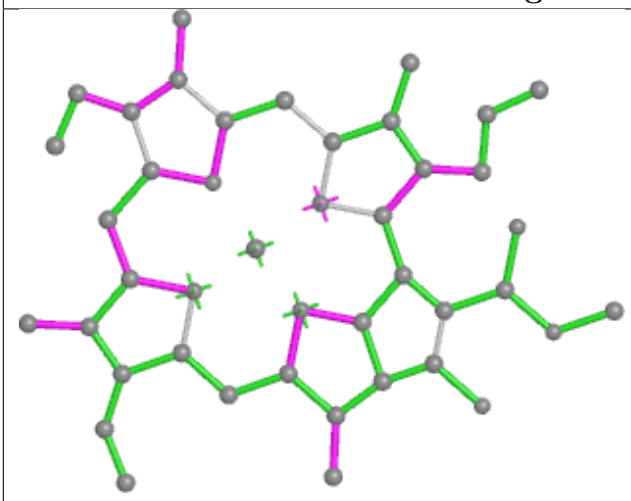


Rings

Ligand CLA P 606



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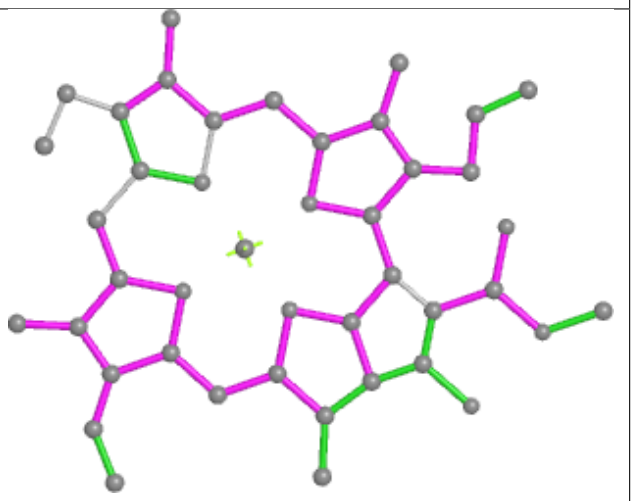
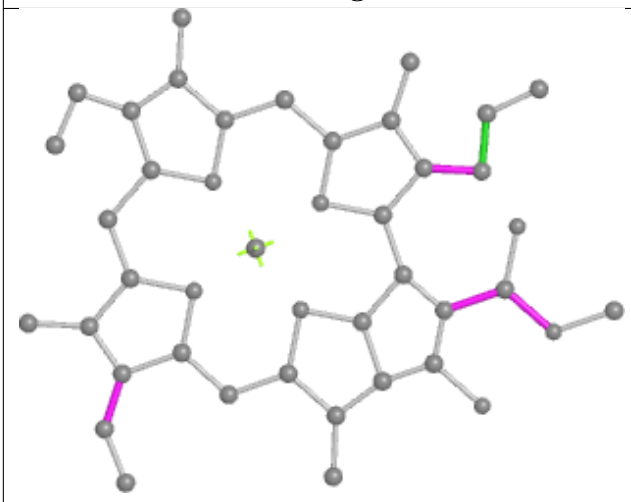
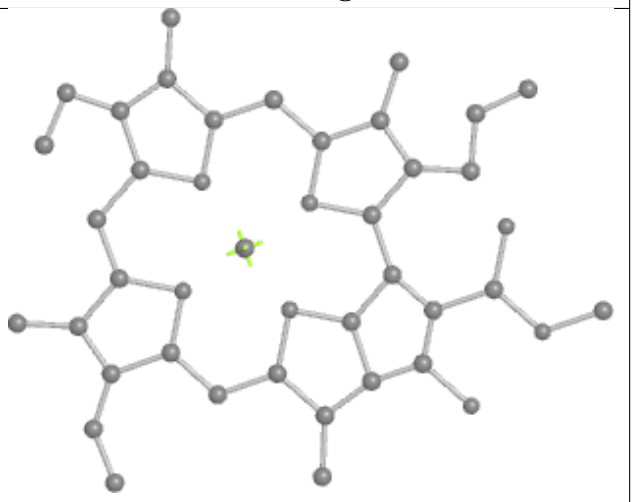


Bond angles

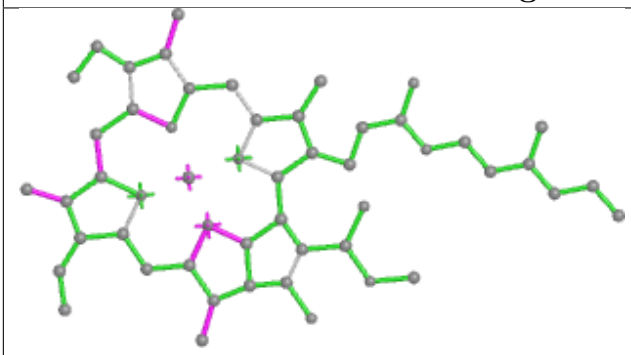


Torsions

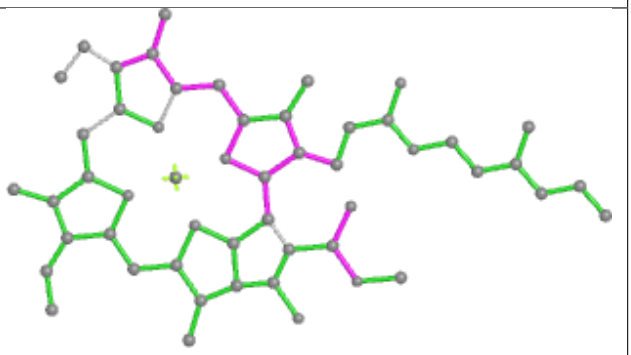


Rings

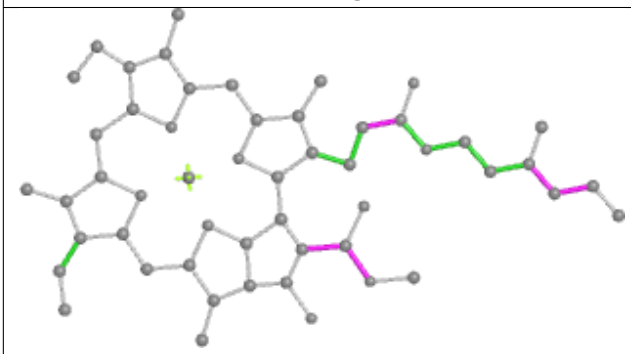
Ligand CLA 18 309



Bond lengths



Bond angles



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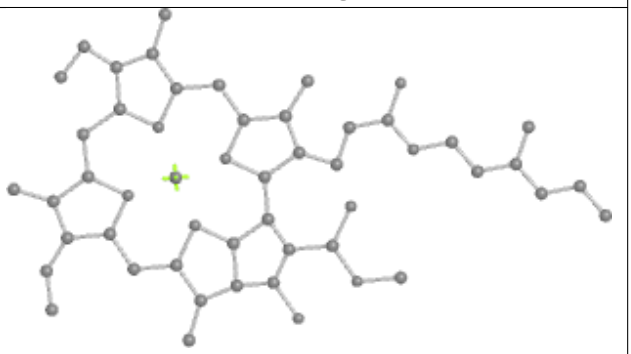
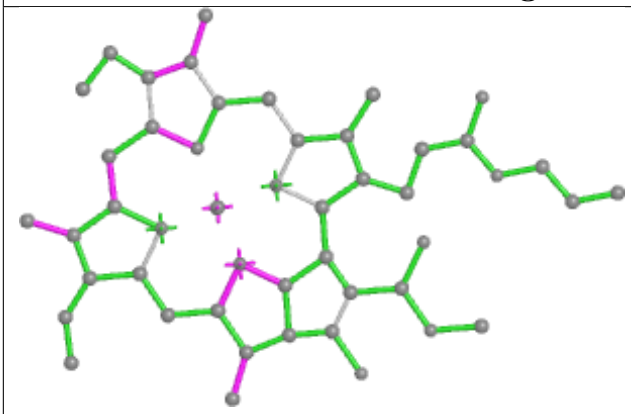


Rings

Ligand CLA 10 317



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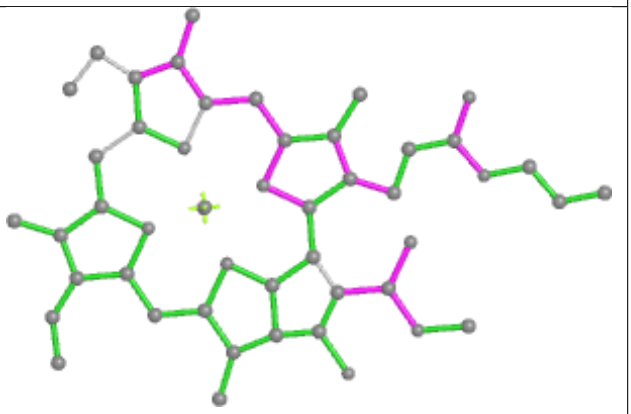
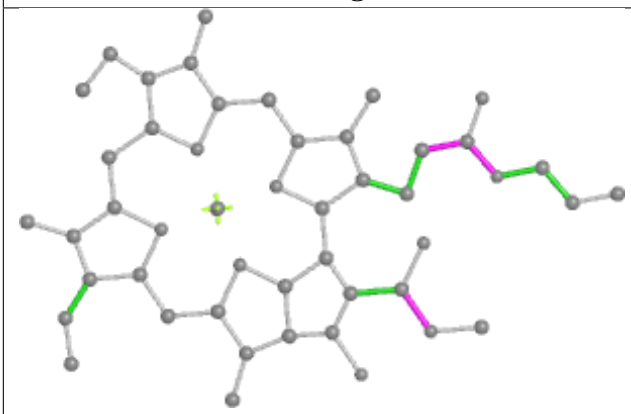


Bond angles



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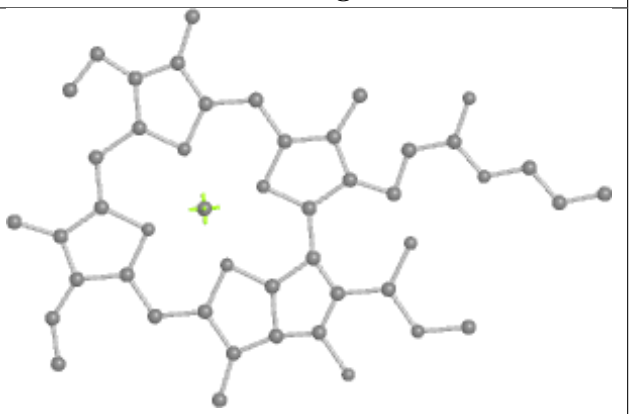
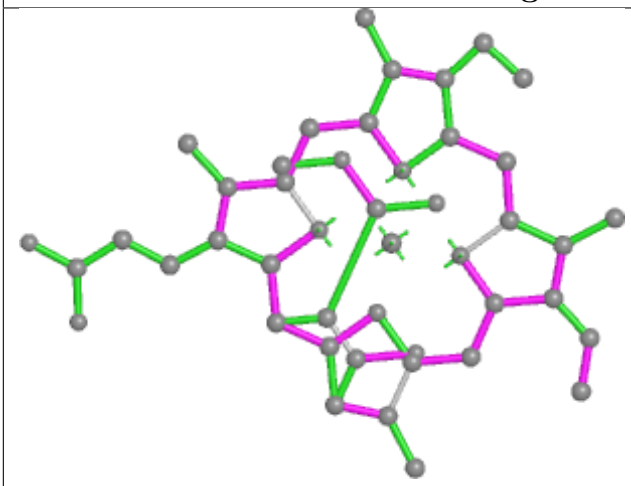


Rings

Ligand KC2 12 311



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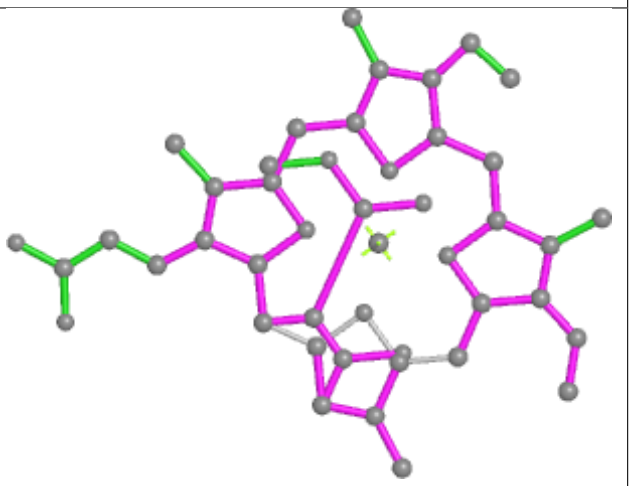

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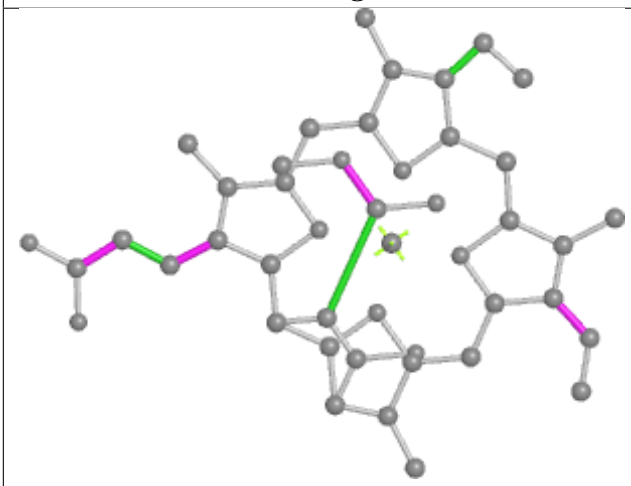

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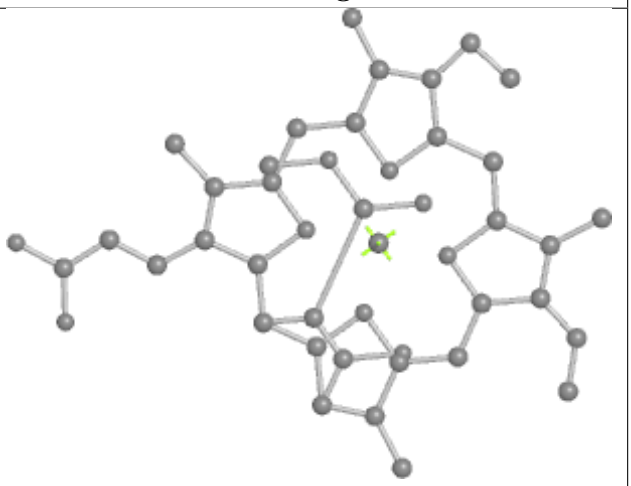
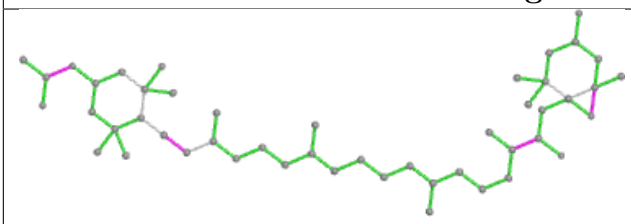


Rings

Ligand A86 13 302



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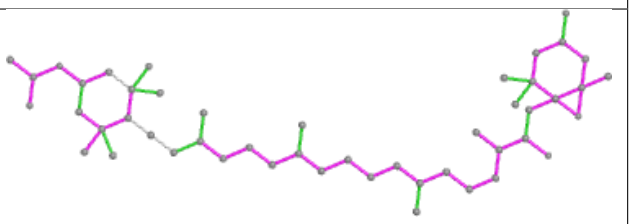

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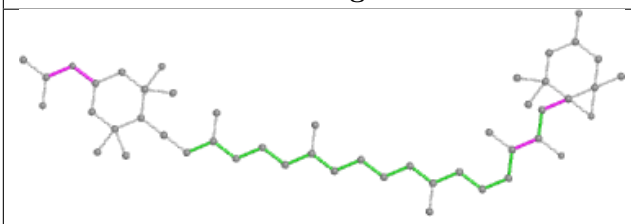

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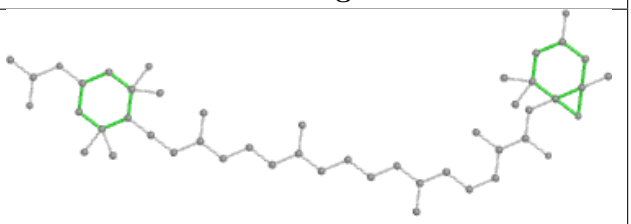
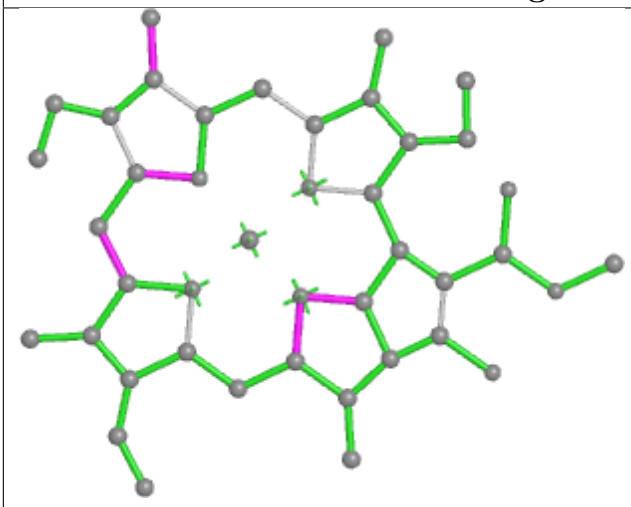


Rings

Ligand CLA 6 308



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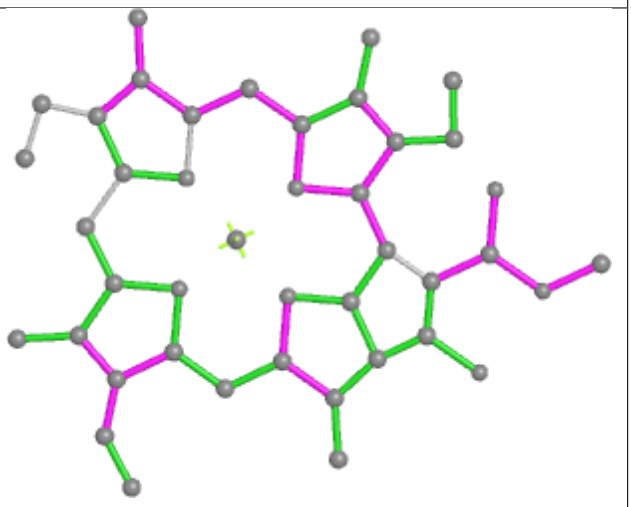

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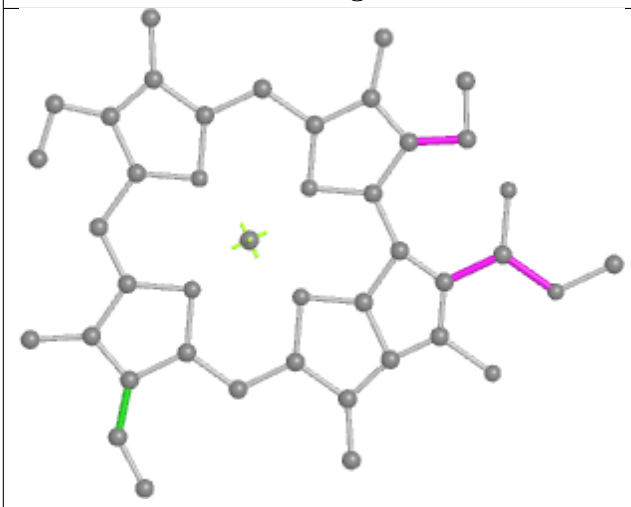

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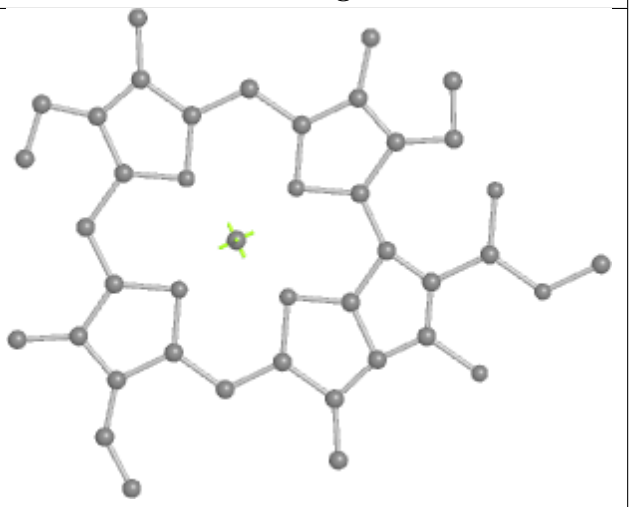
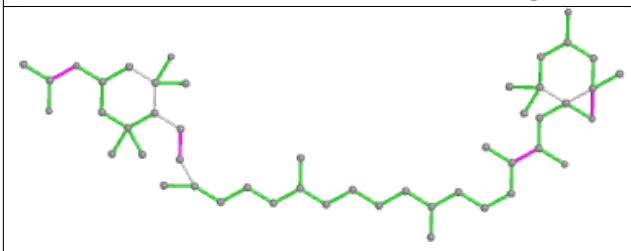


Rings

Ligand A86 19 302



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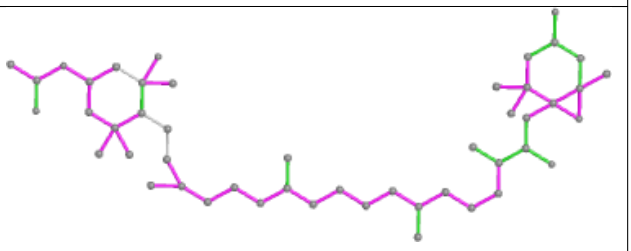

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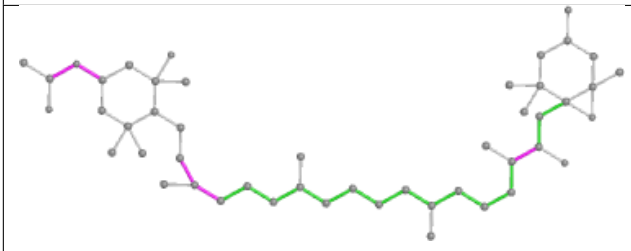

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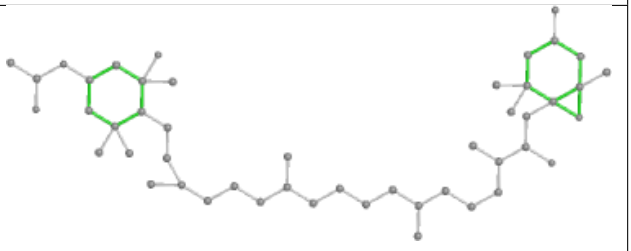
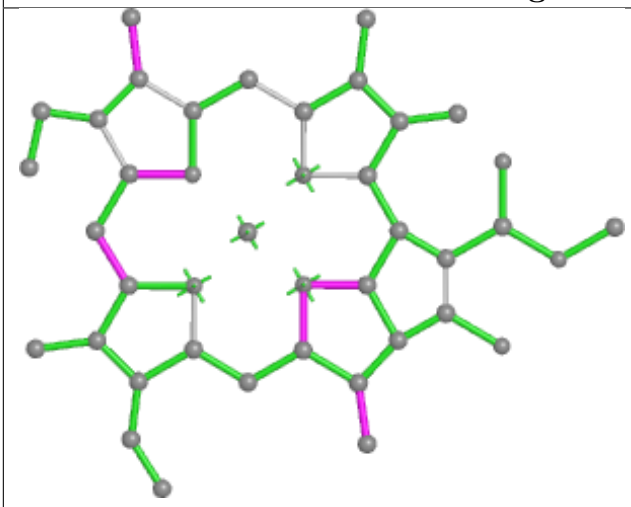


Rings

Ligand CLA 6 311



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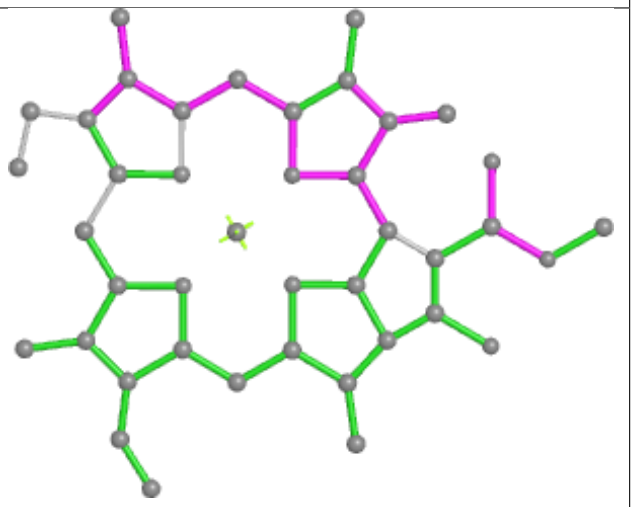

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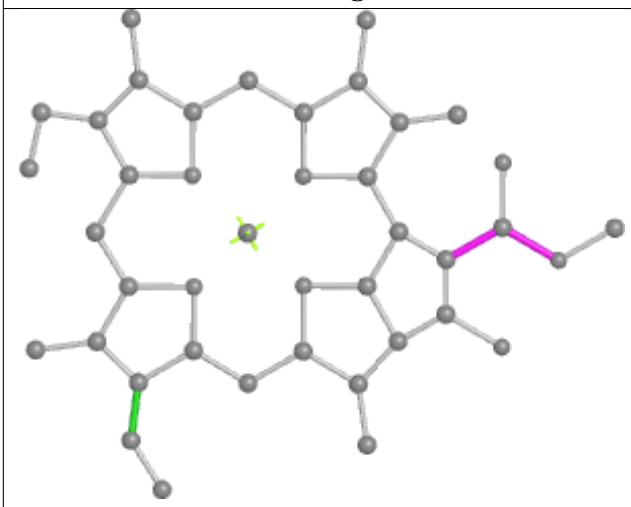

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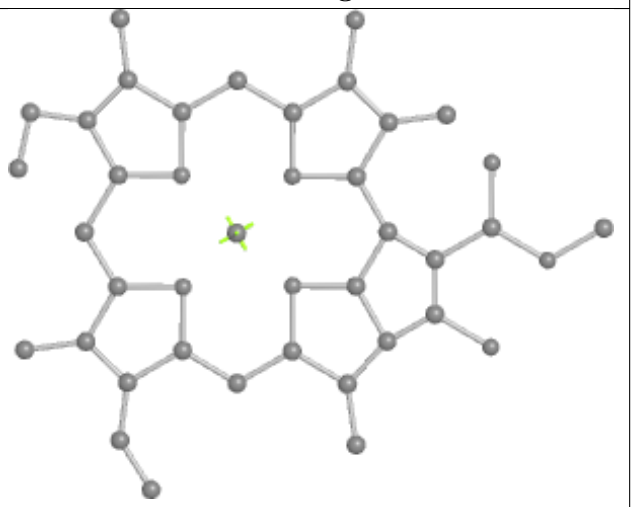
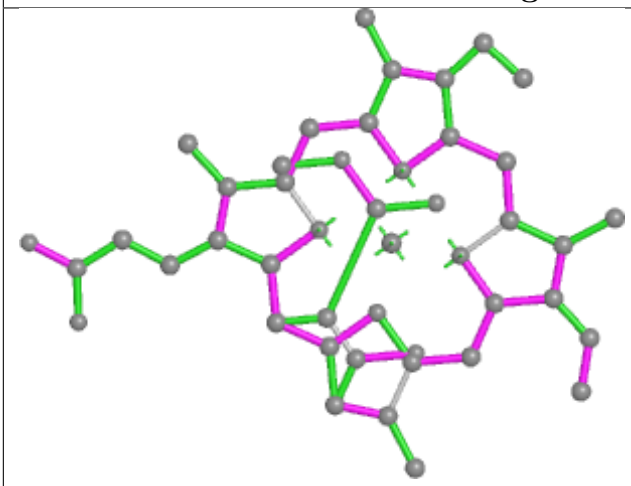


Rings

Ligand KC2 18 308



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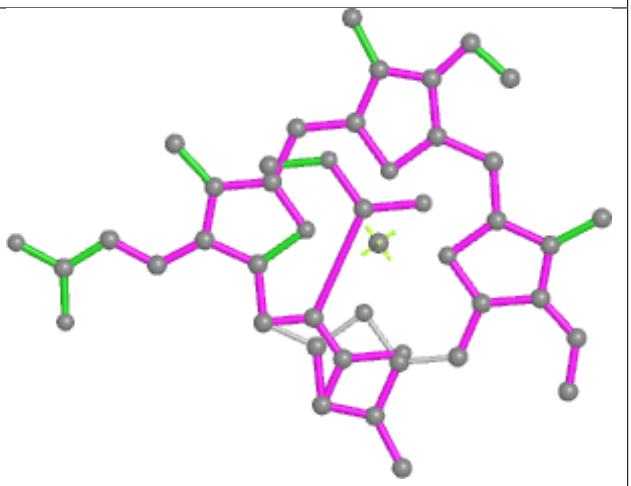

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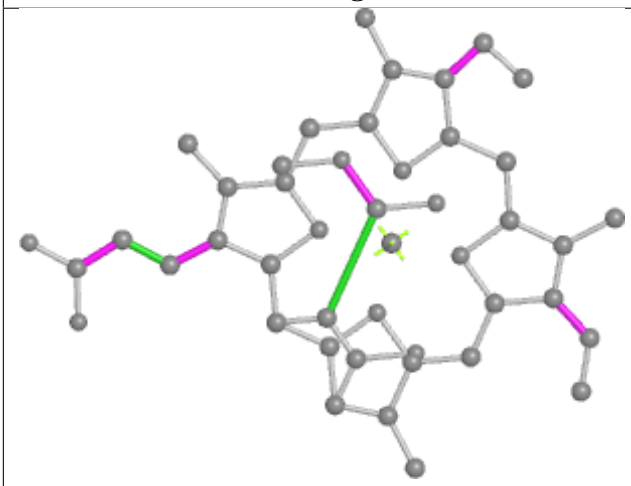

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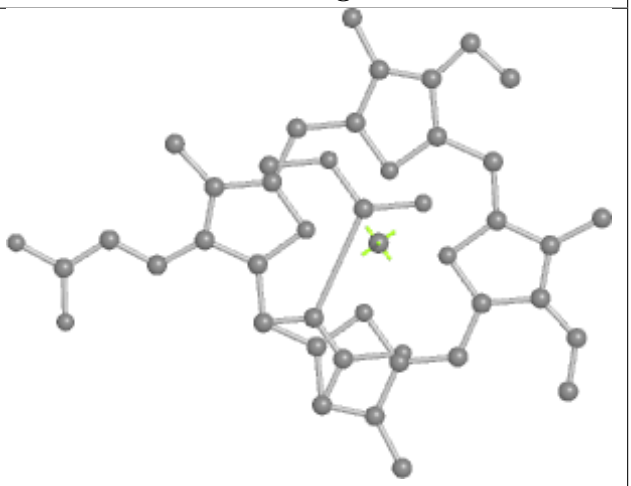
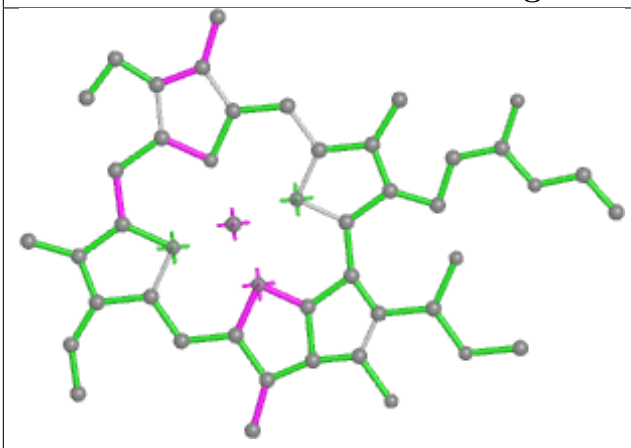


Rings

Ligand CLA R 101



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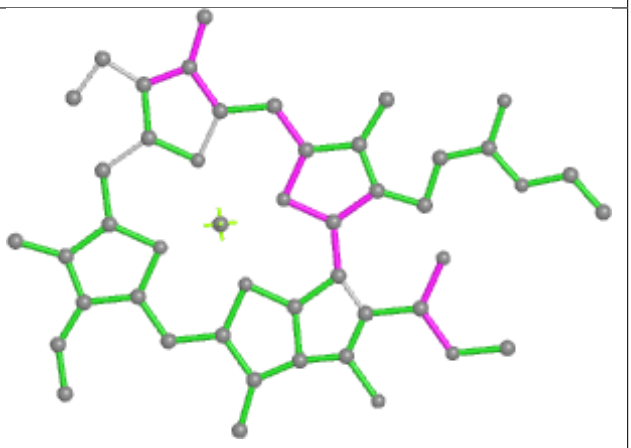

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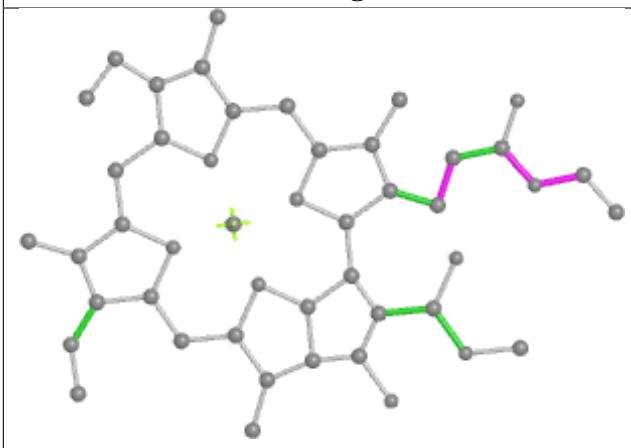

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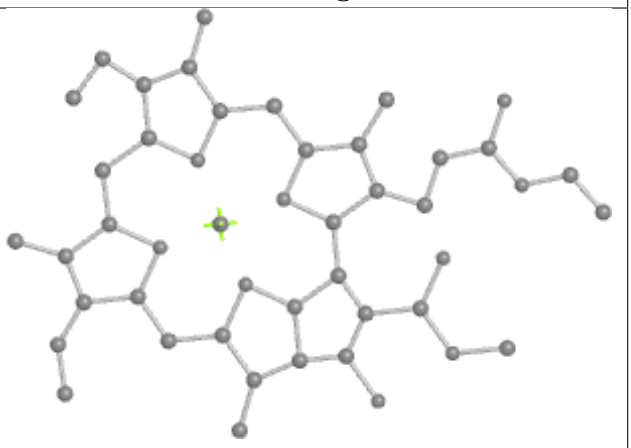
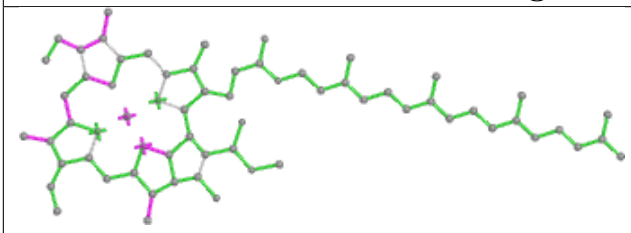


Rings

Ligand CLA 1 313



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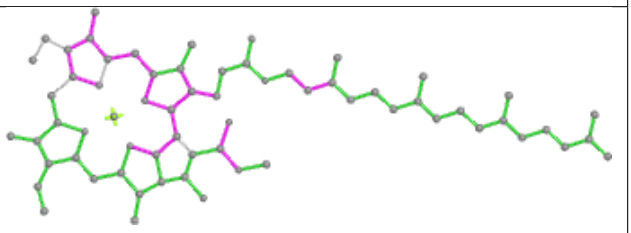

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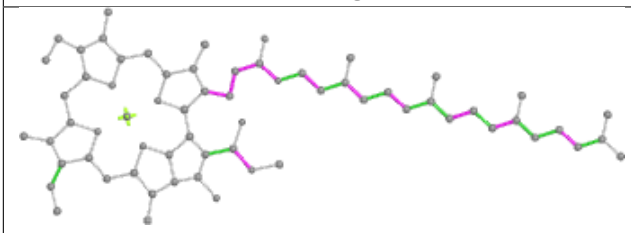

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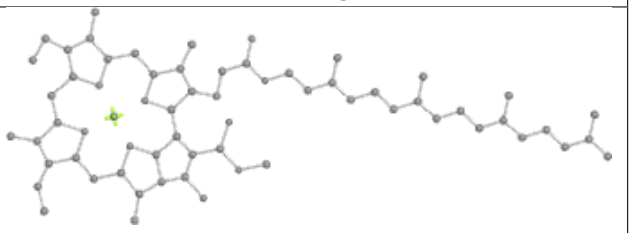
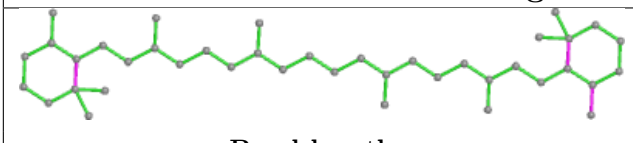


Rings

Ligand BCR a 407



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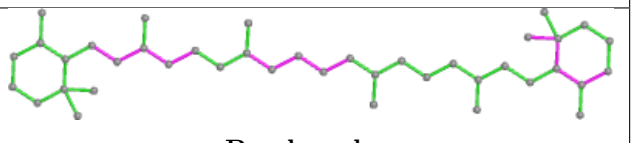

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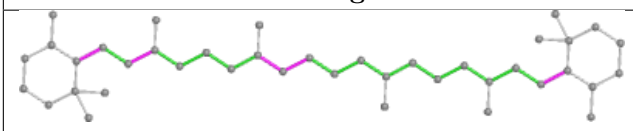

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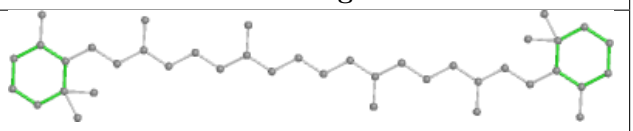
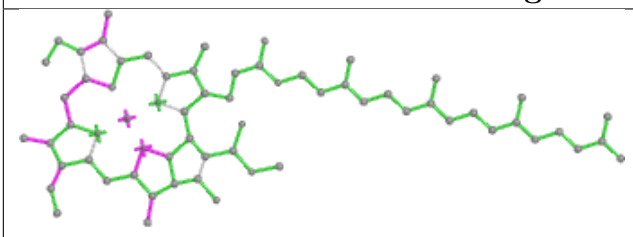


Rings

Ligand CLA B 611



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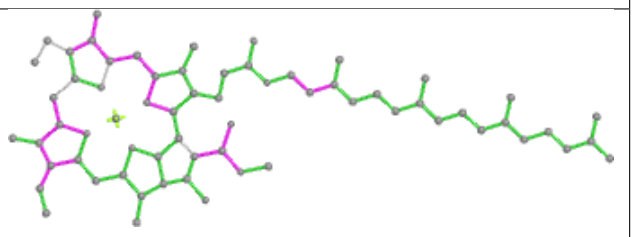
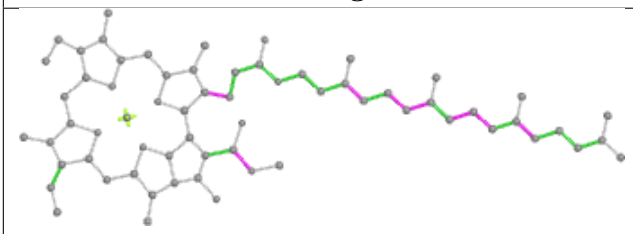


Bond angles



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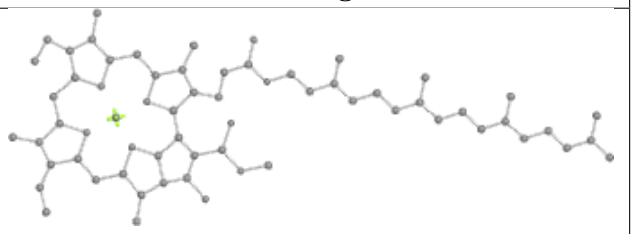
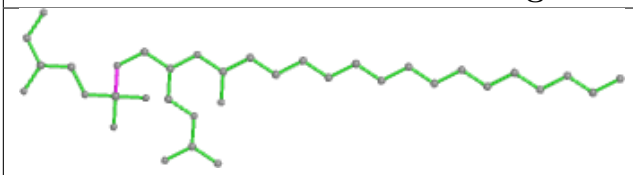


Rings

Ligand LHG 4 317



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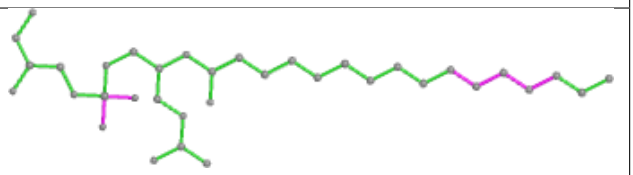
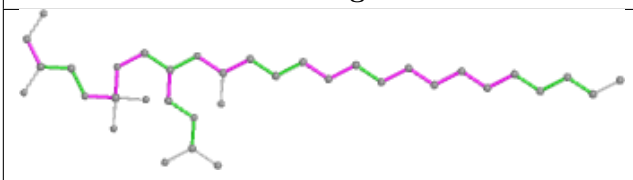


Bond angles



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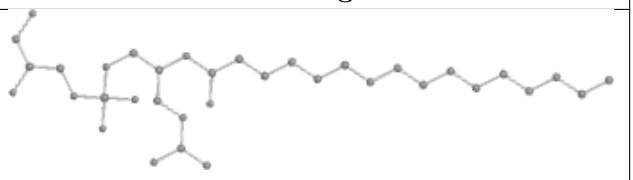
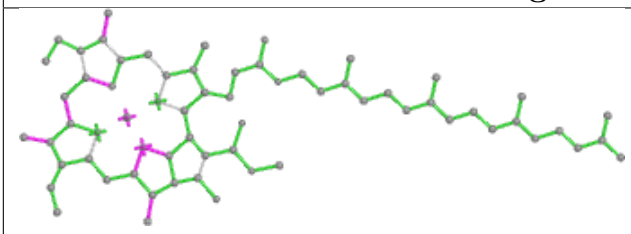
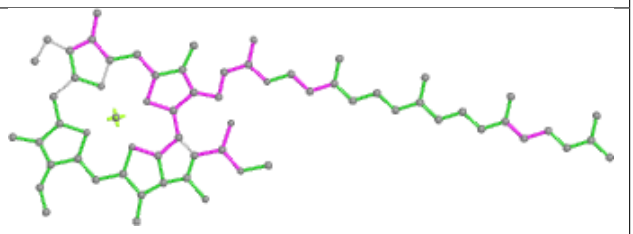


Rings

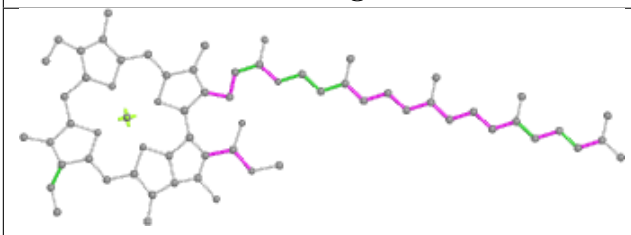
Ligand CLA c 504



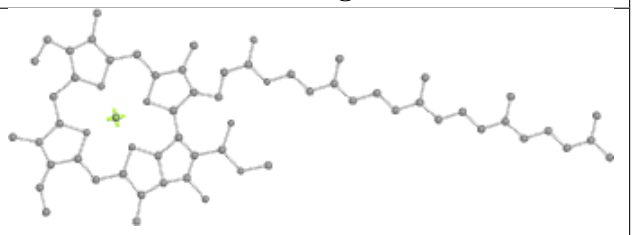
Bond lengths



Bond angles

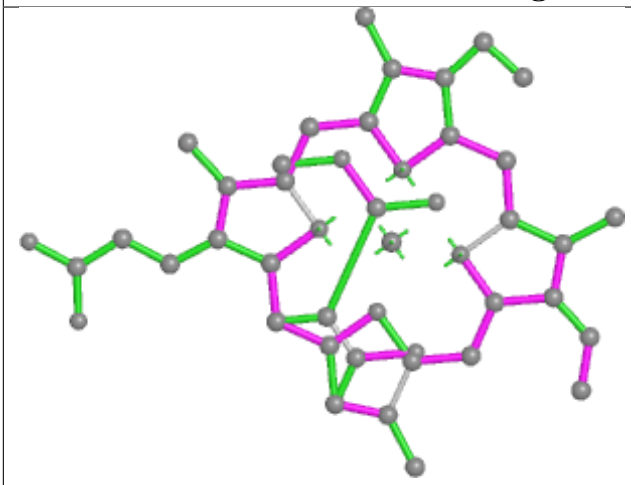


Torsions



Rings

Ligand KC2 6 310



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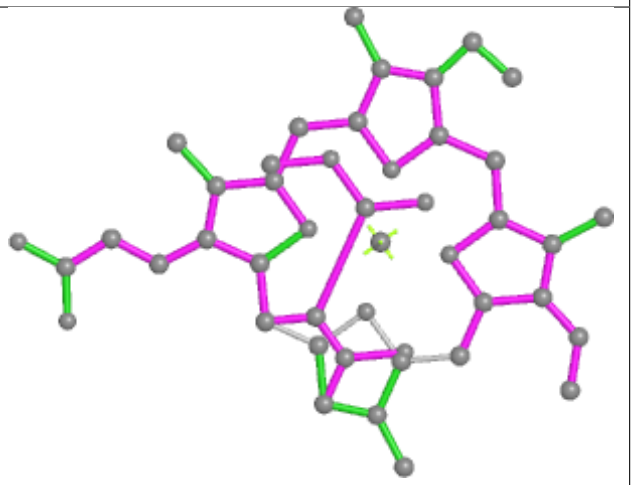

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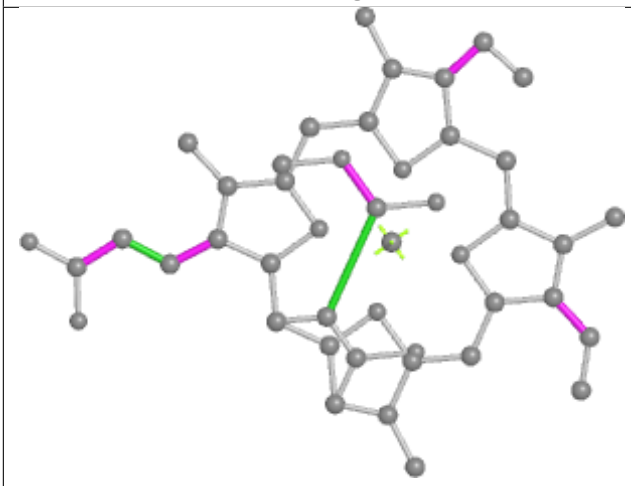

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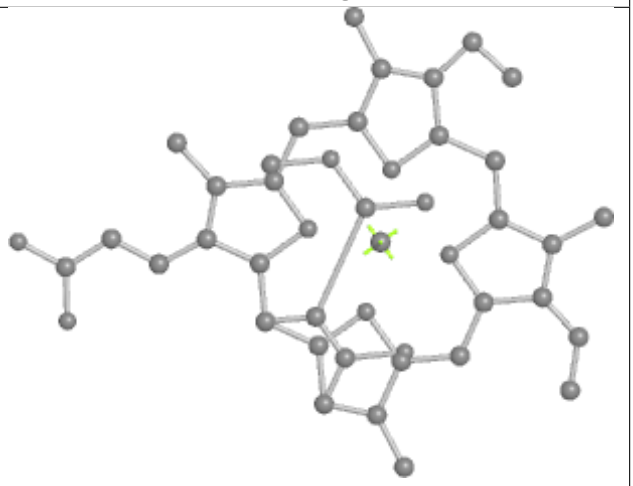
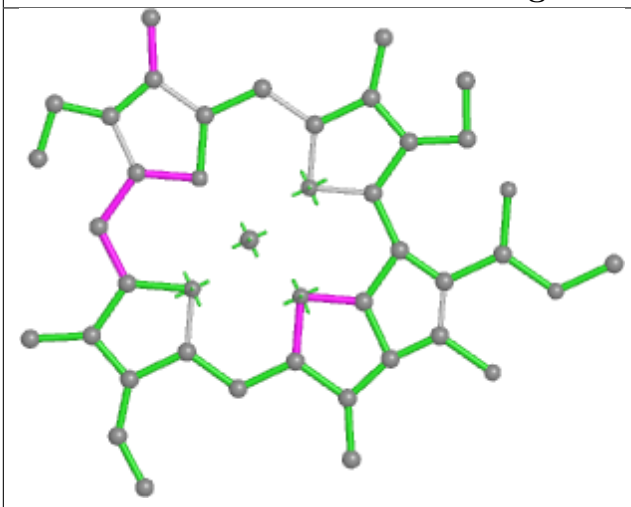


Rings

Ligand CLA 3 307



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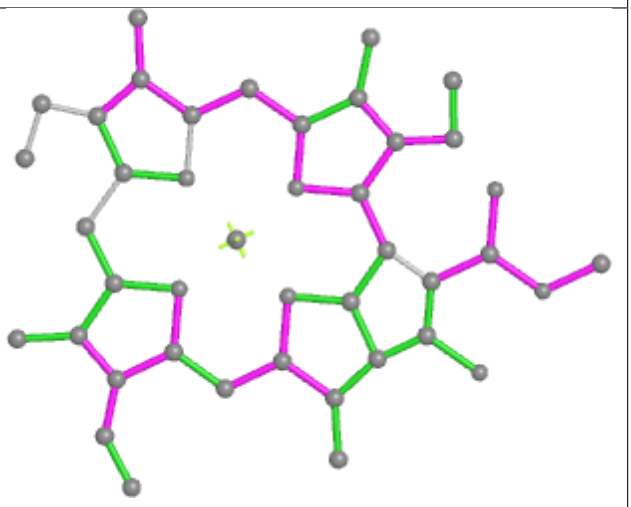

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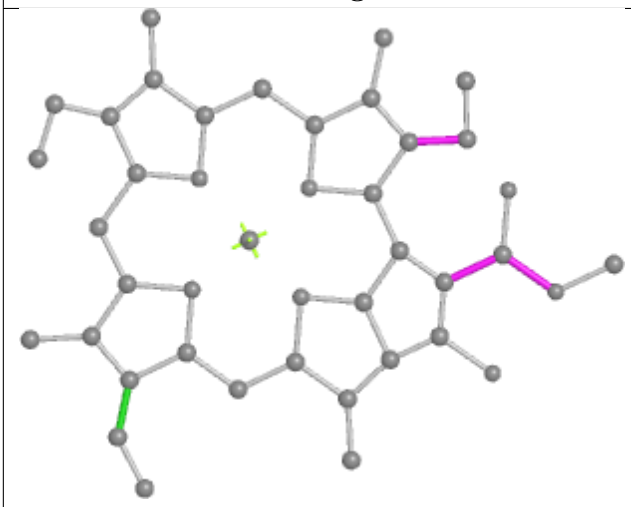

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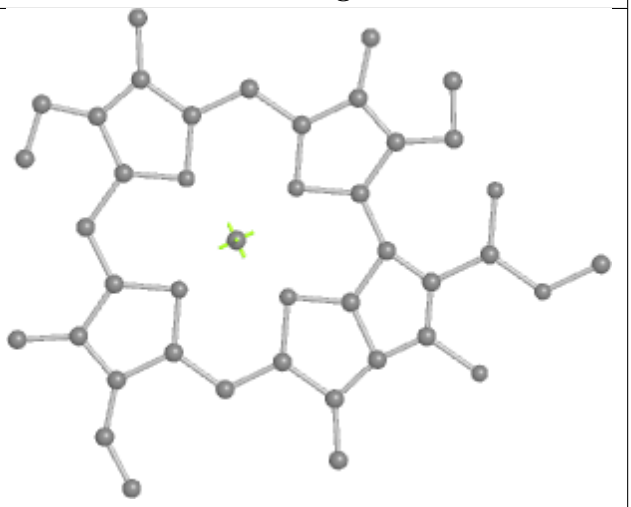
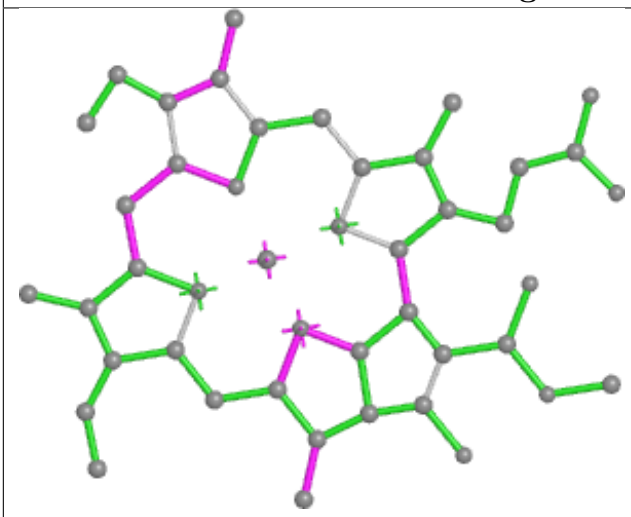


Rings

Ligand CLA 15 311



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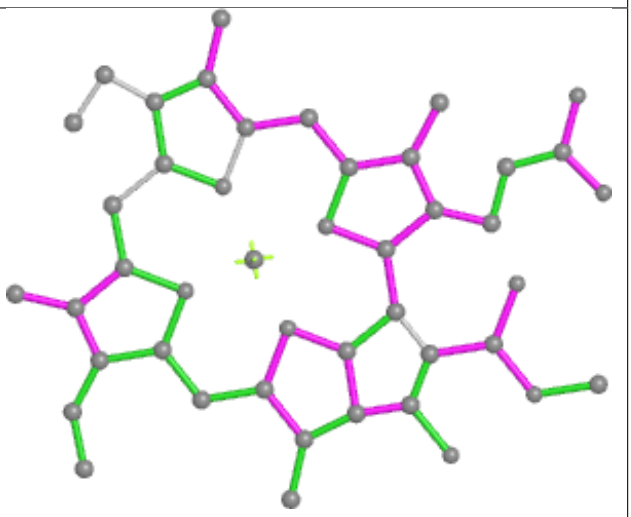

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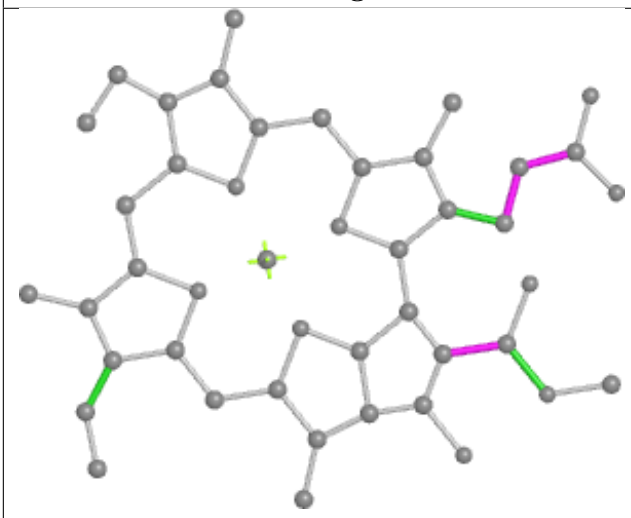

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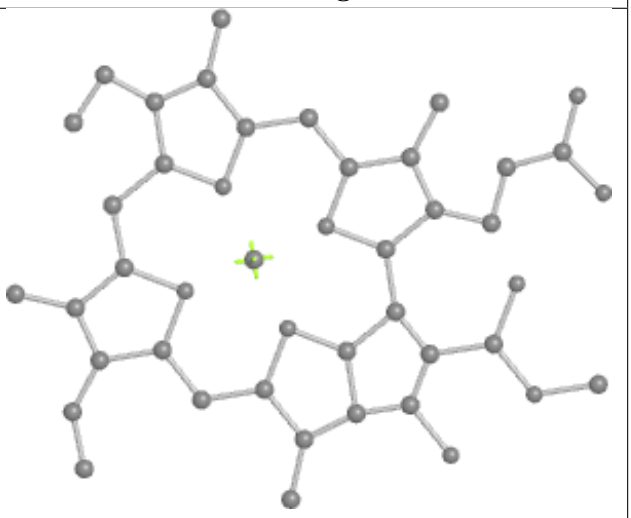
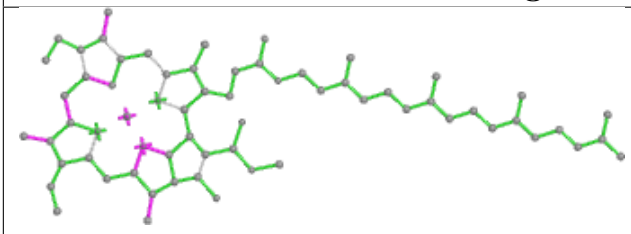


Rings

Ligand CLA C 502



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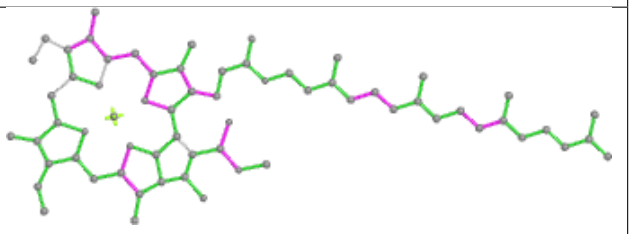

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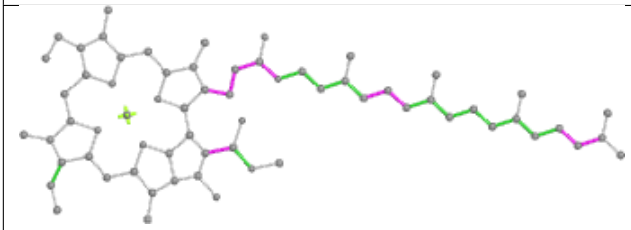

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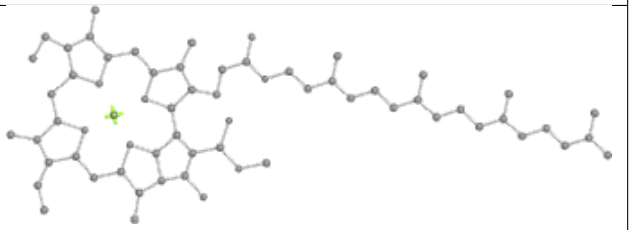
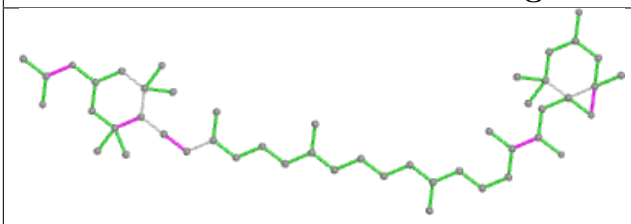


Rings

Ligand A86 12 302



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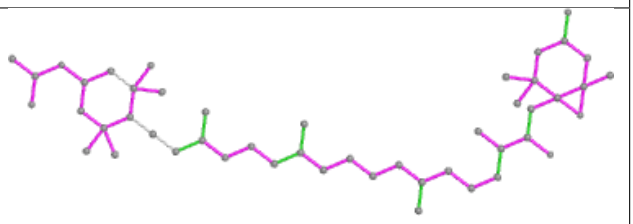

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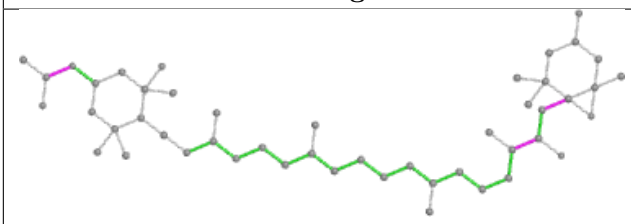

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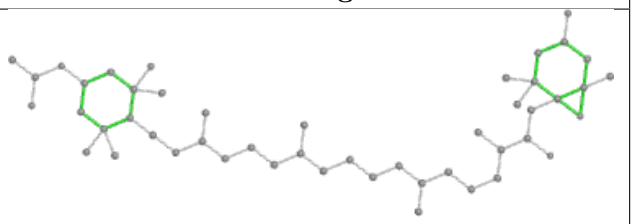

Rings

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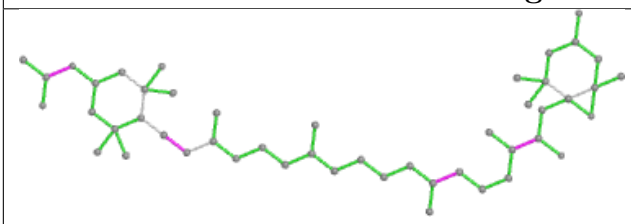

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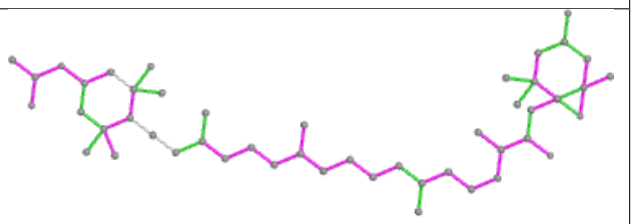

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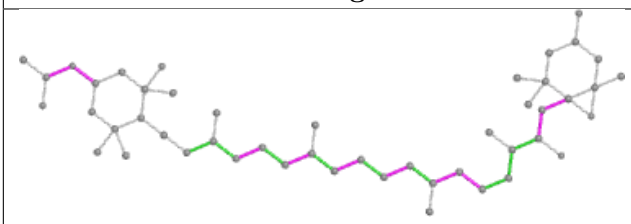

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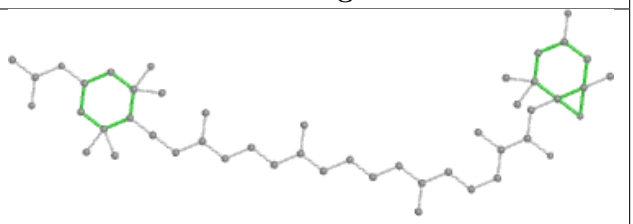
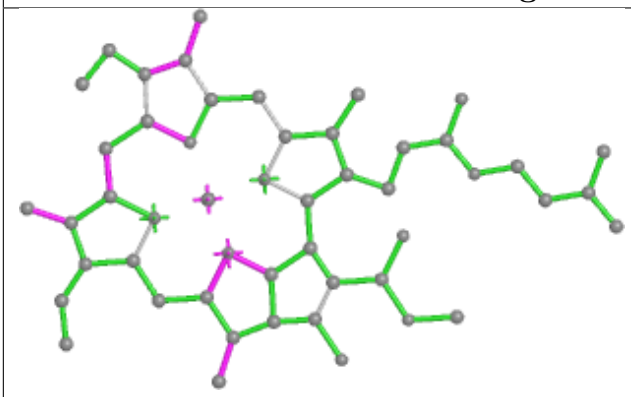


Rings

Ligand CLA 18 306



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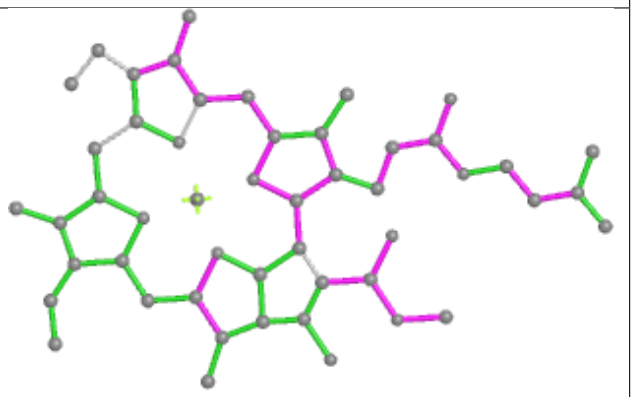

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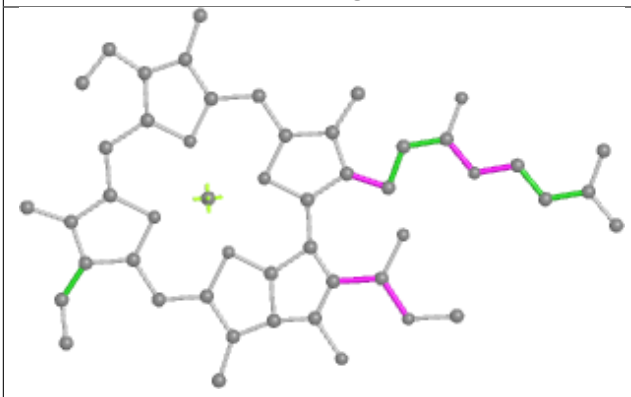

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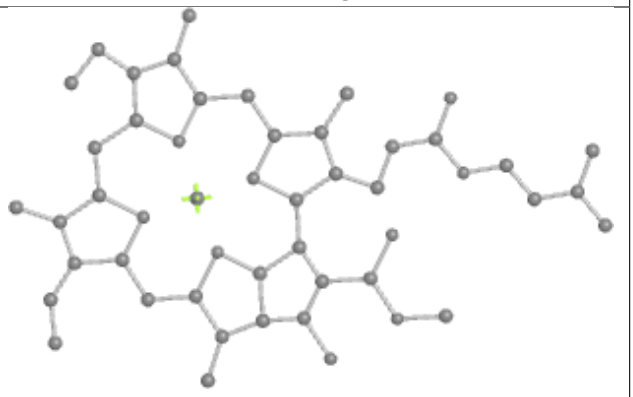
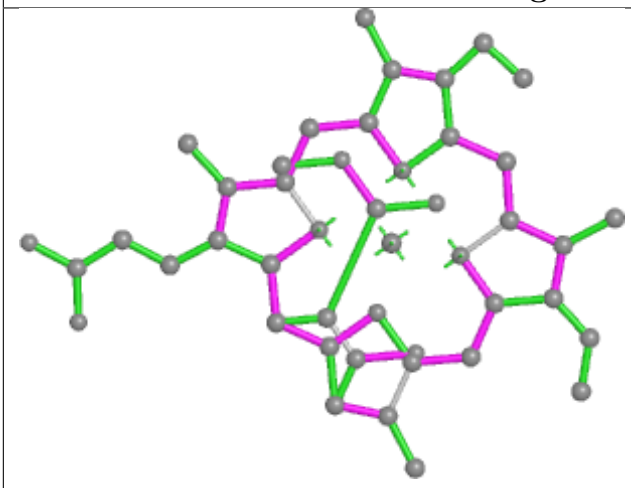


Rings

Ligand KC1 3 314



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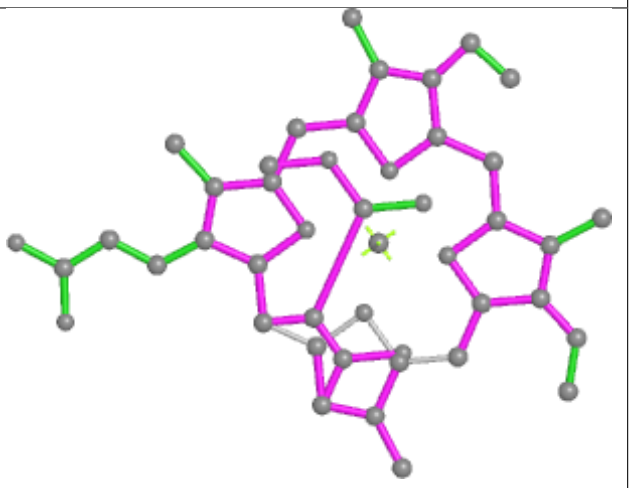

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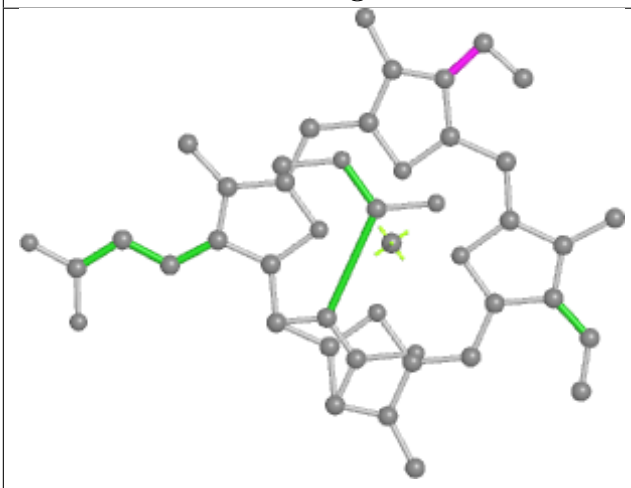

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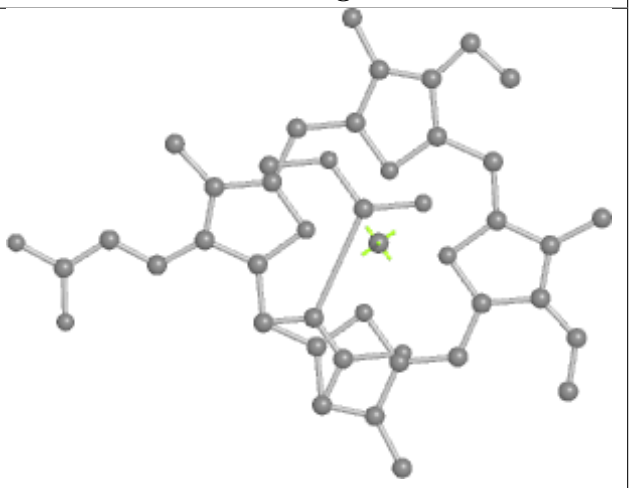
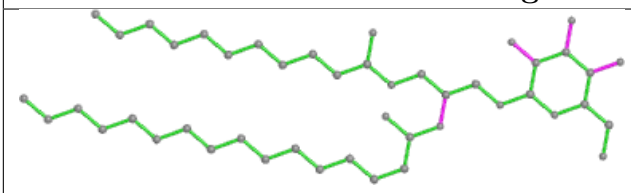


Rings

Ligand LMG F 102



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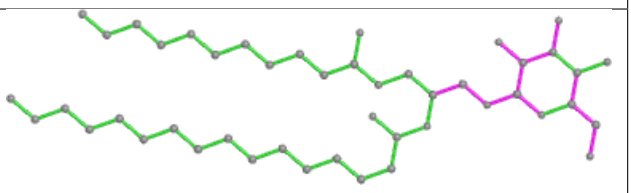

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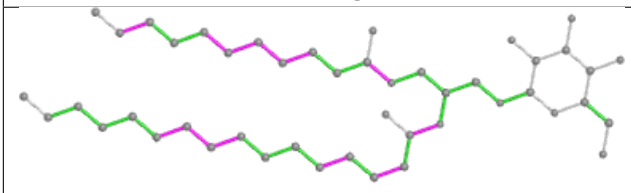

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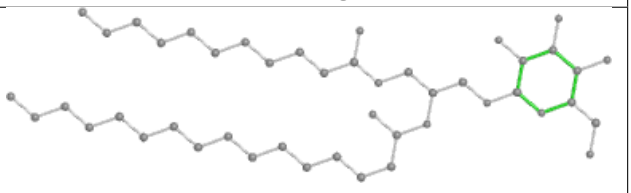
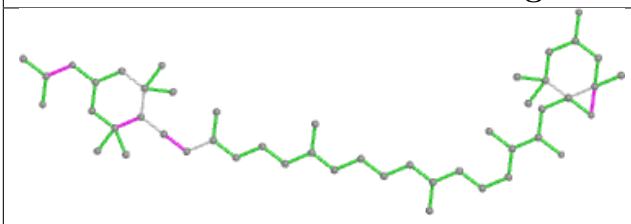


Rings

Ligand A86 18 302



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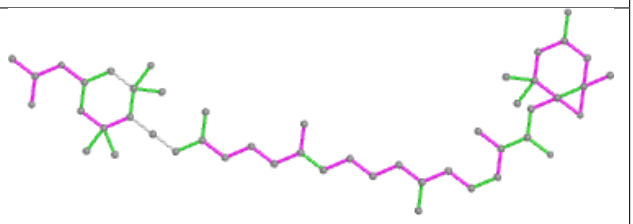

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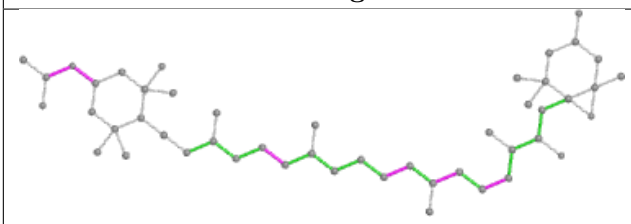

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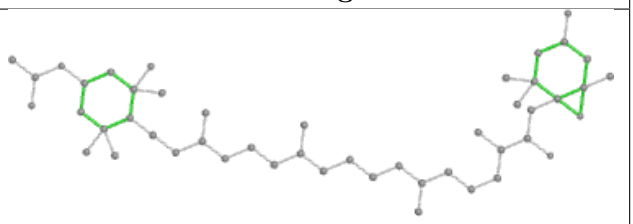
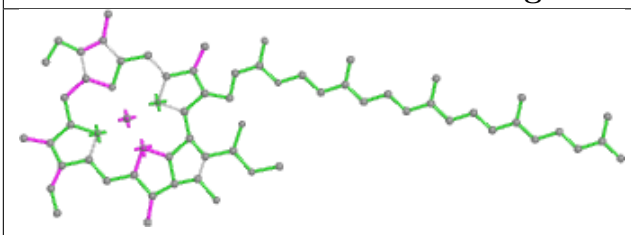


Rings

Ligand CLA B 604



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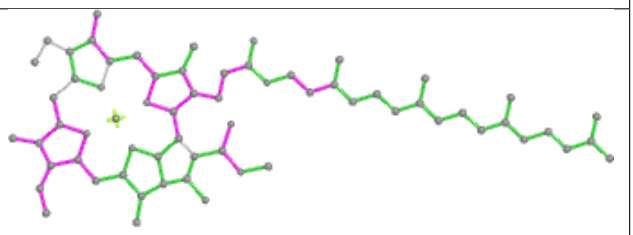

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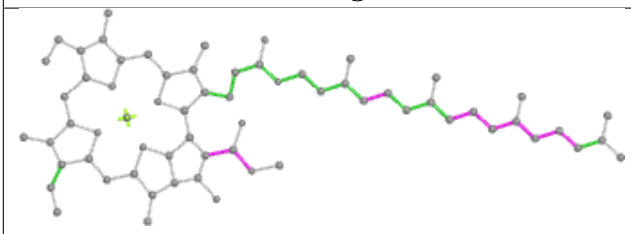

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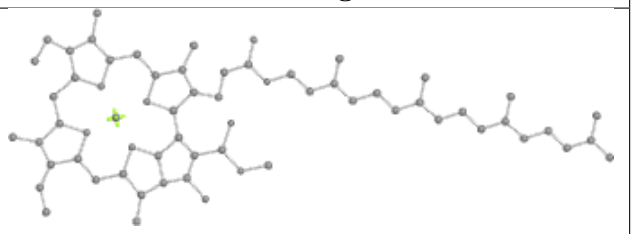
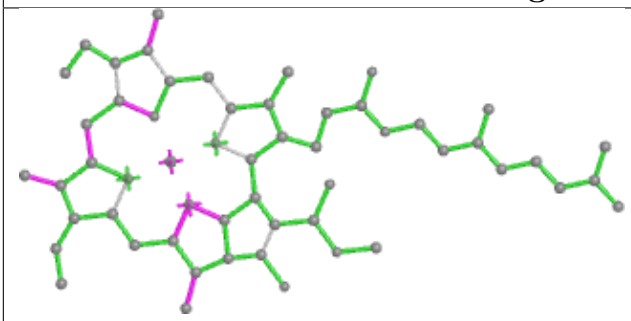


Rings

Ligand CLA 0 311



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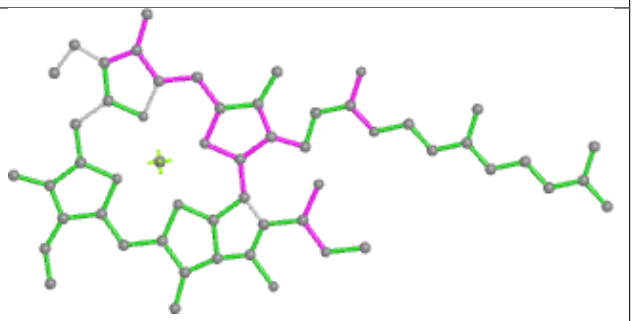

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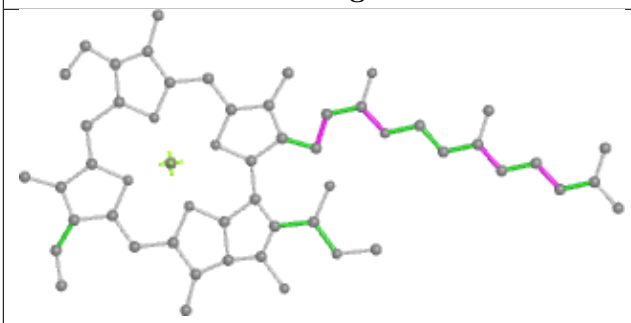

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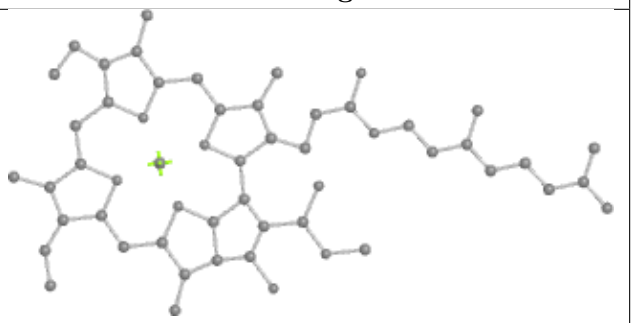
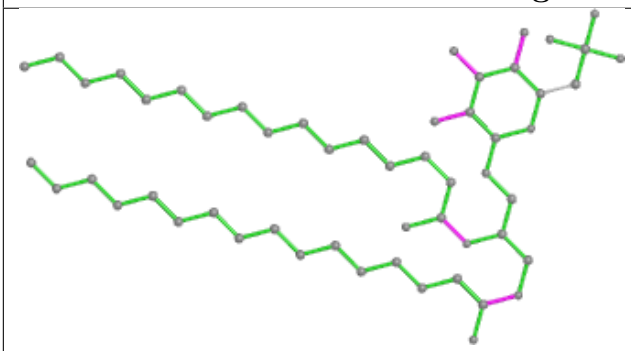


Rings

Ligand SQD l 101



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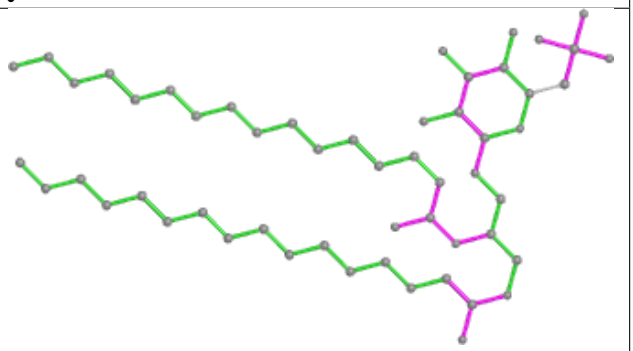
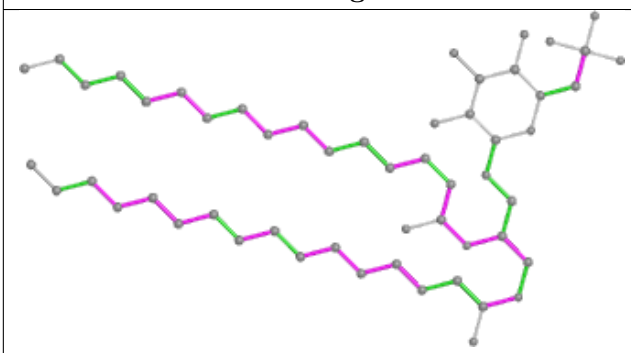


Bond angles



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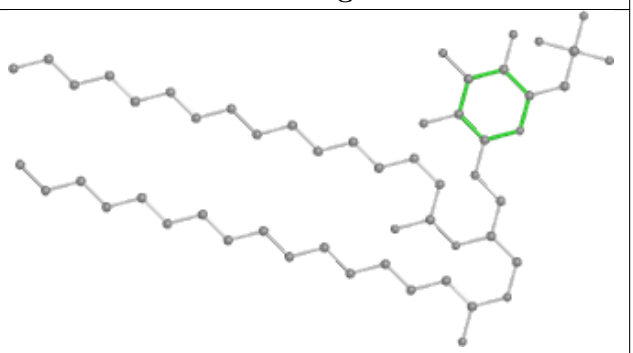
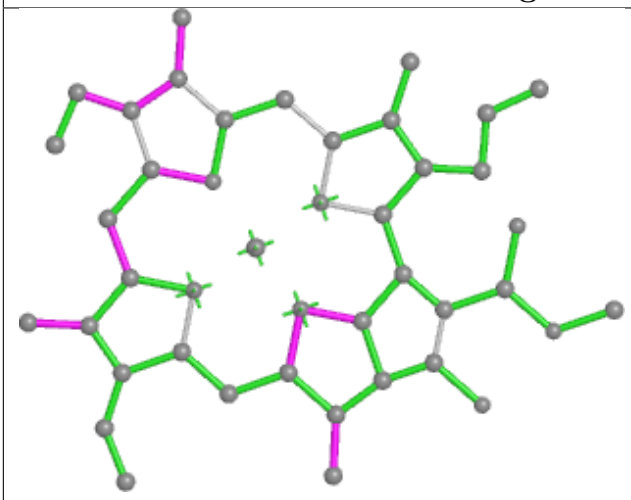
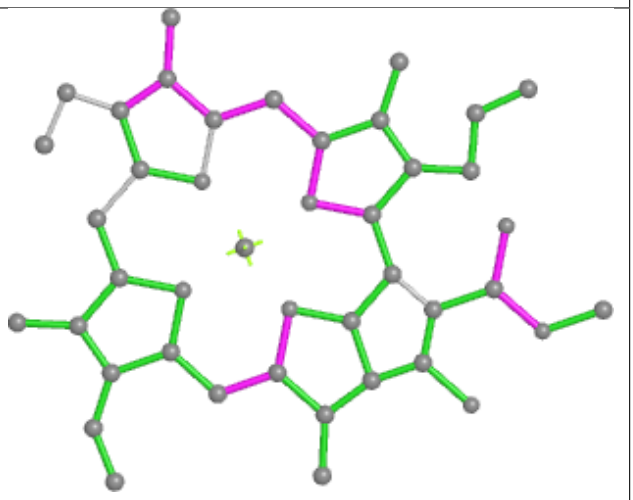


Rings

Ligand CLA 14 314



Bond lengths



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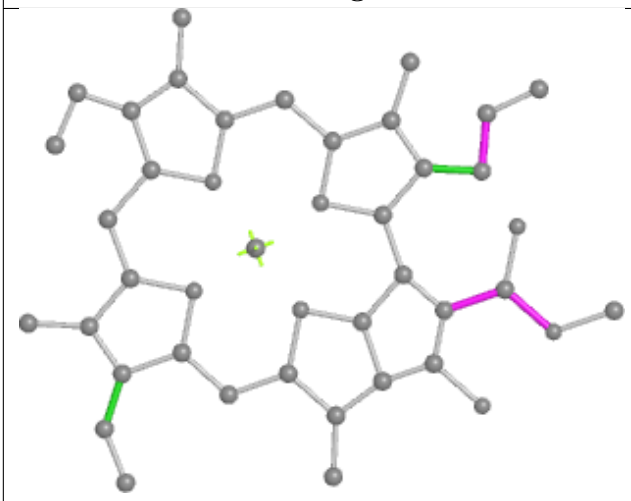

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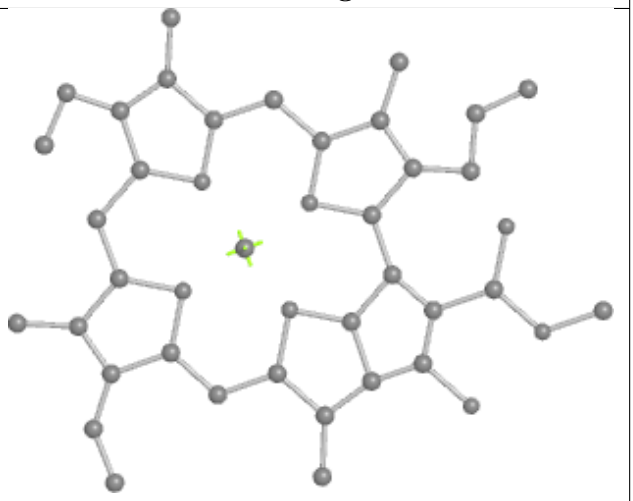
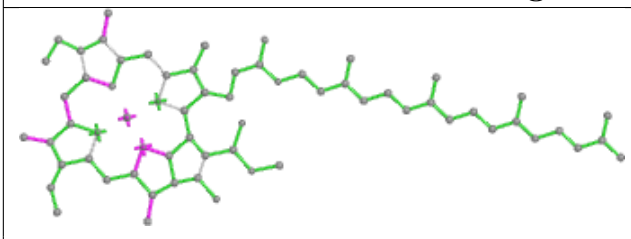


Rings

Ligand CLA b 614



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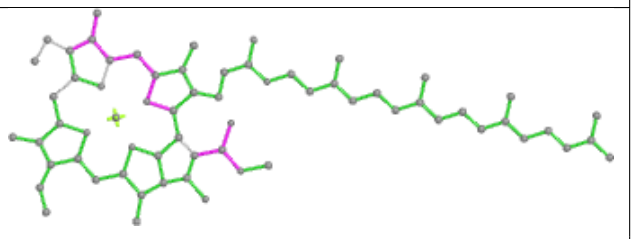

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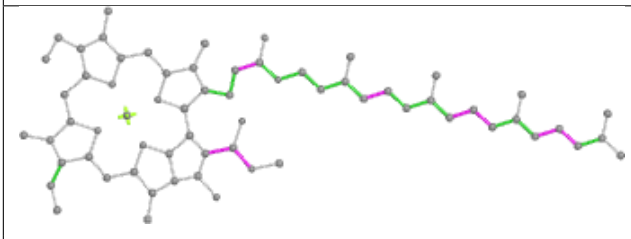

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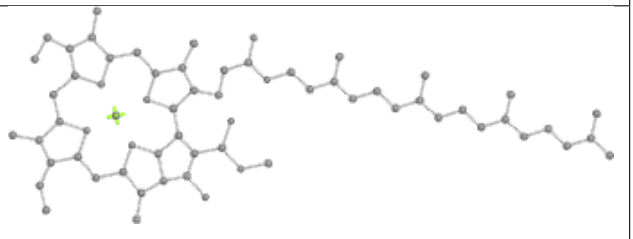
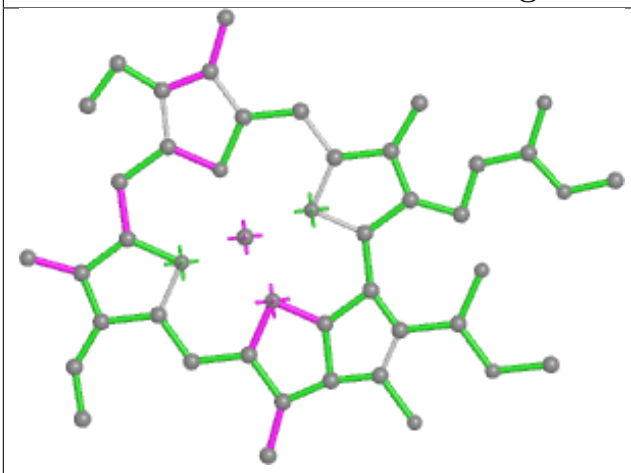


Rings

Ligand CLA 11 312



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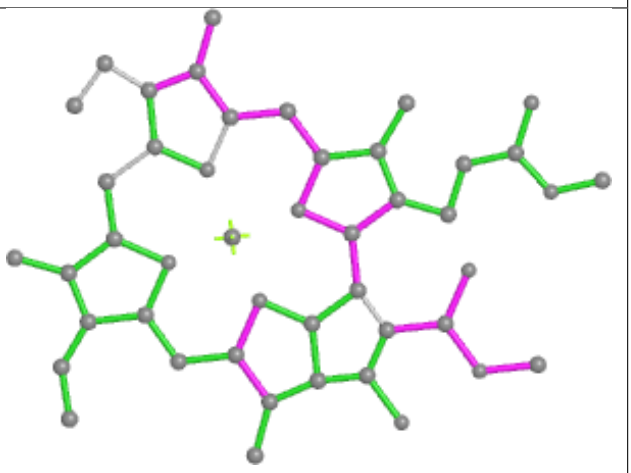

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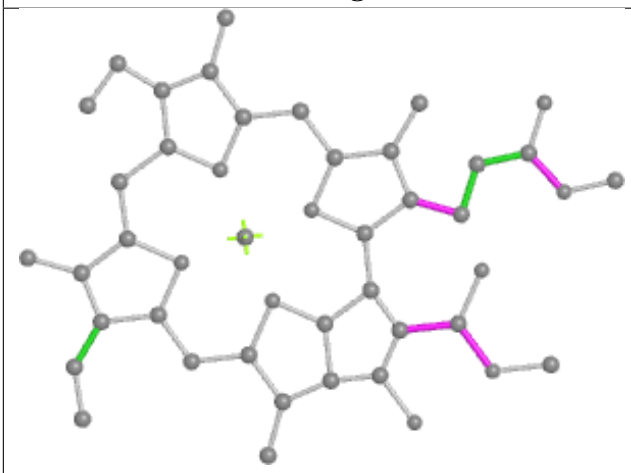

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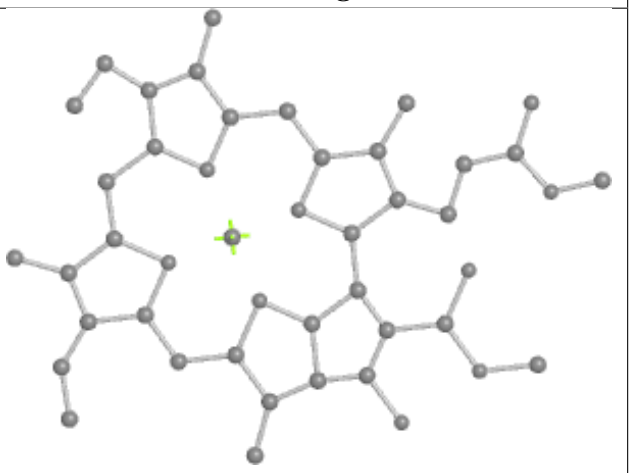
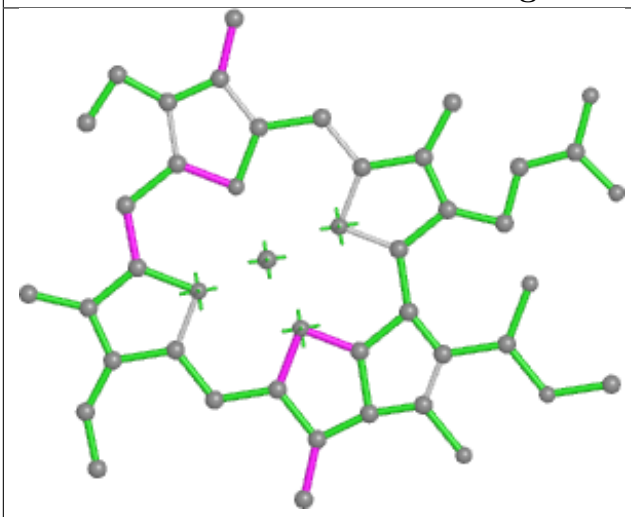


Rings

Ligand CLA 13 312



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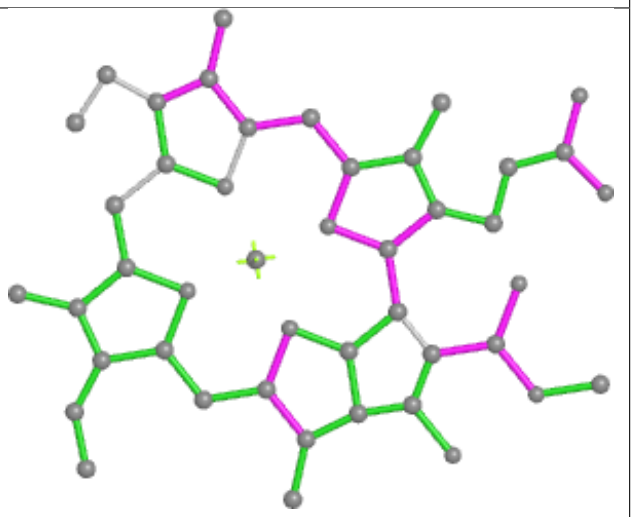

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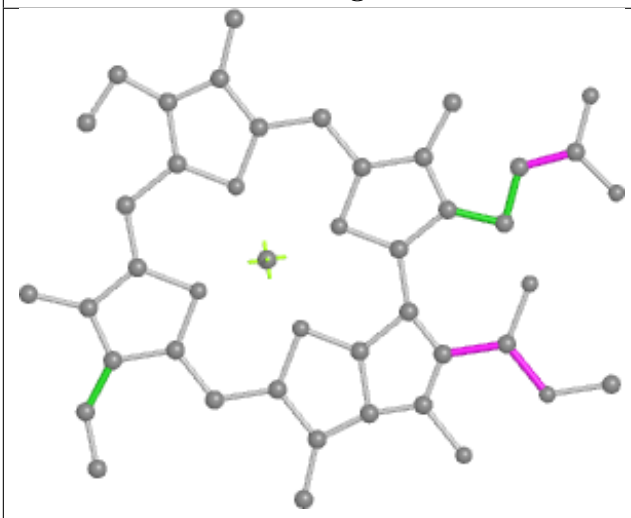

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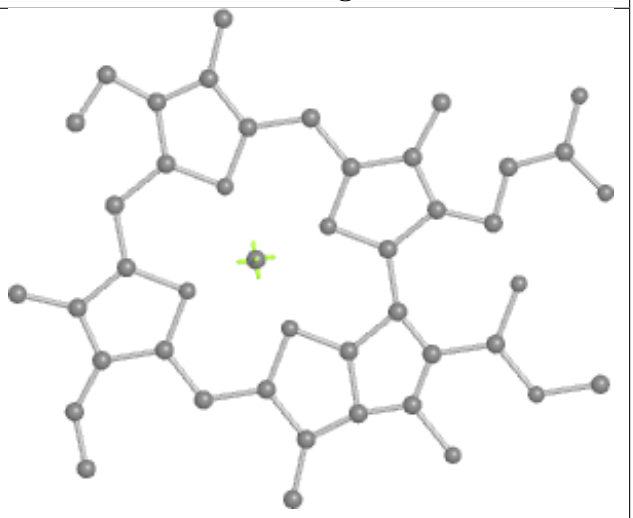
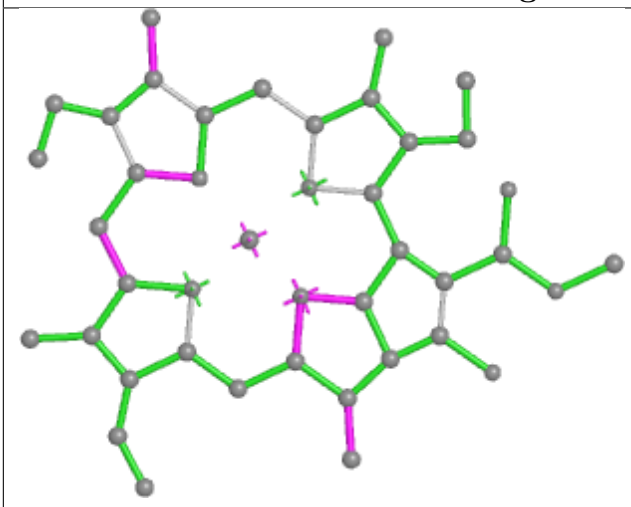


Rings

Ligand CLA 12 307



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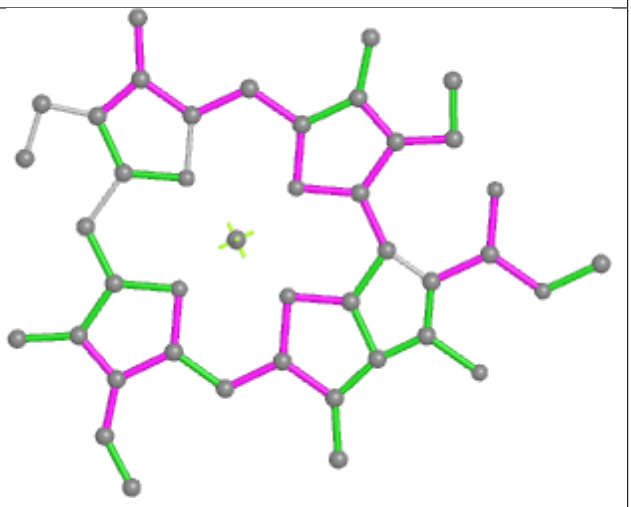

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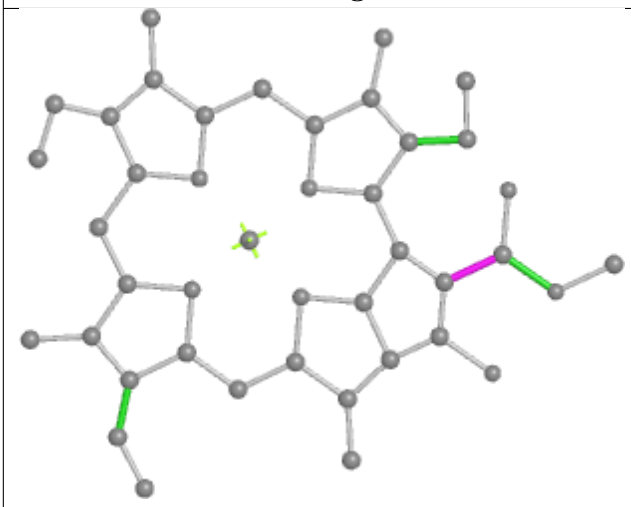

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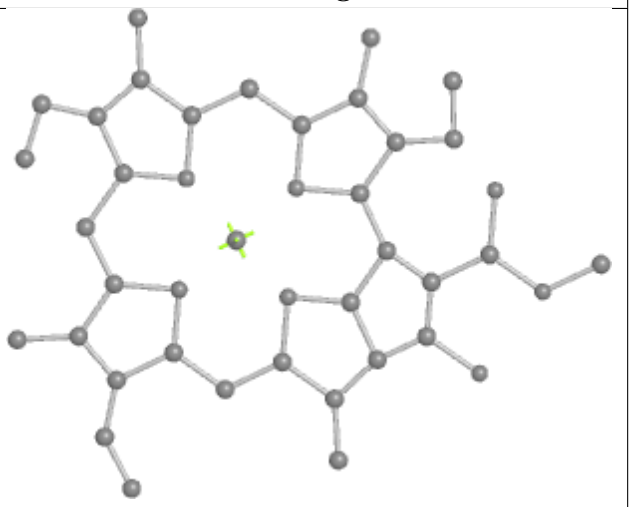
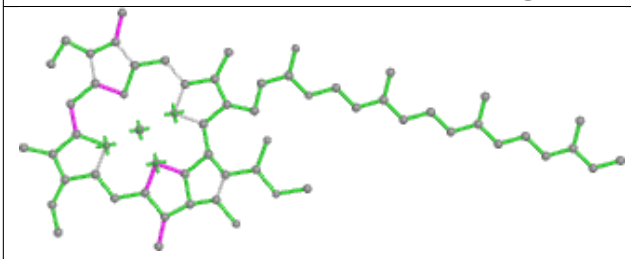


Rings

Ligand CLA 19 307



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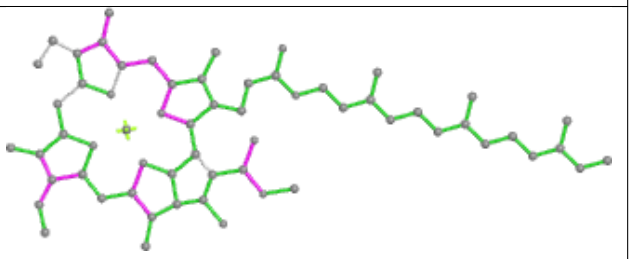

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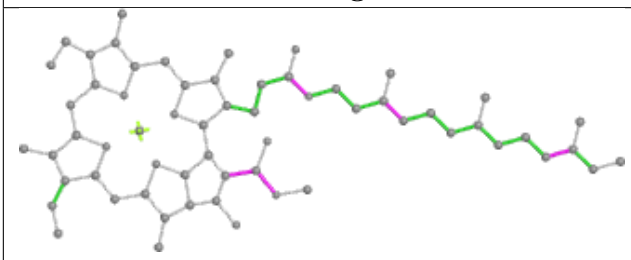

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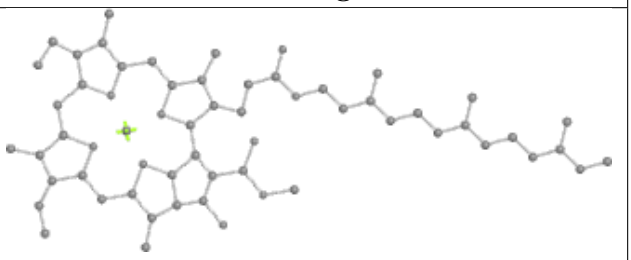
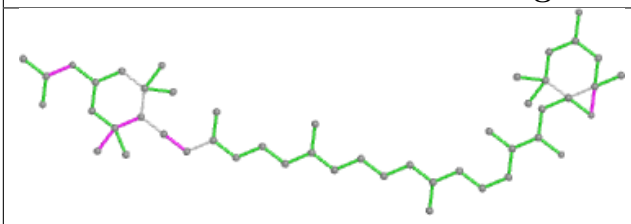


Rings

Ligand A86 5 304



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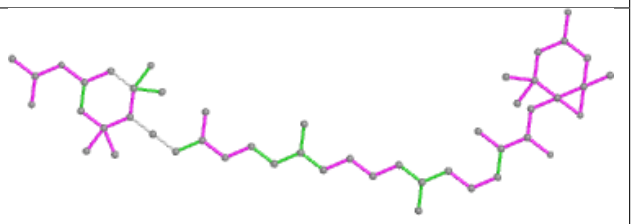

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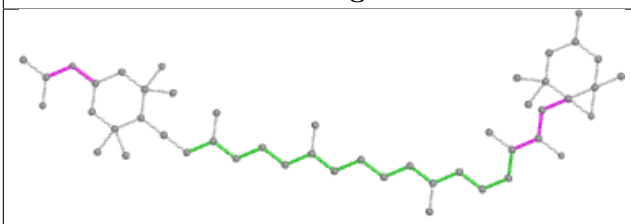

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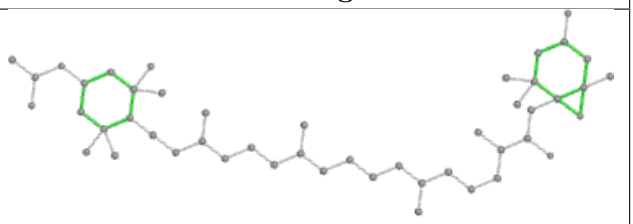
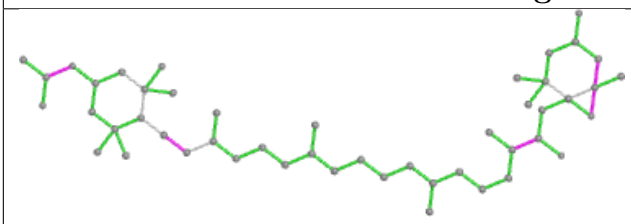


Rings

Ligand A86 6 303



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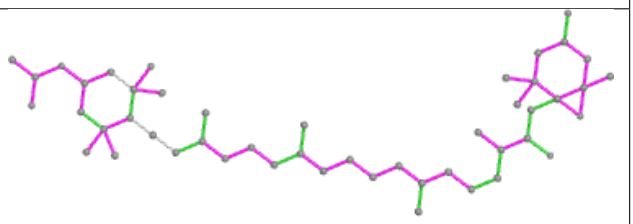

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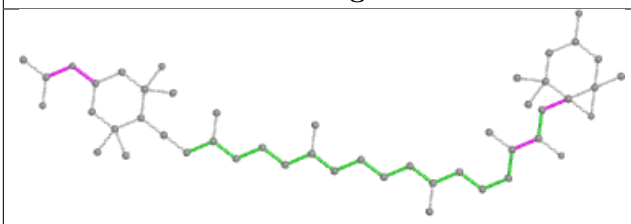

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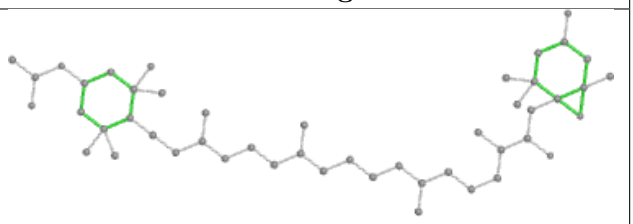
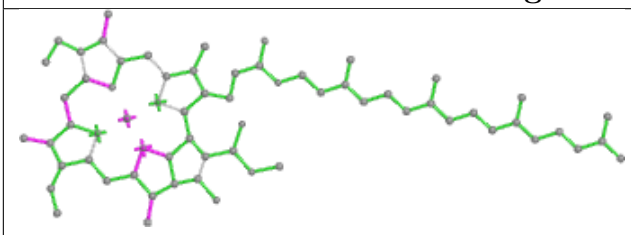


Rings

Ligand CLA C 506



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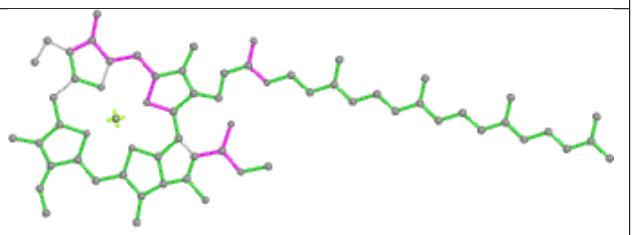

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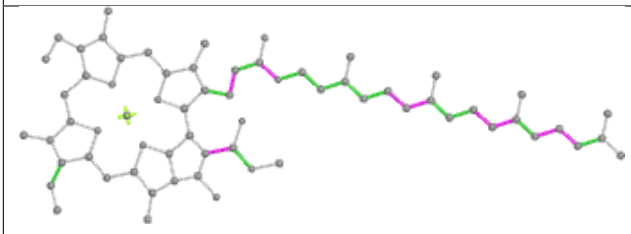

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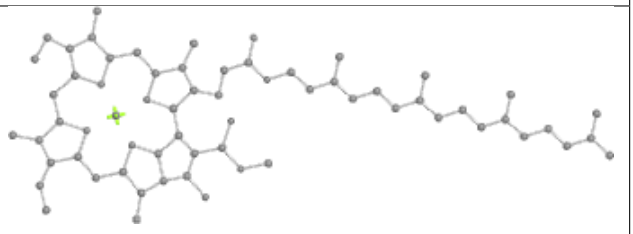
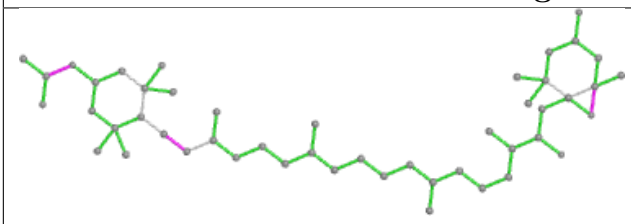


Rings

Ligand A86 3 306



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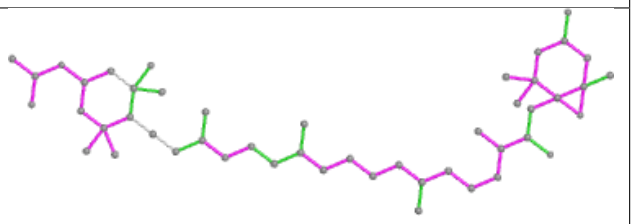

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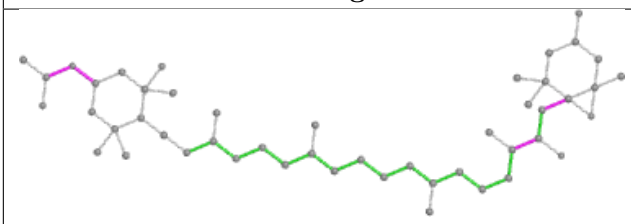

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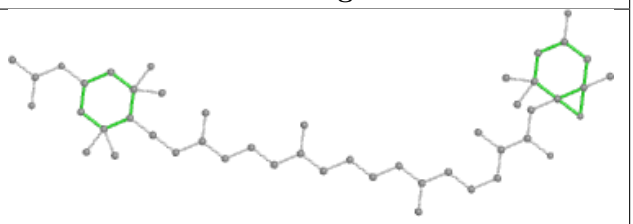
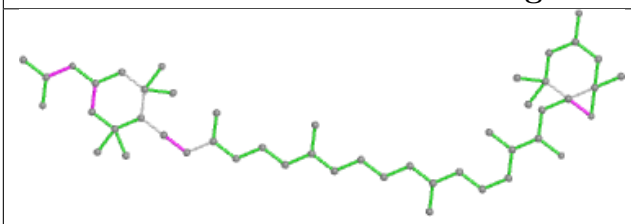


Rings

Ligand A86 19 301



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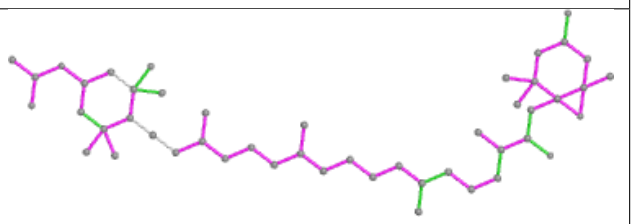

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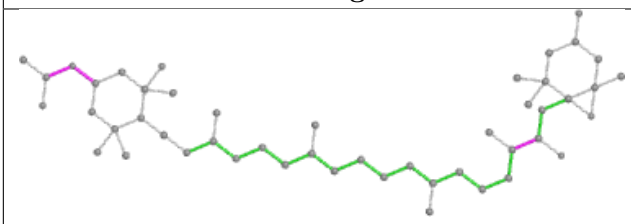

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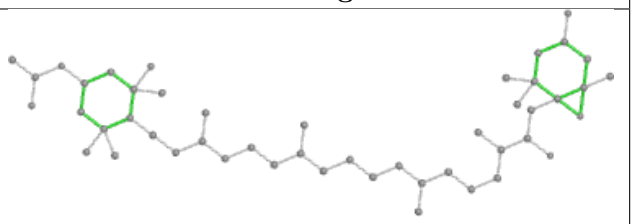
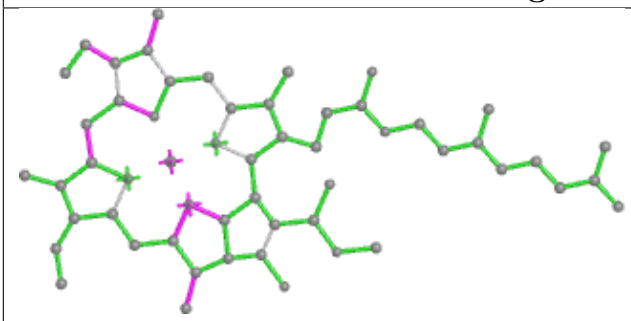


Rings

Ligand CLA 5 309



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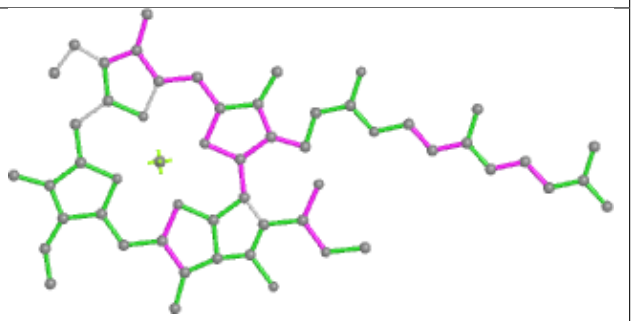

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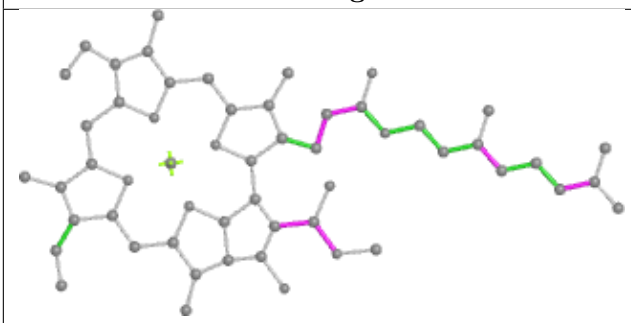

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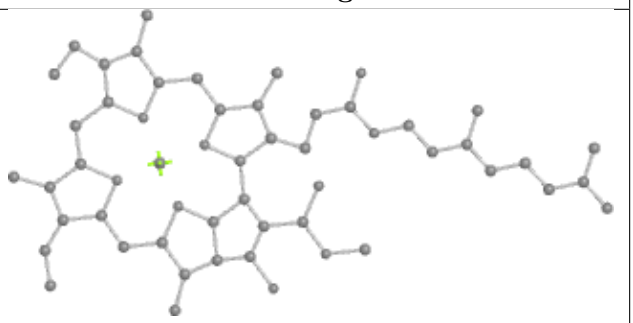
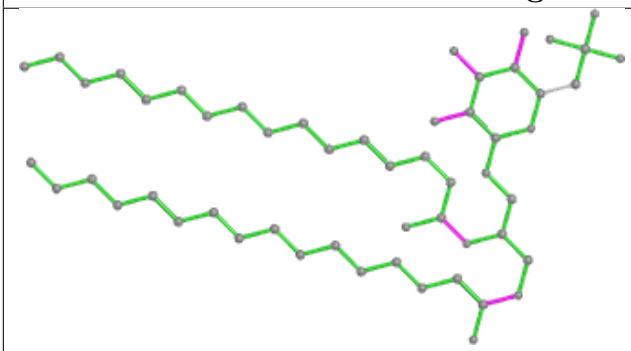


Rings

Ligand SQD L 102



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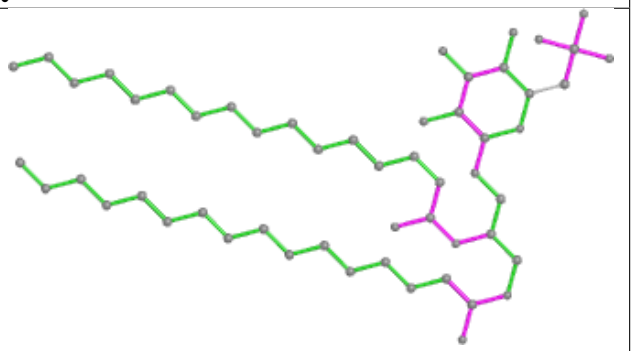

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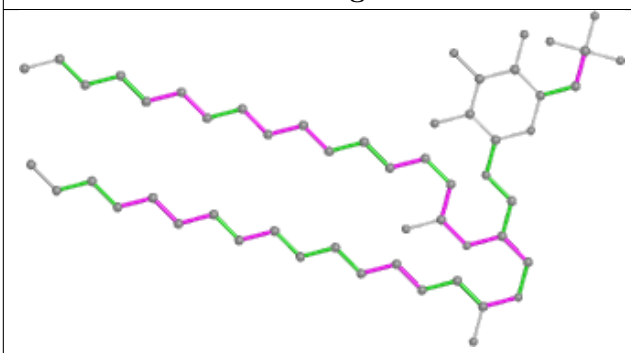

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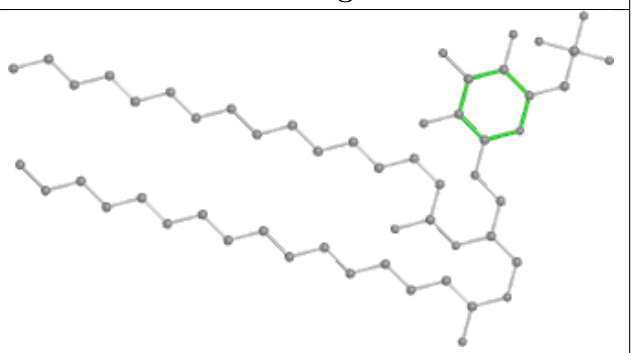
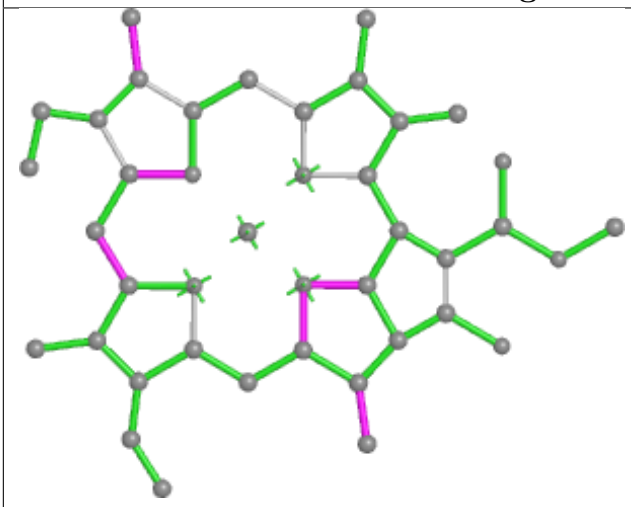


Rings

Ligand CLA 15 313



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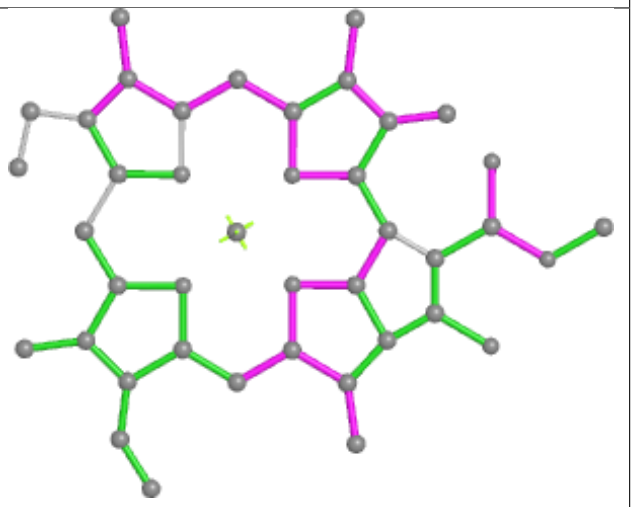

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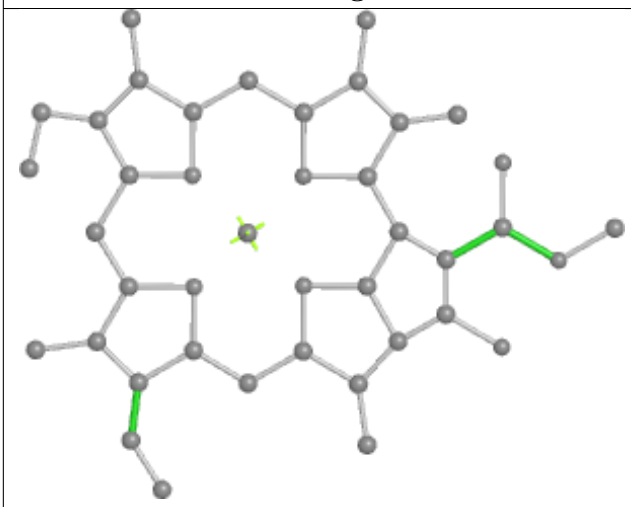

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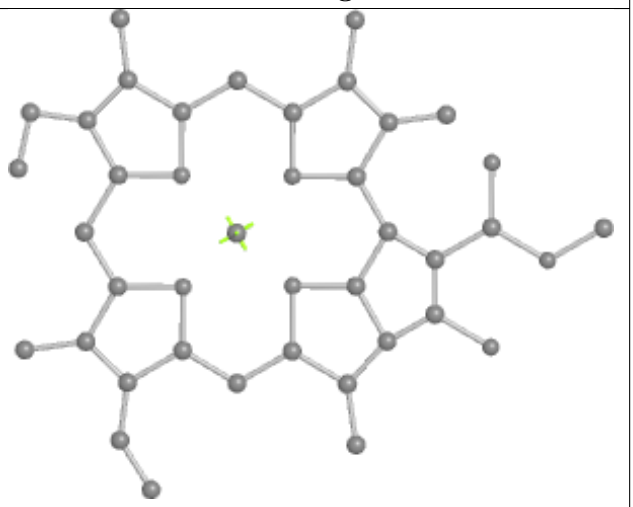
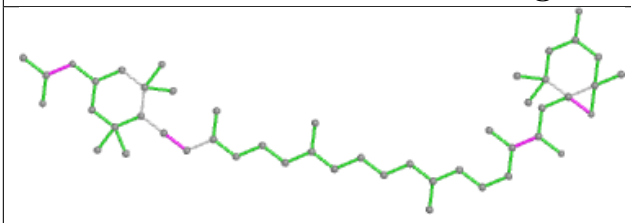


Rings

Ligand A86 9 304



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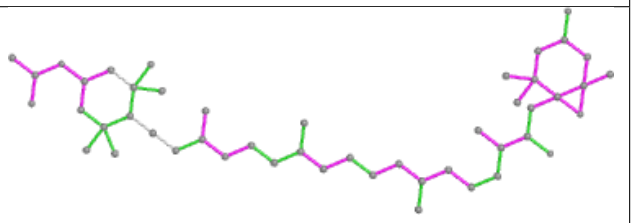

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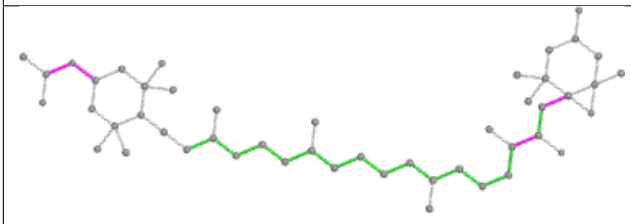
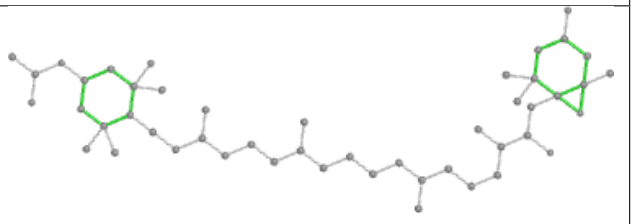
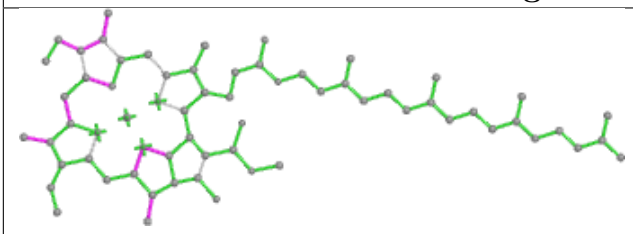


Torsions



Rings

Ligand CLA D 405



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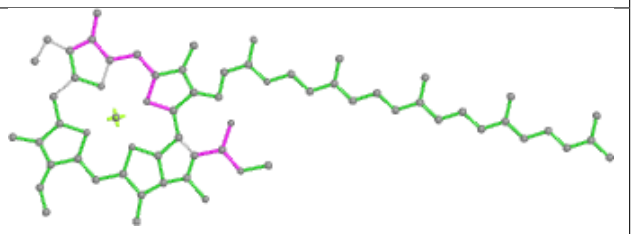

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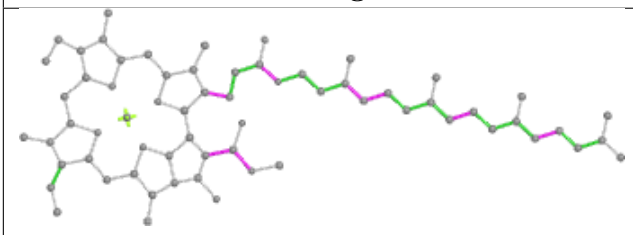

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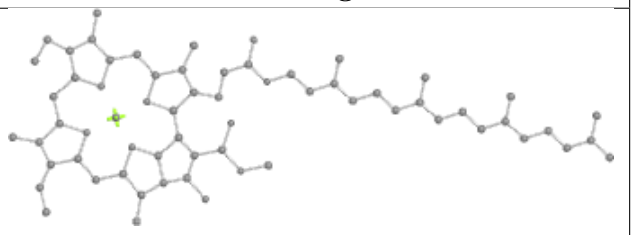
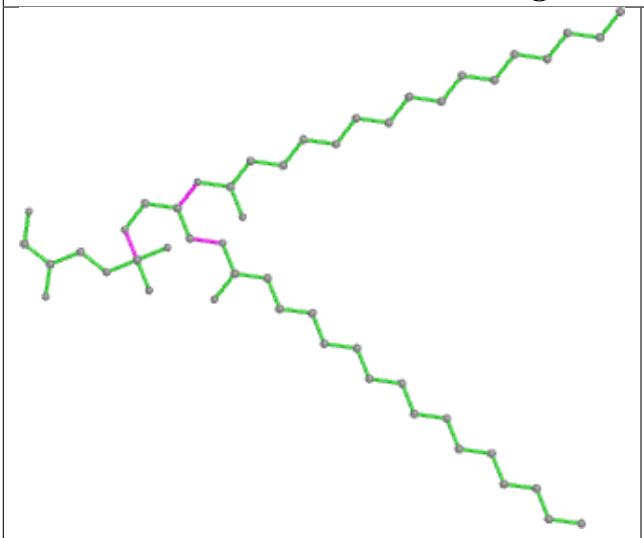


Rings

Ligand LHG l 102



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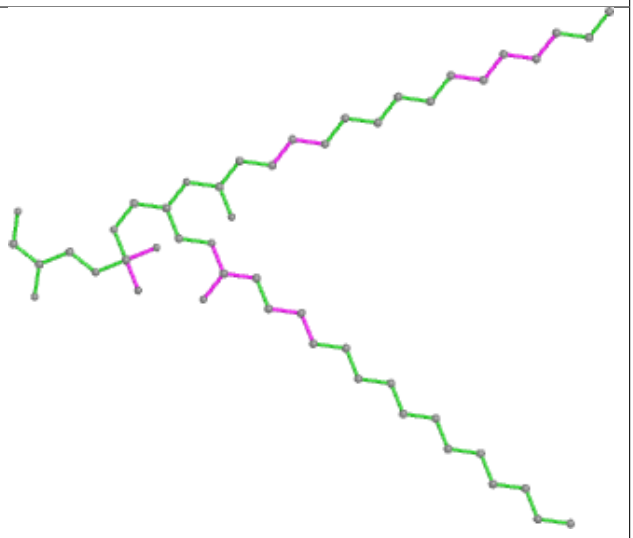

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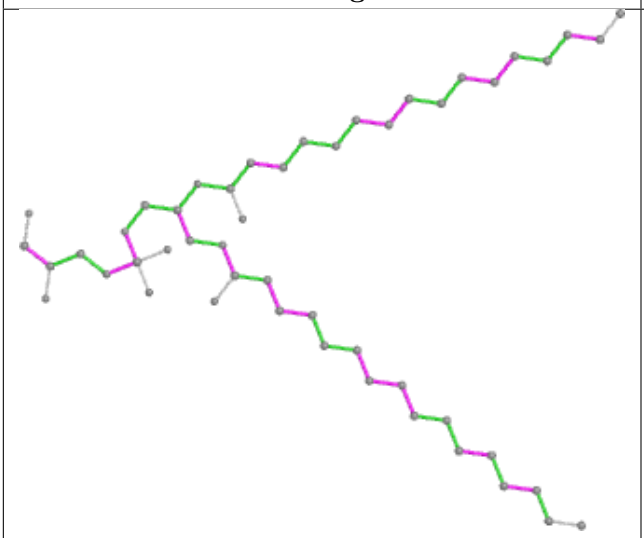

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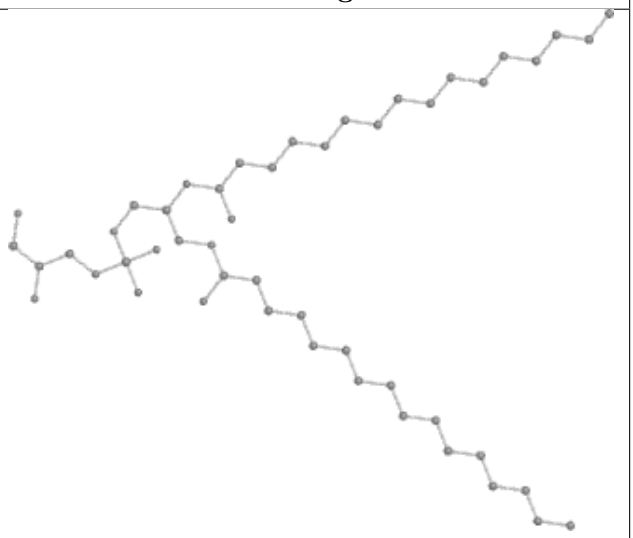
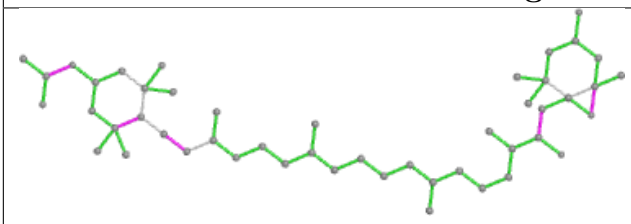


Rings

Ligand A86 15 305



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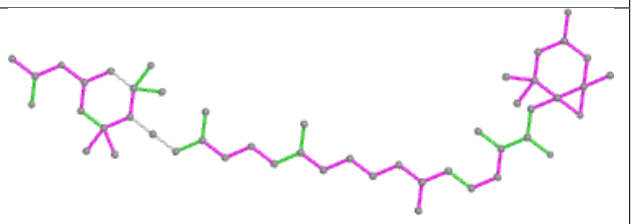

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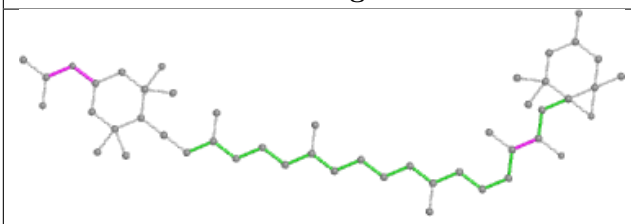

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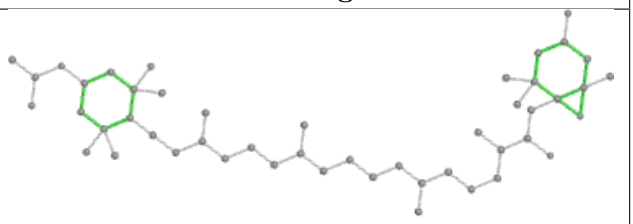
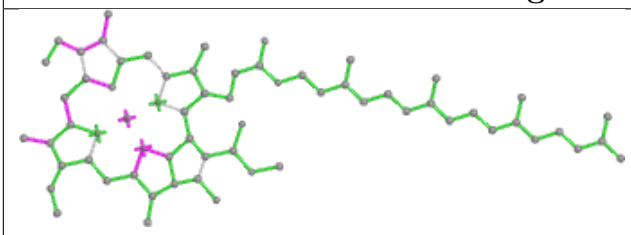


Rings

Ligand CLA p 602



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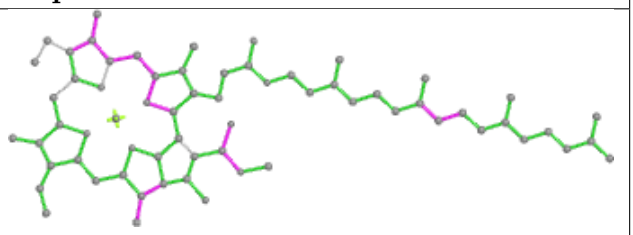

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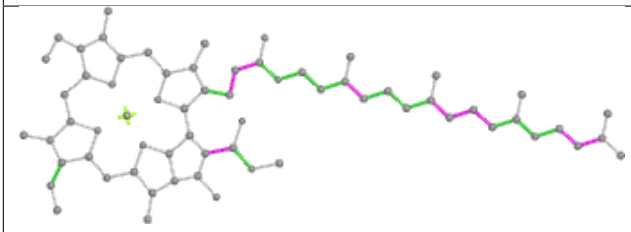

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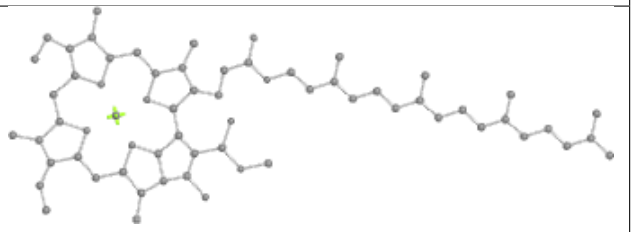
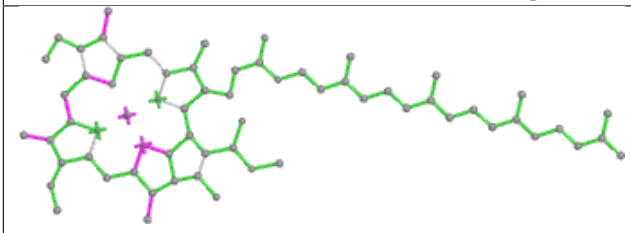


Rings

Ligand CLA C 504



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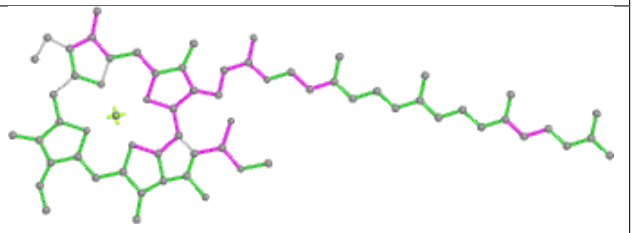

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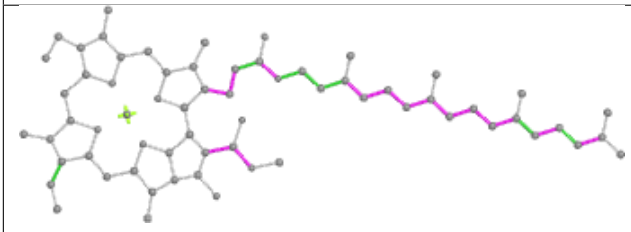

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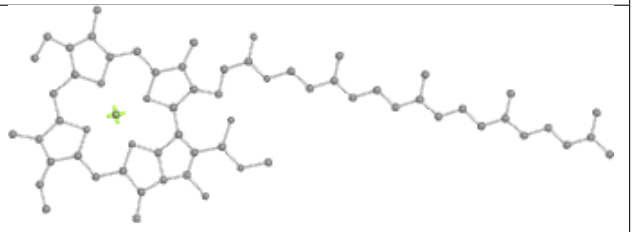
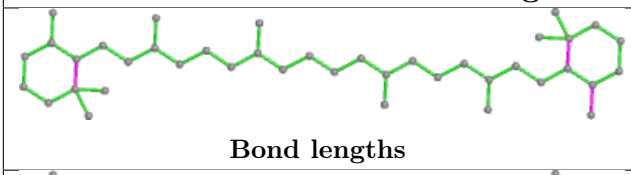


Rings

Ligand BCR A 407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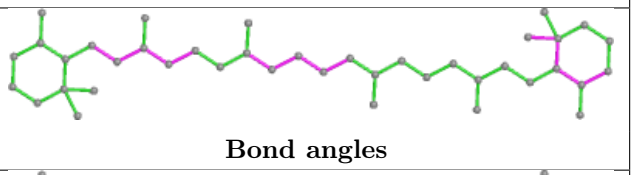
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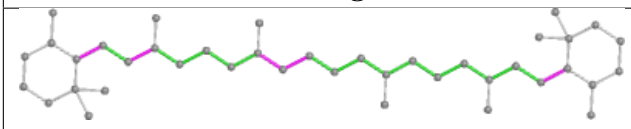
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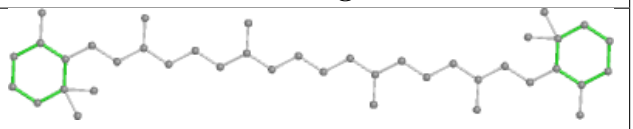
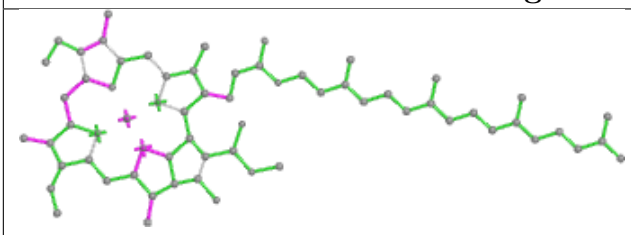

Rings

Ligand CLA B 602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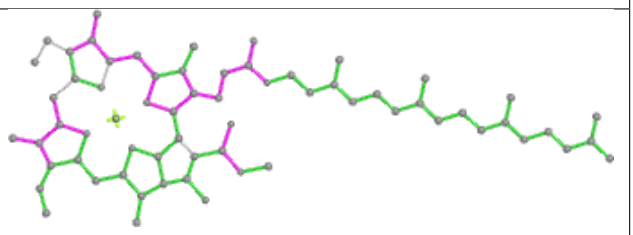
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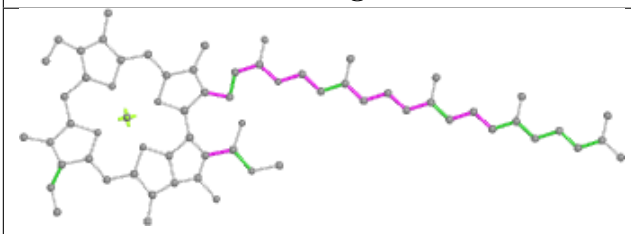
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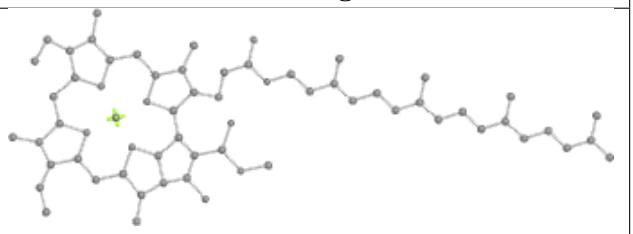
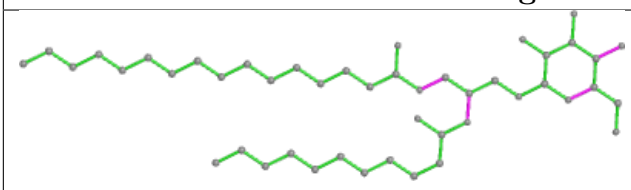

Rings

Ligand LMG K 101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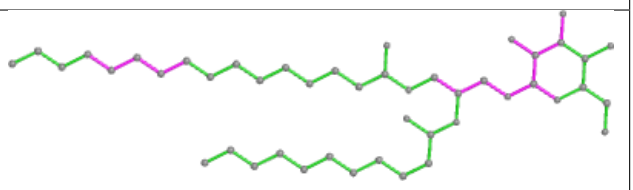
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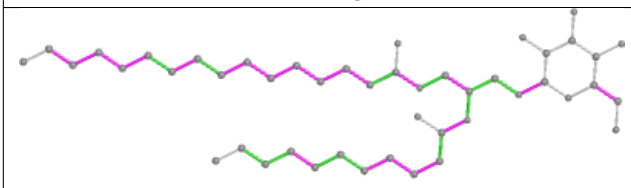
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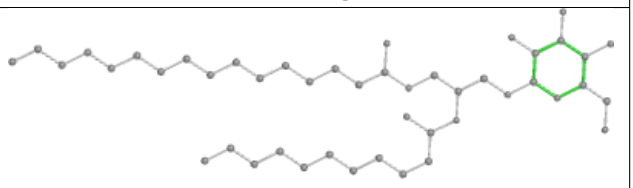
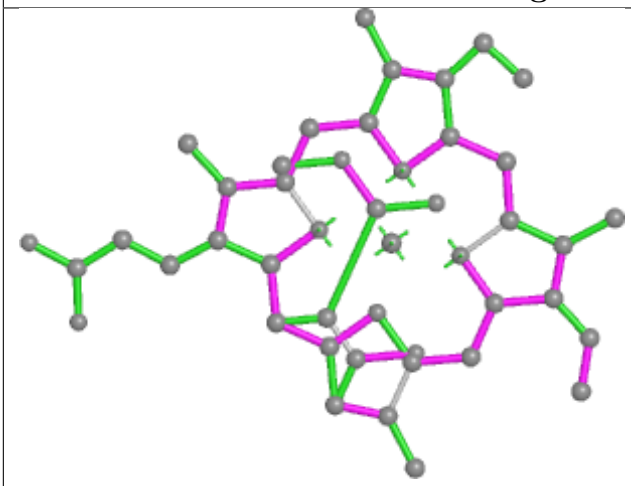

Rings

Ligand KC2 7 309



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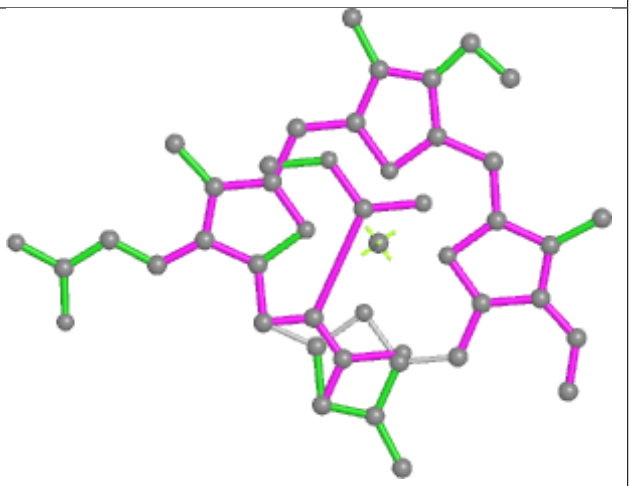

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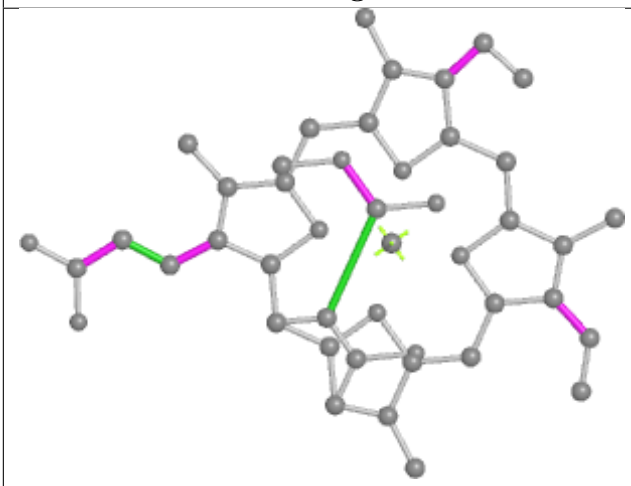

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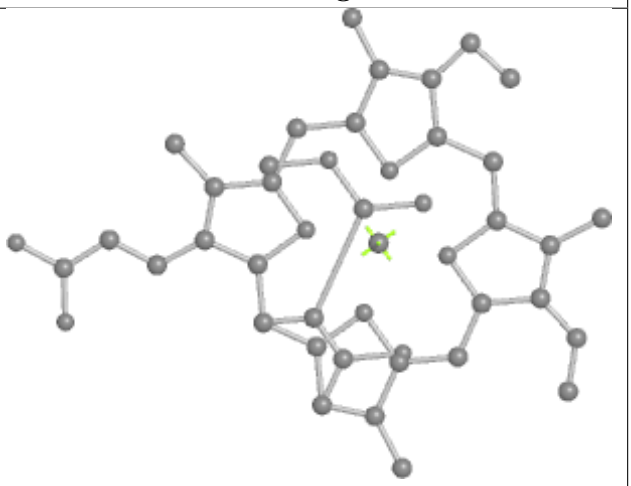
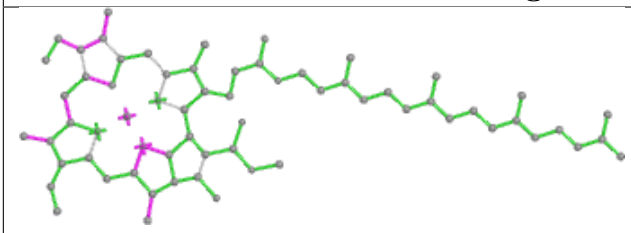


Rings

Ligand CLA P 602



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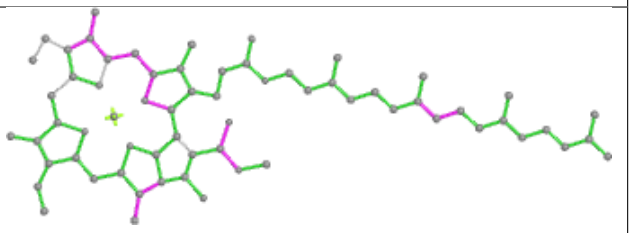

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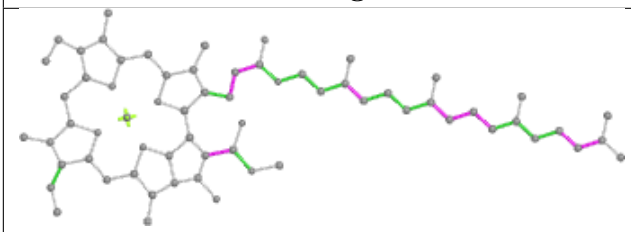

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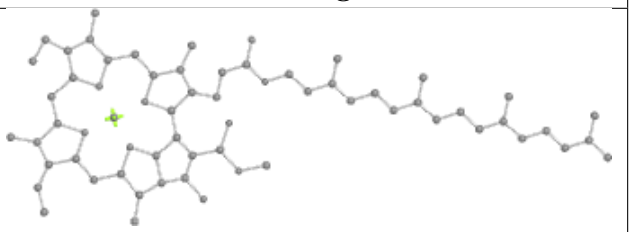
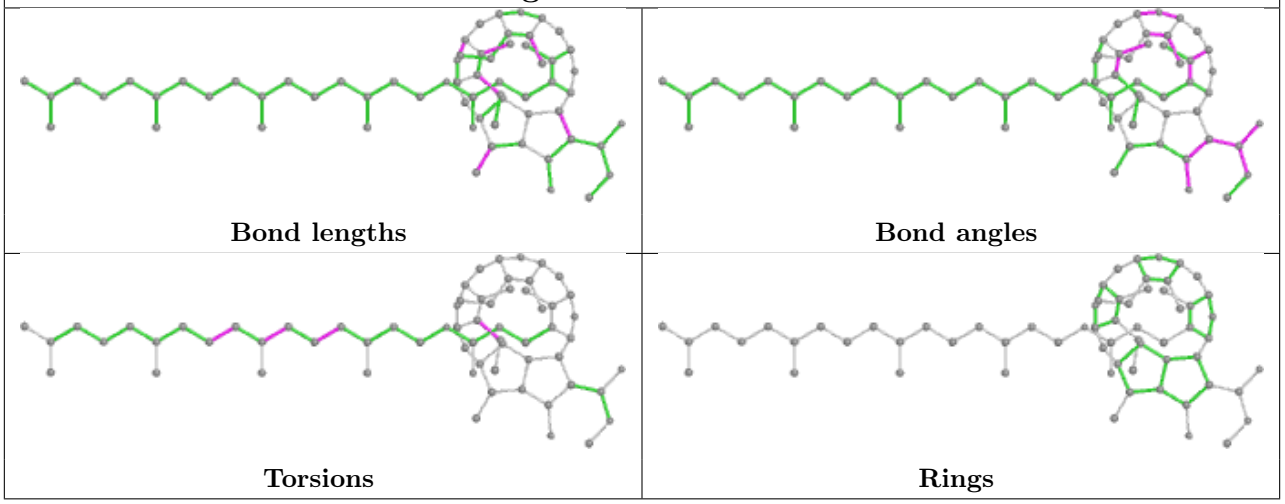
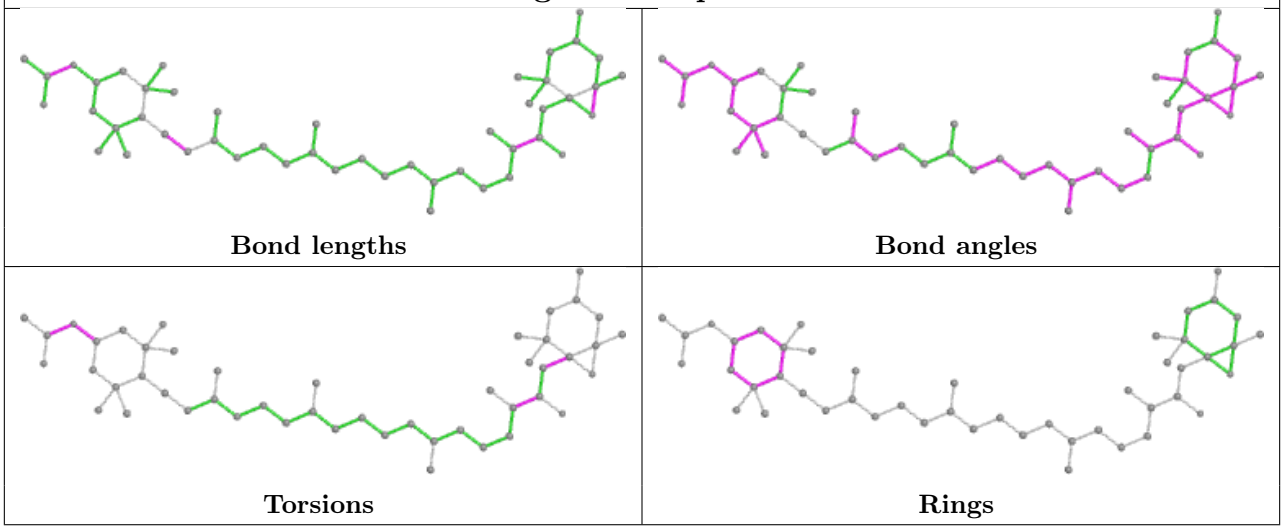


Rings

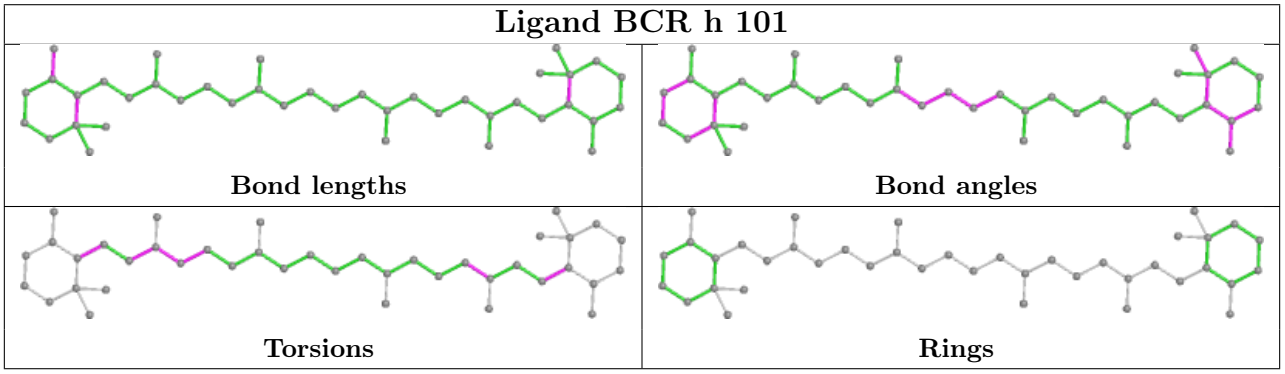
Ligand PHO D 402



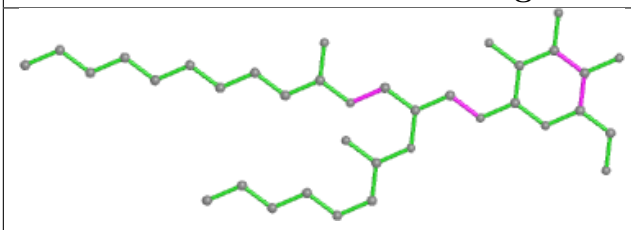
Ligand A86 p 613



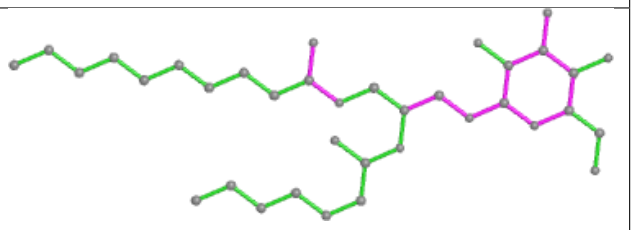
Ligand BCR h 101



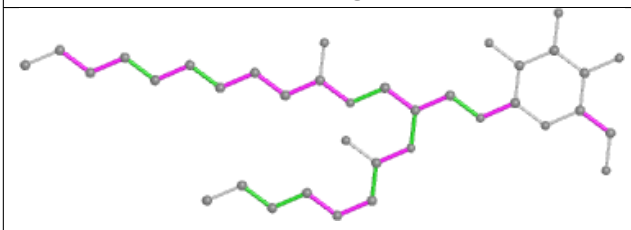
Ligand LMG 15 315



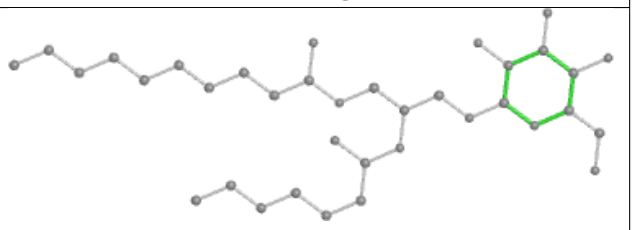
Bond lengths



Bond angles

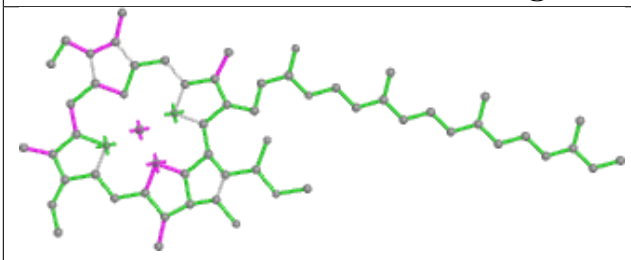


Torsions



Rings

Ligand CLA 8 307



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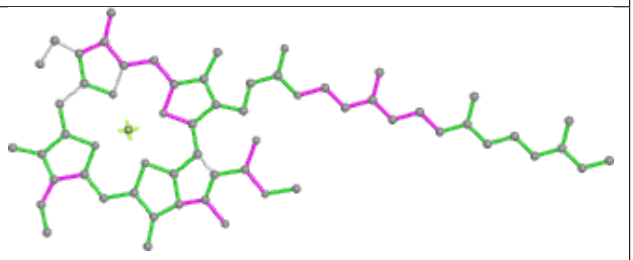
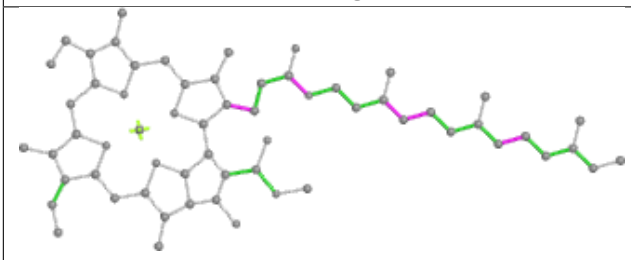


Bond angles



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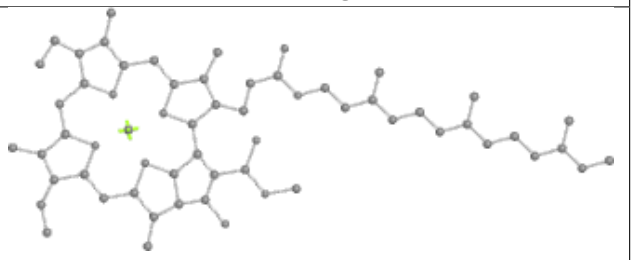
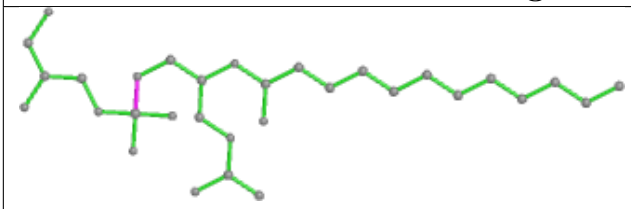
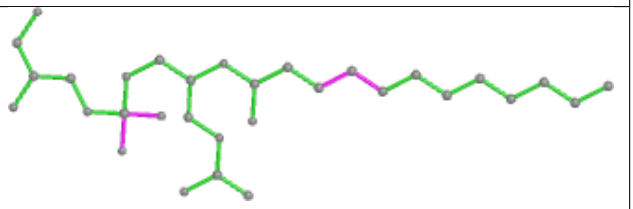


Rings

Ligand LHG 8 316



Bond lengths



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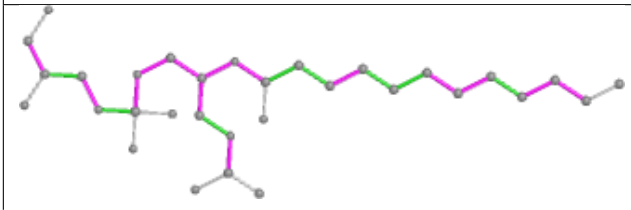

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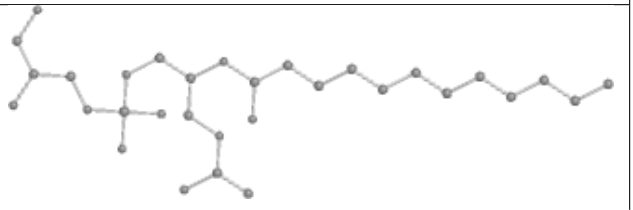
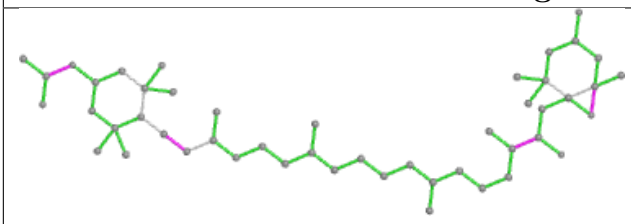


Rings

Ligand A86 4 304



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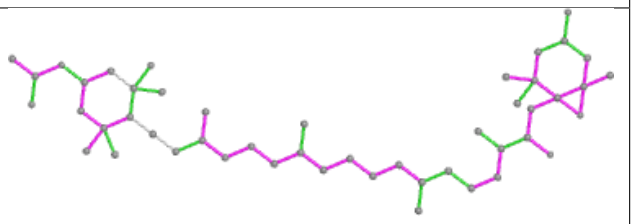

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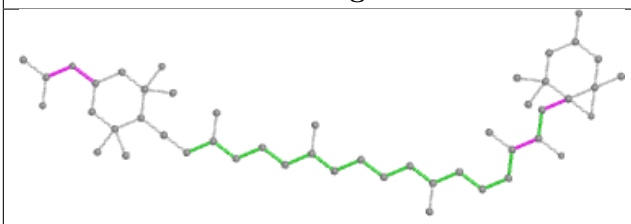

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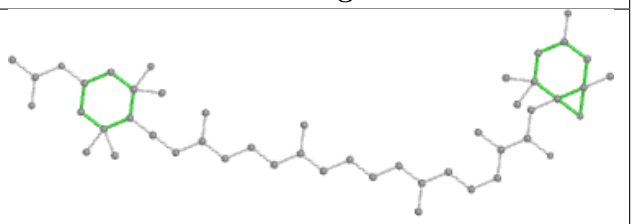
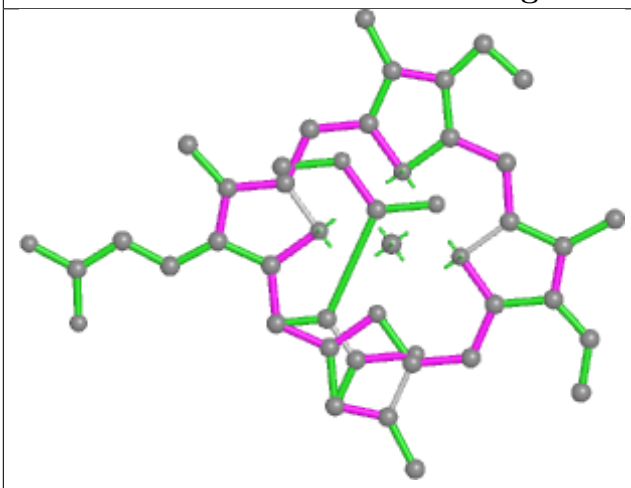


Rings

Ligand KC1 17 314



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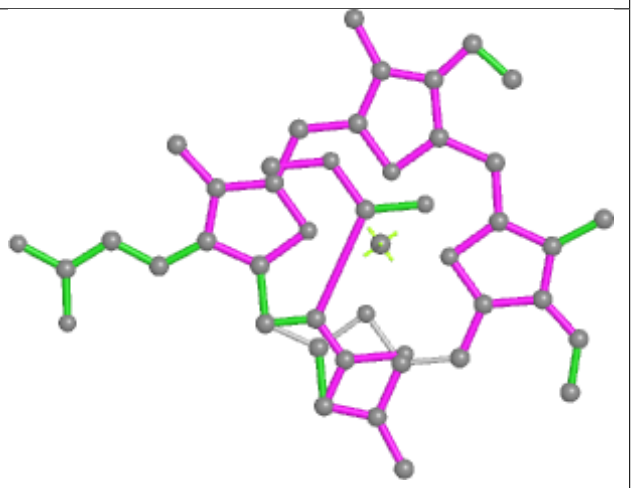

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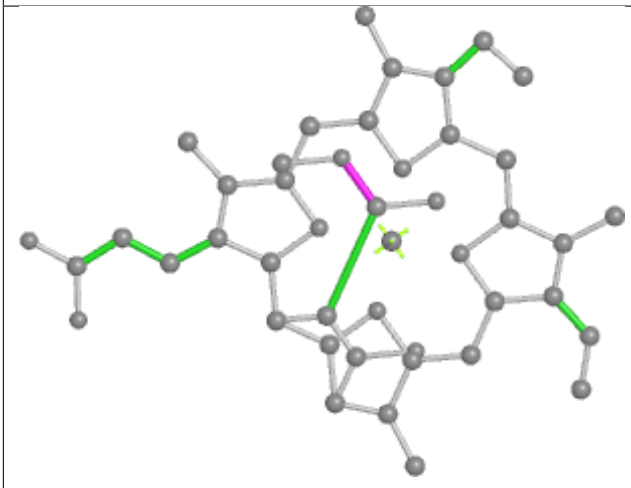

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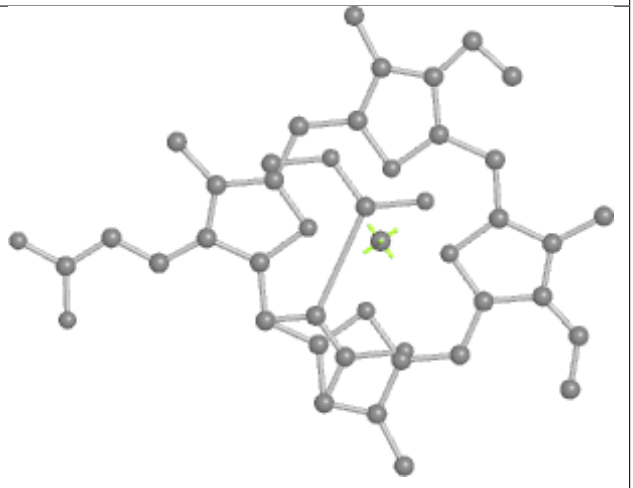

Rings

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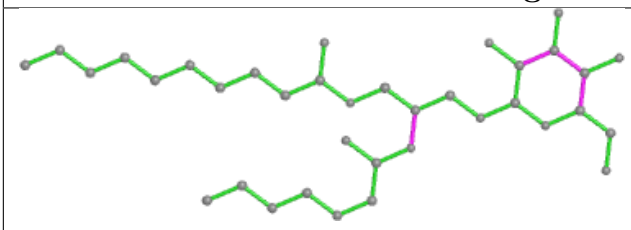

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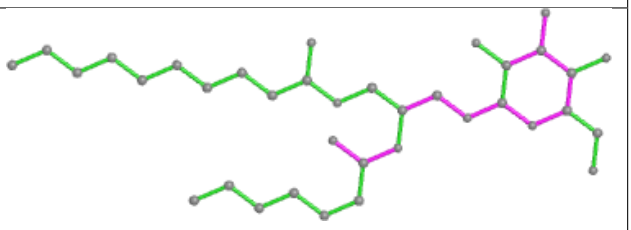

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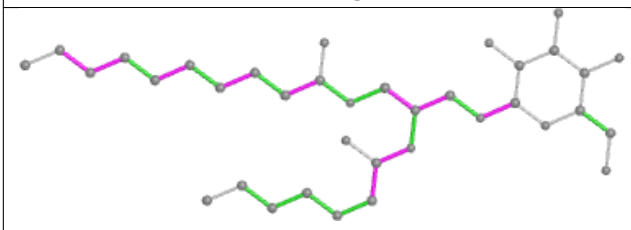

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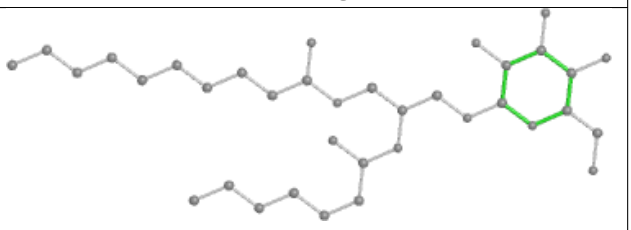
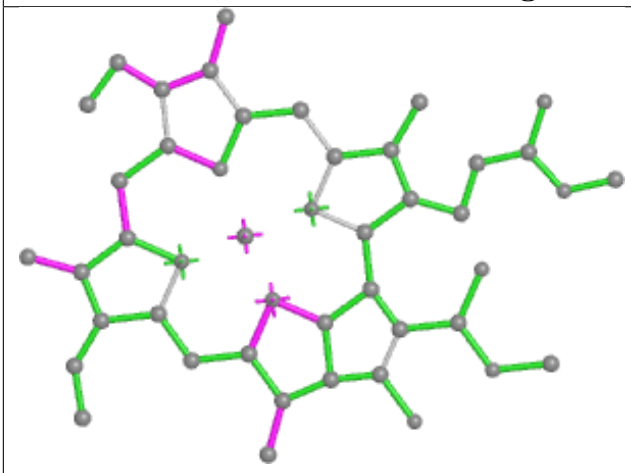


Rings

Ligand CLA 18 311



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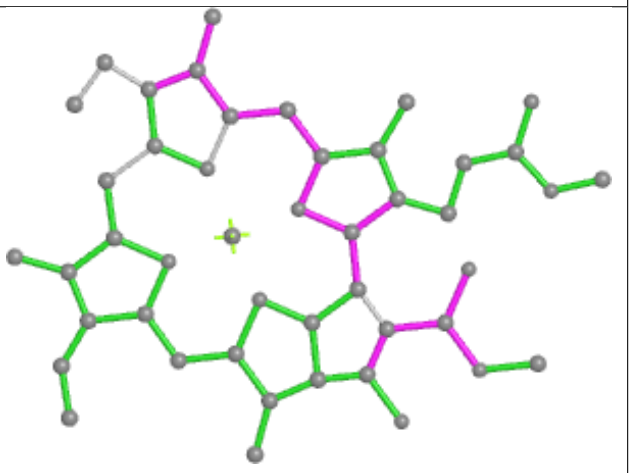

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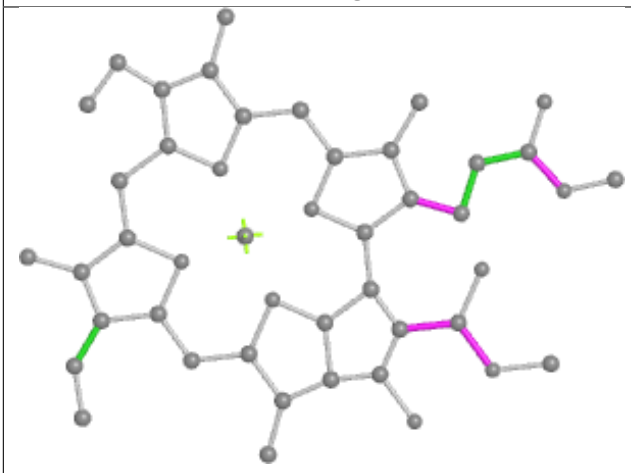

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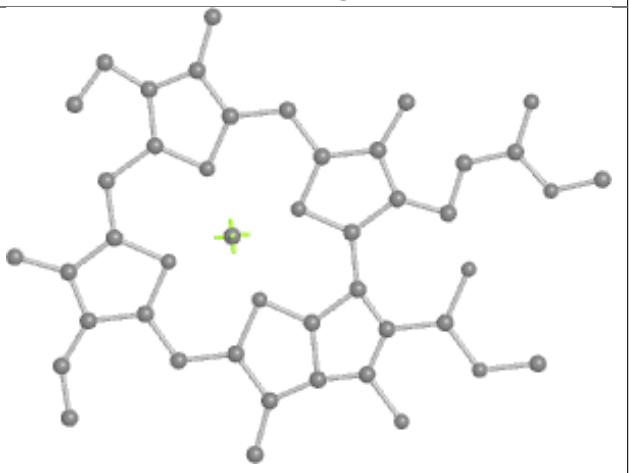

Rings

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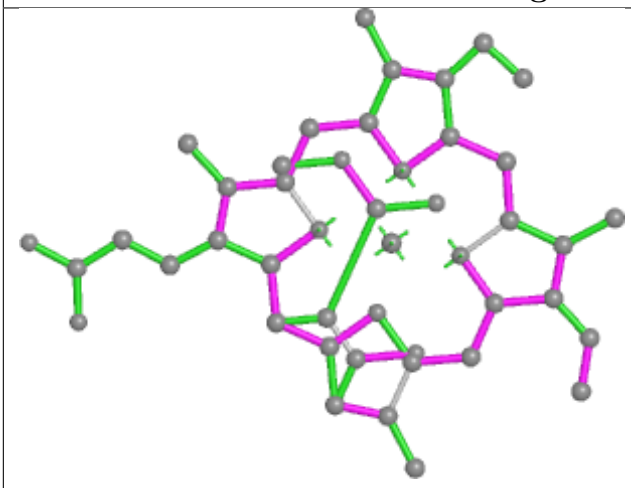

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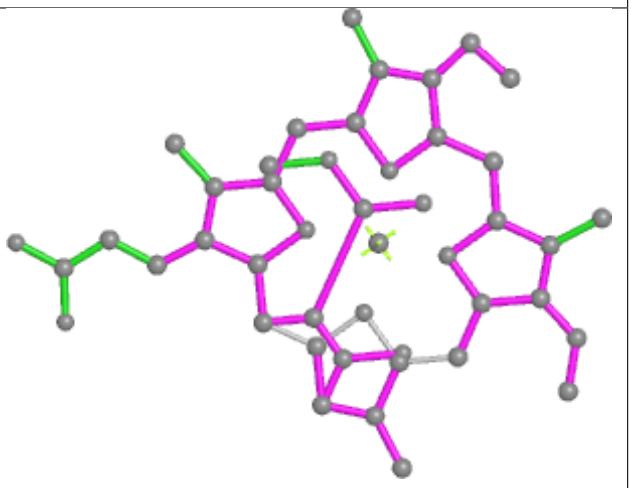

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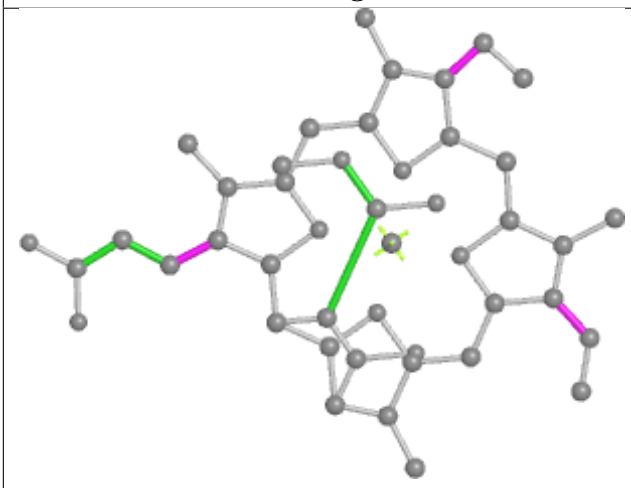

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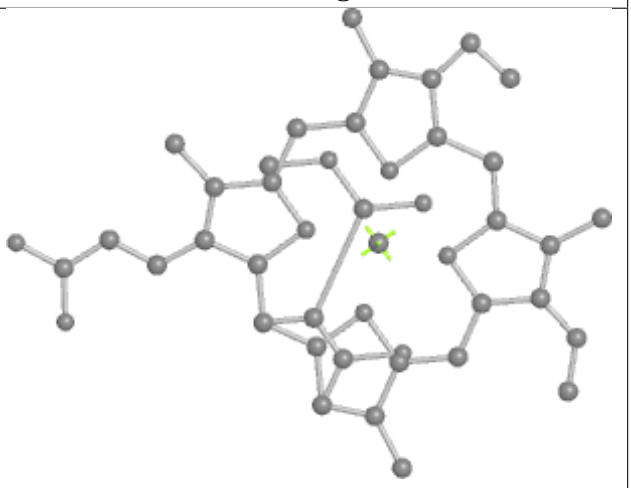

Rings

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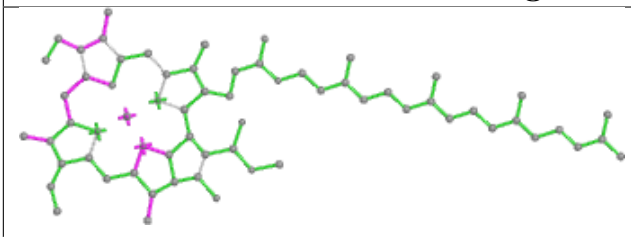

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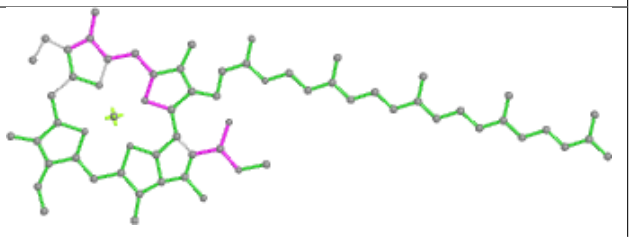

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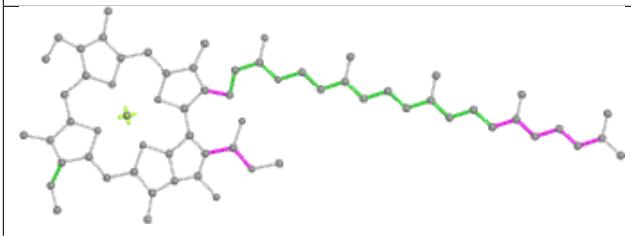

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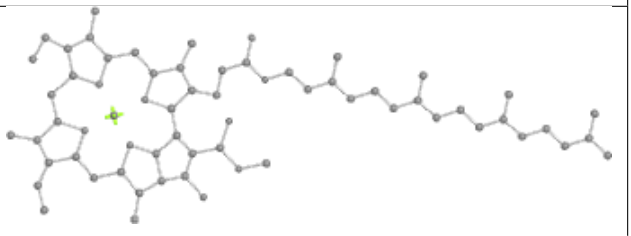
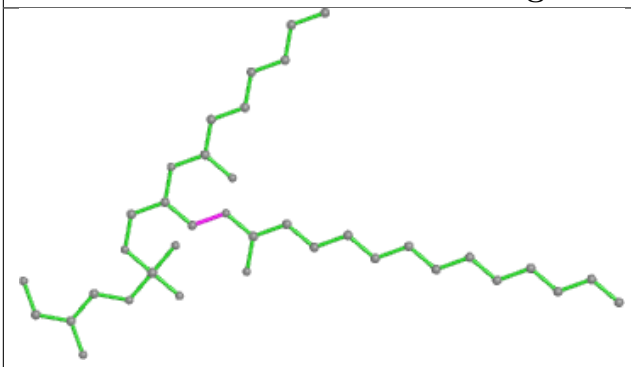


Rings

Ligand LHG a 410



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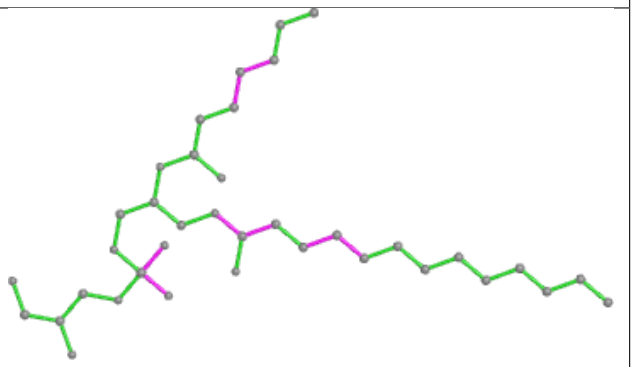

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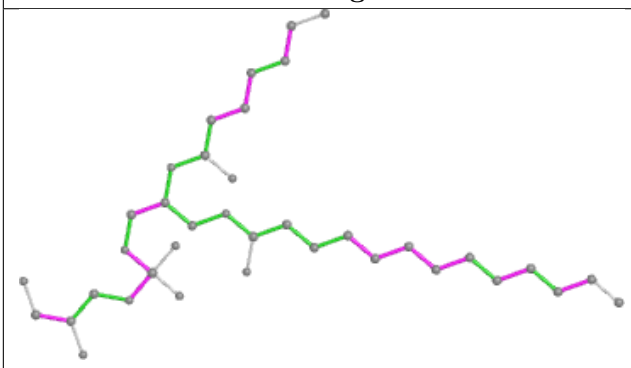

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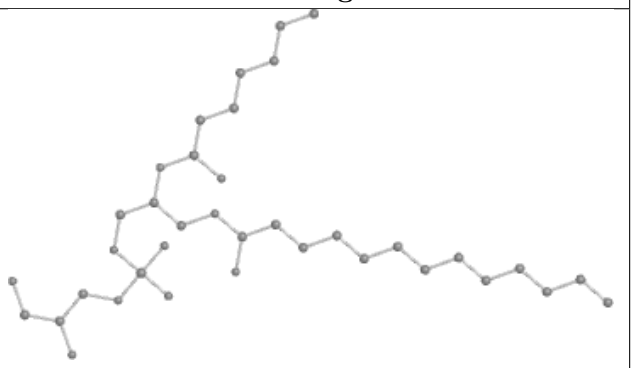
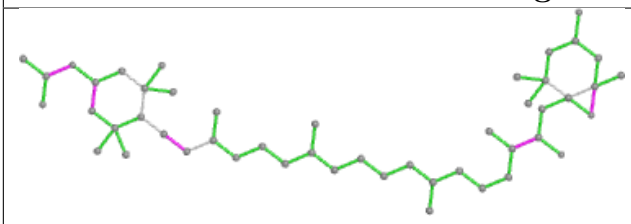


Rings

Ligand A86 4 302



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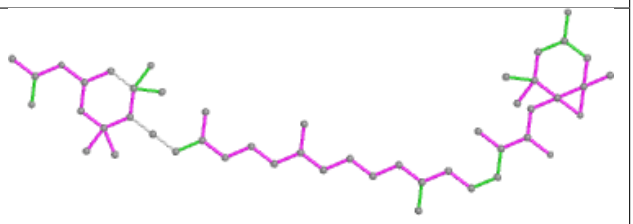

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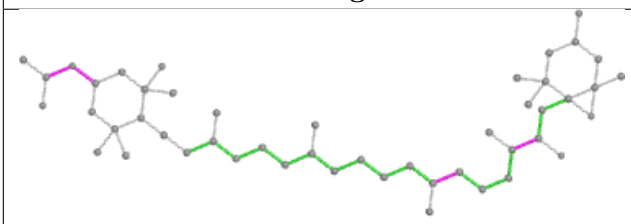

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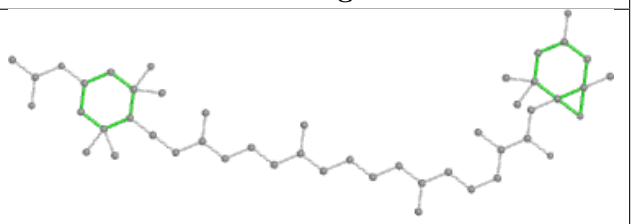

Rings

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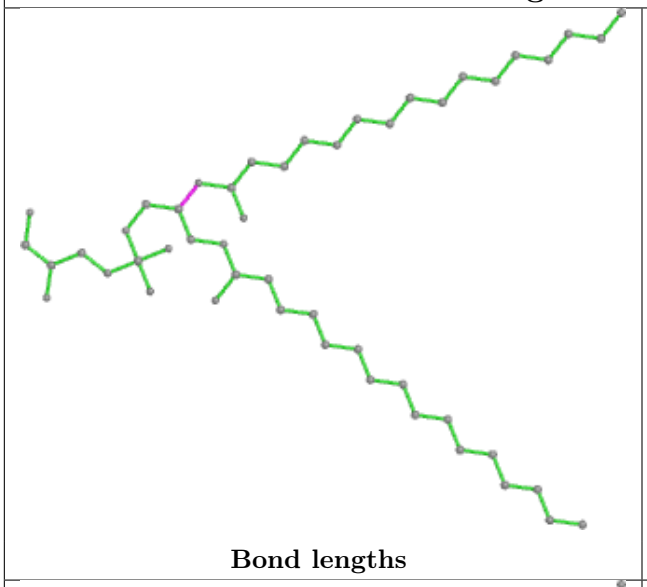

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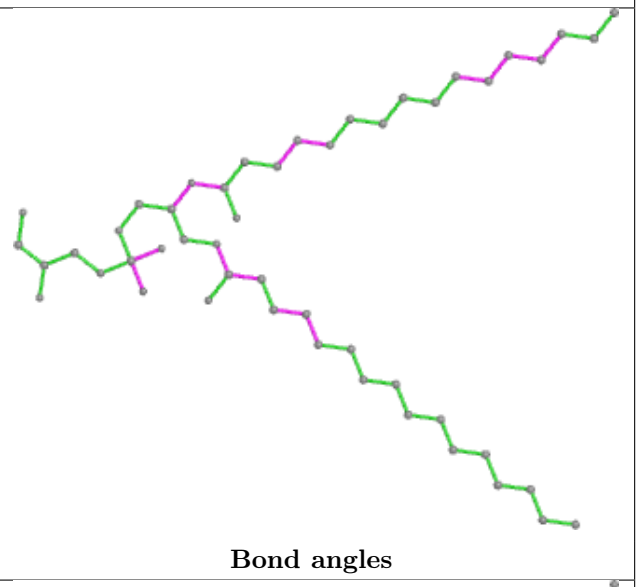

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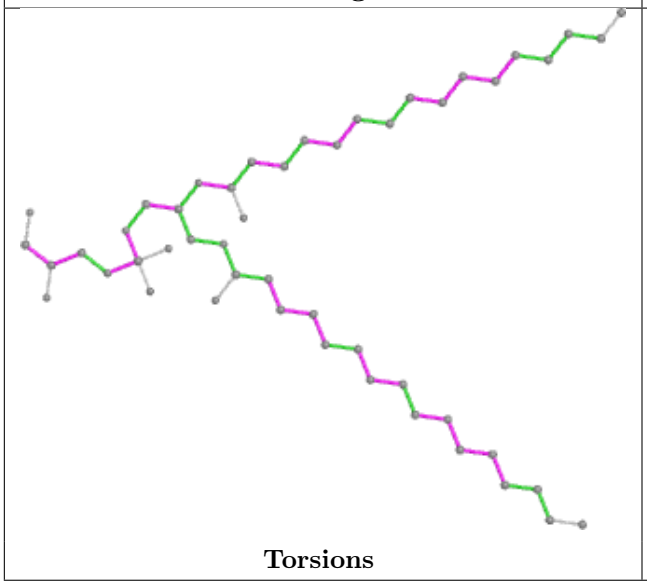

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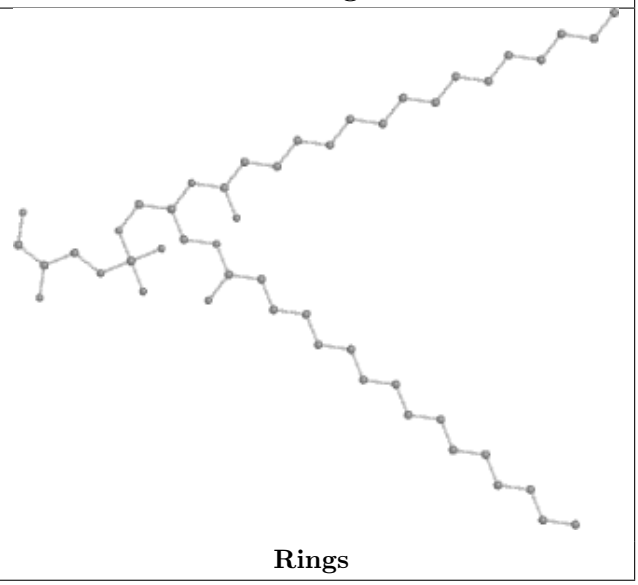
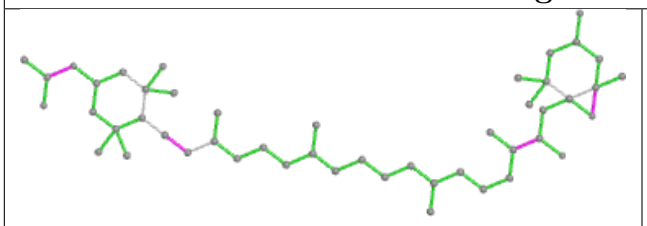


Rings

Ligand A86 5 318



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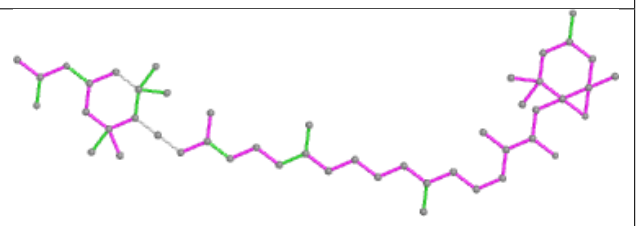

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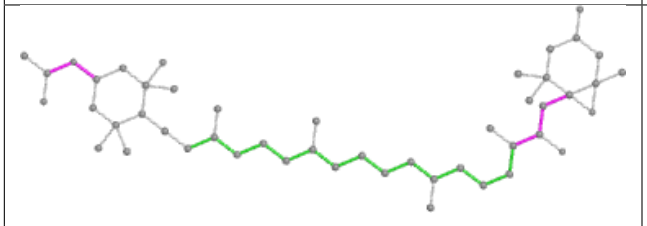

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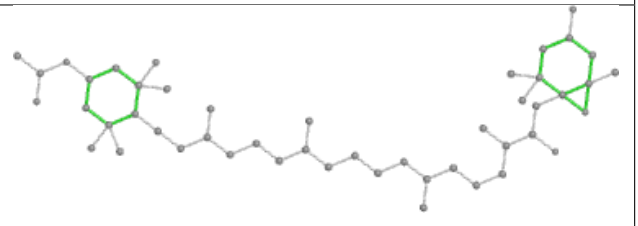

Rings

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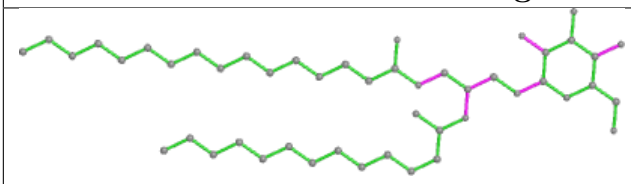

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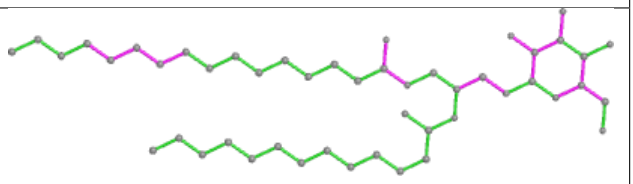

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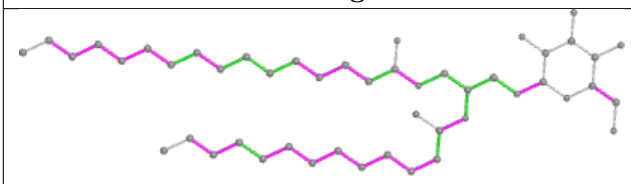

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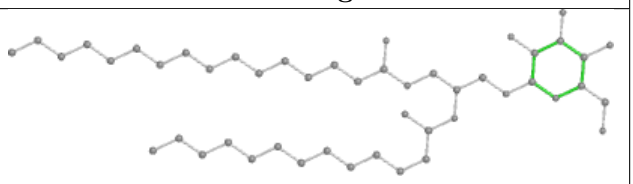
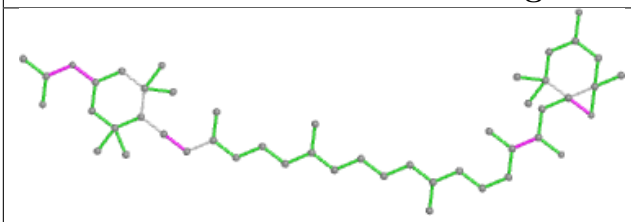


Rings

Ligand A86 12 304



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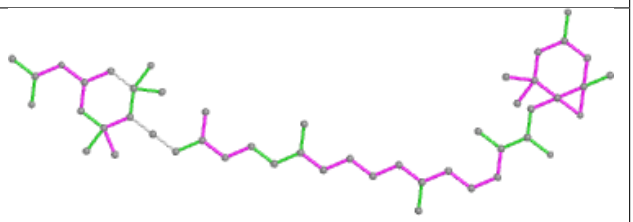

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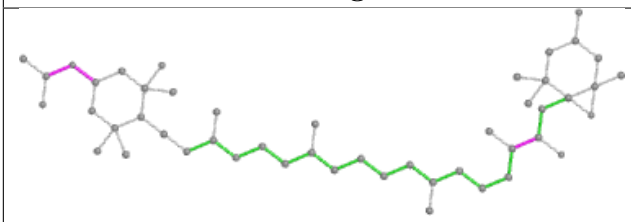

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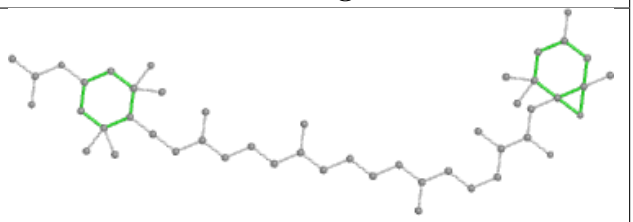
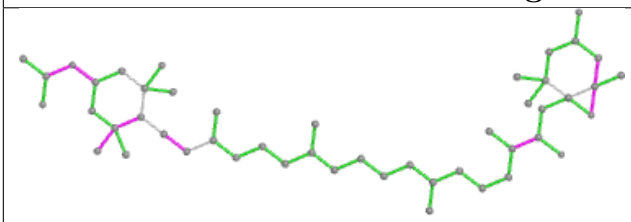


Rings

Ligand A86 13 304



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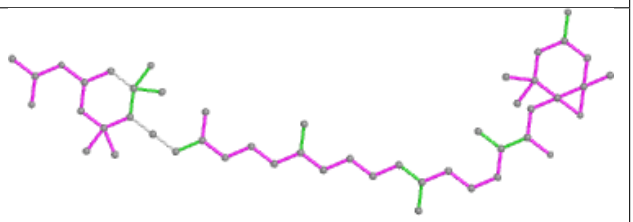
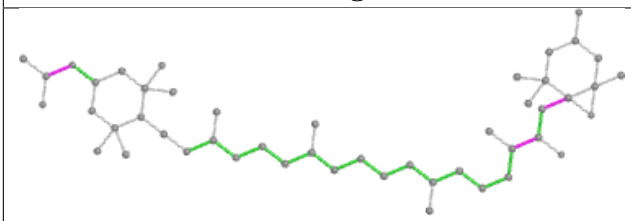


Bond angles



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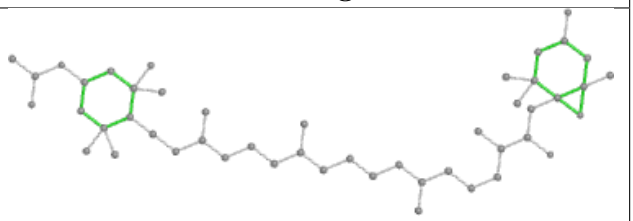
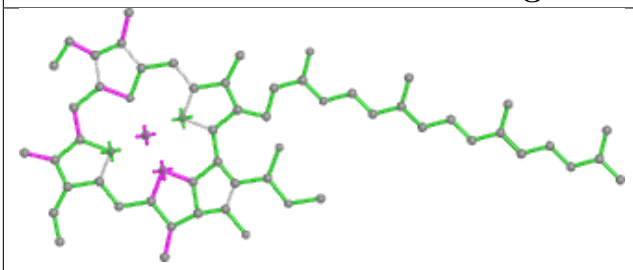


Rings

Ligand CLA A 406



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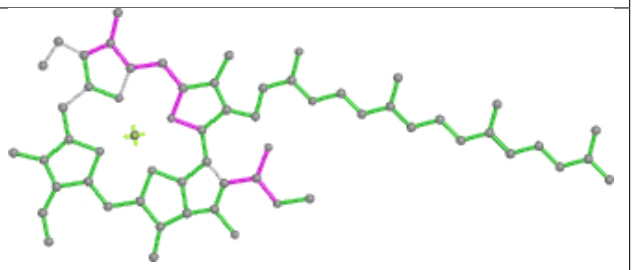

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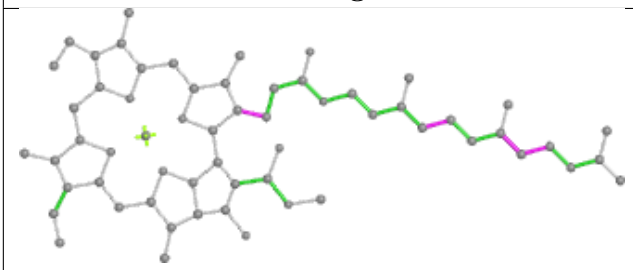
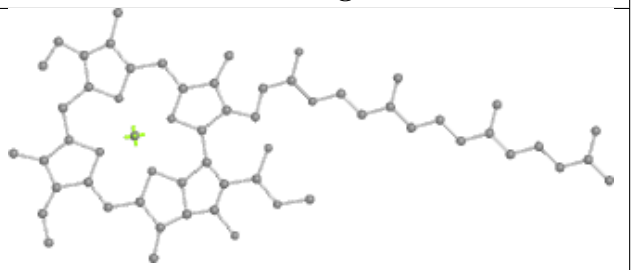
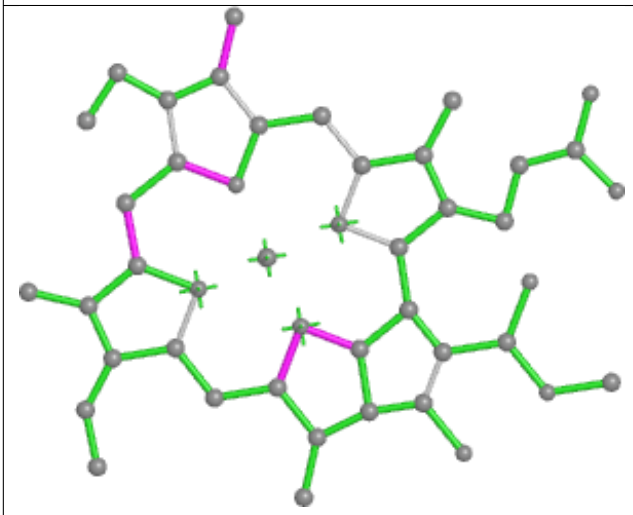


Torsions



Rings

Ligand CLA 17 310



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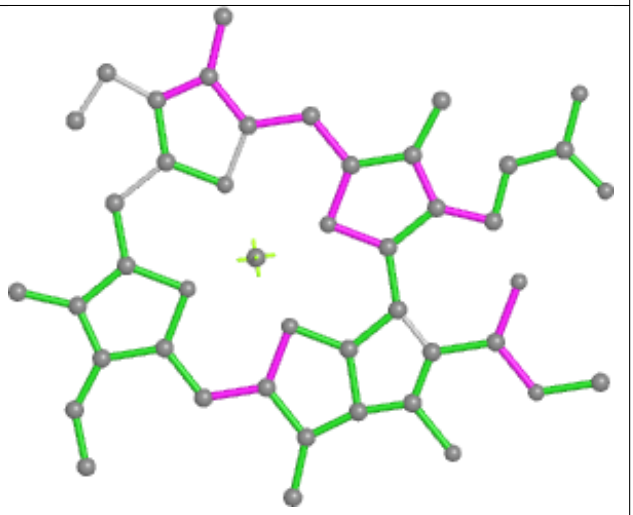

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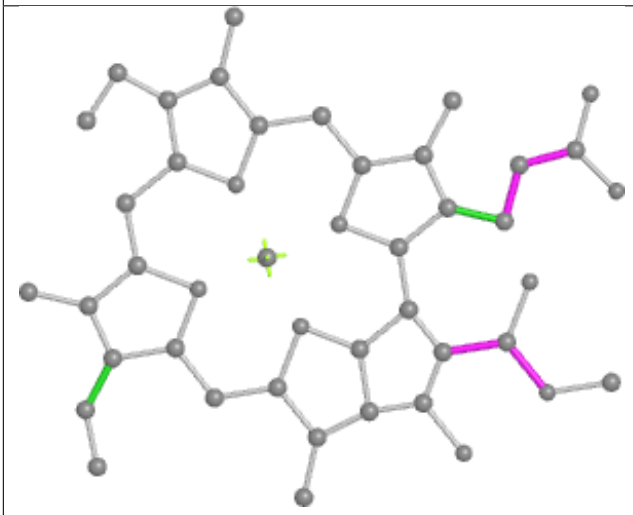

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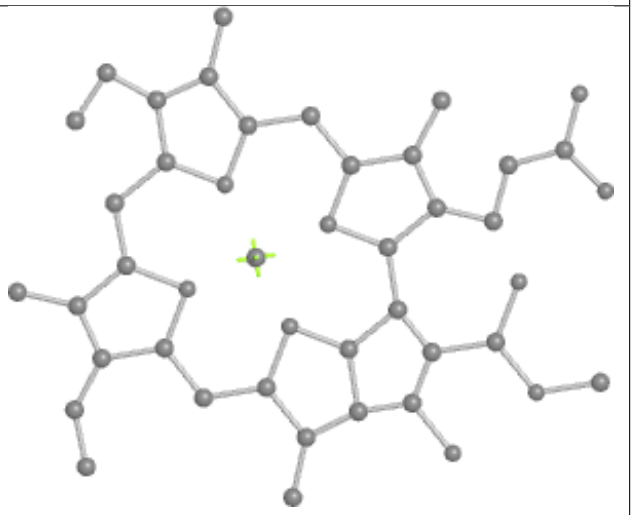
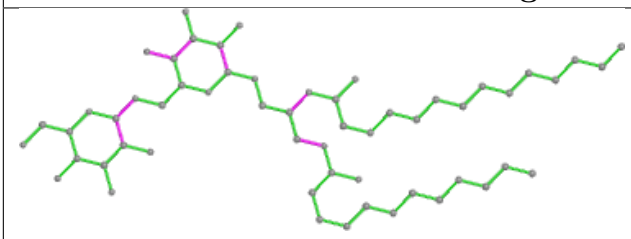


Rings

Ligand DGD w 204



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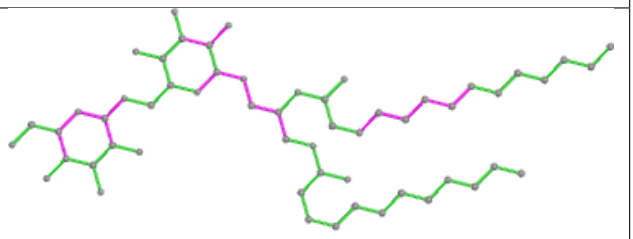

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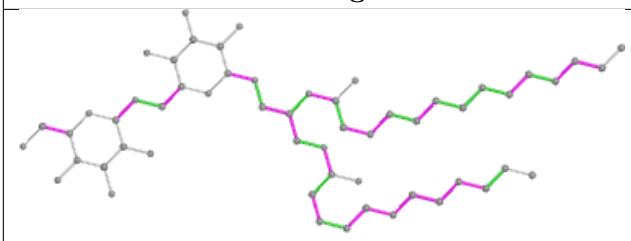

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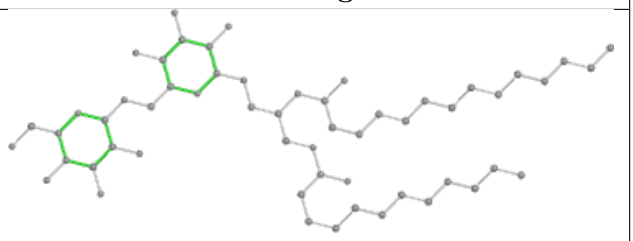
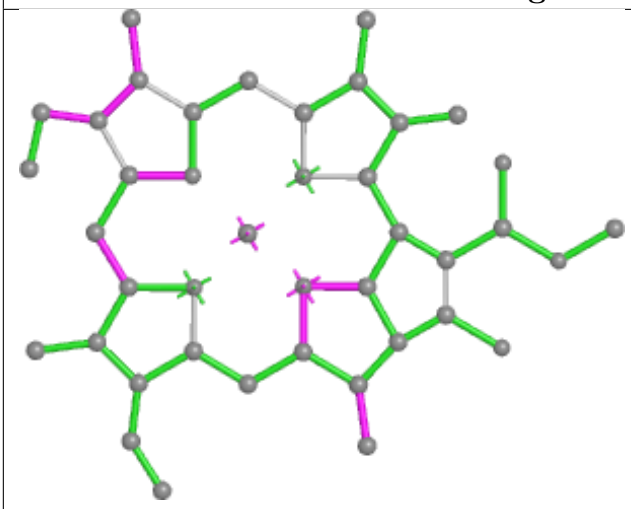


Rings

Ligand CLA 7 308



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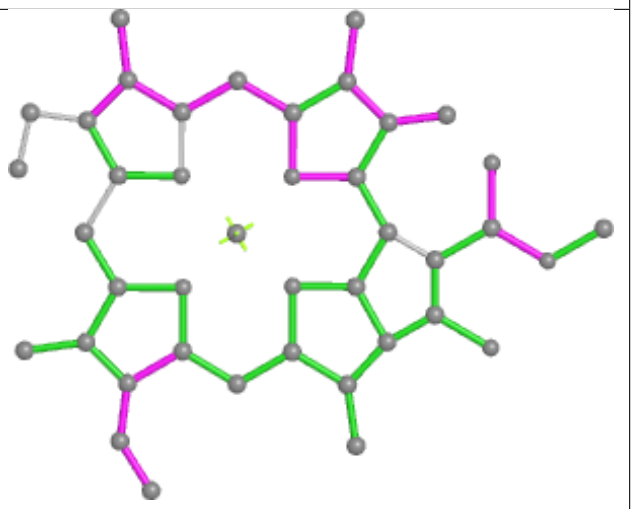

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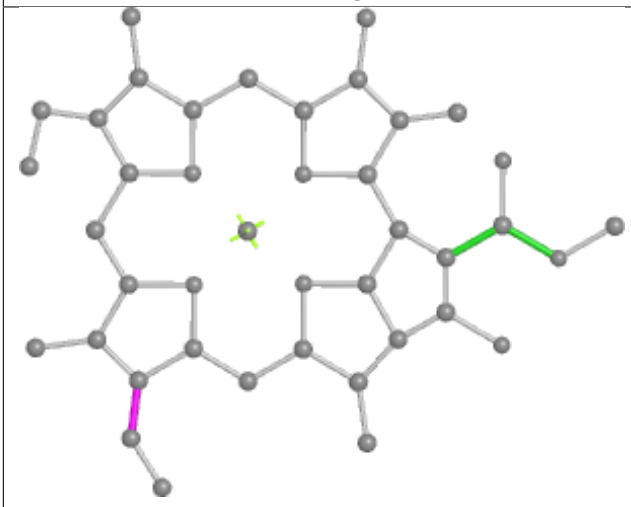

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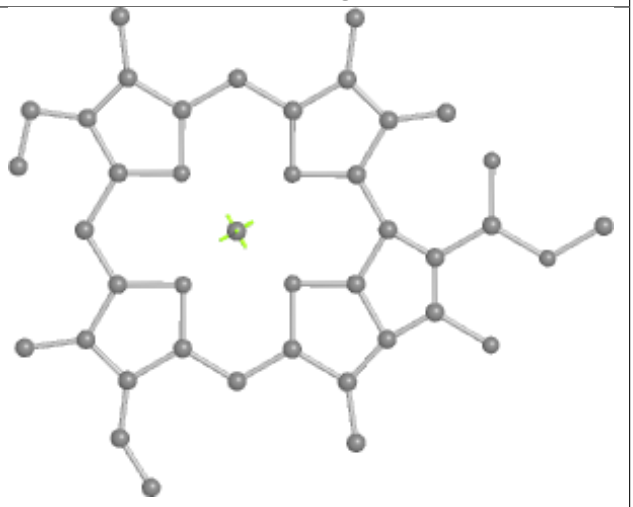
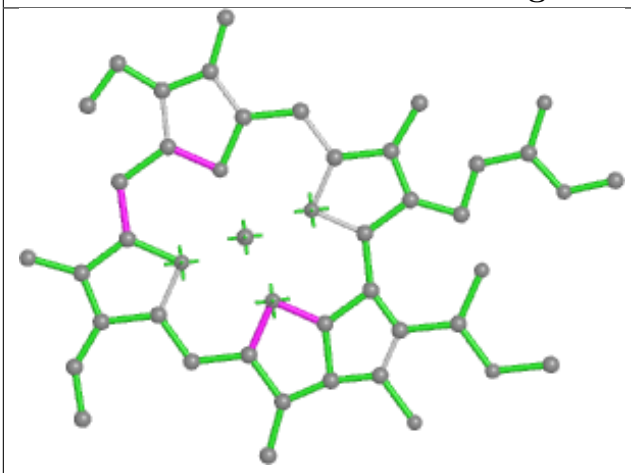


Rings

Ligand CLA 9 311



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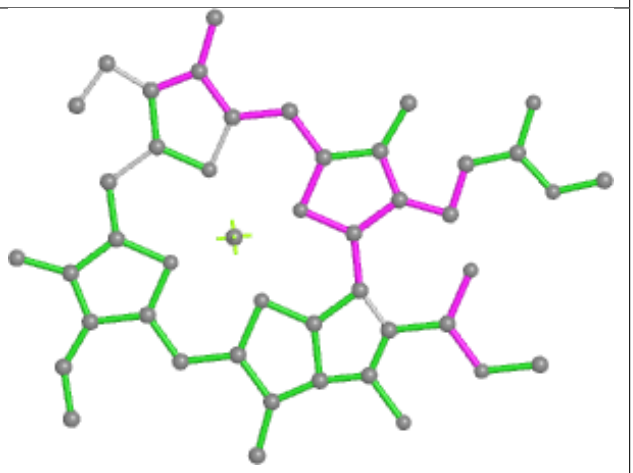

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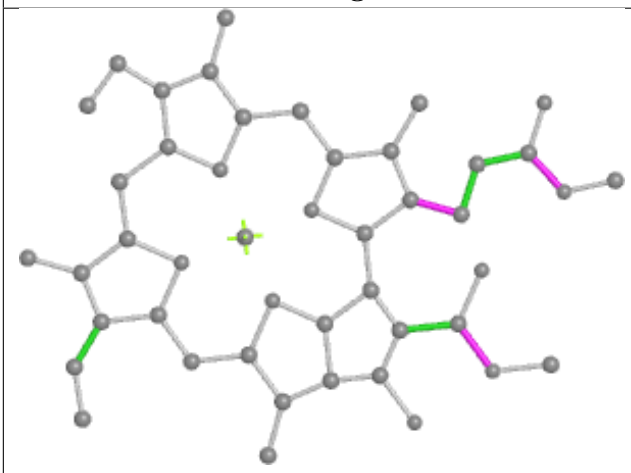

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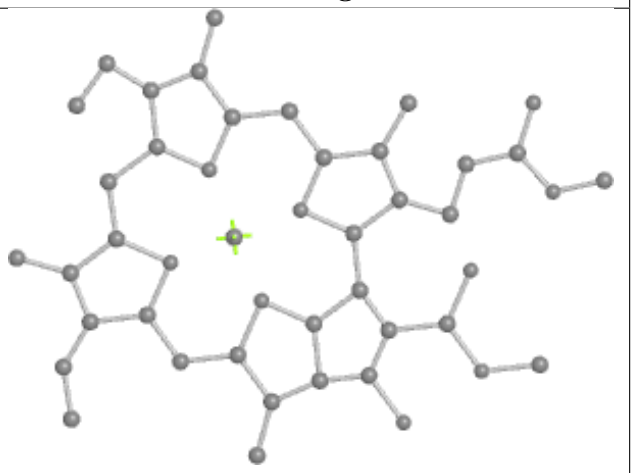
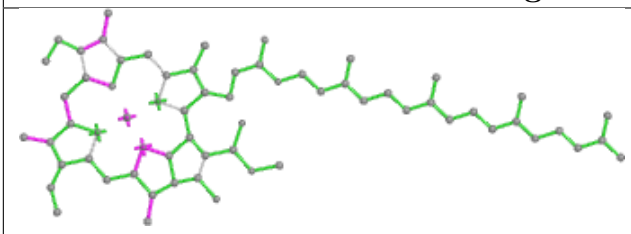


Rings

Ligand CLA B 609



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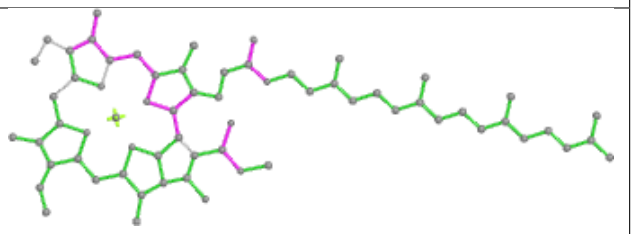

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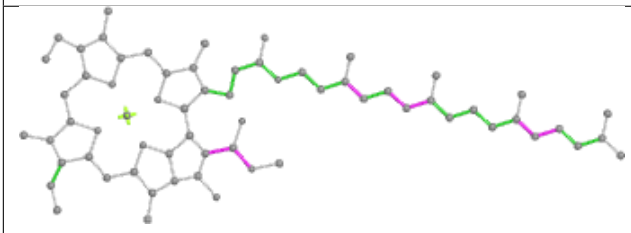

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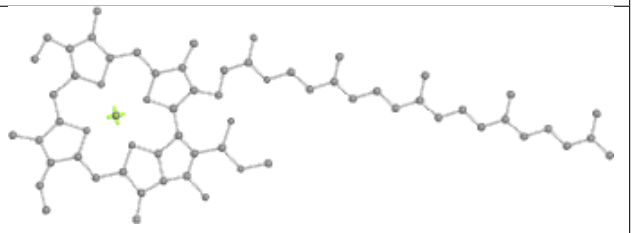
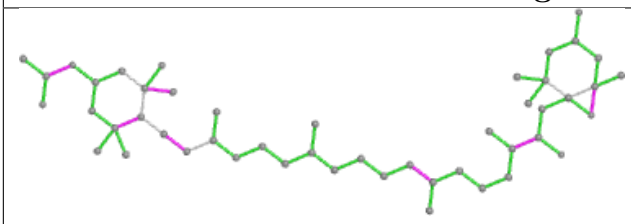


Rings

Ligand A86 0 303



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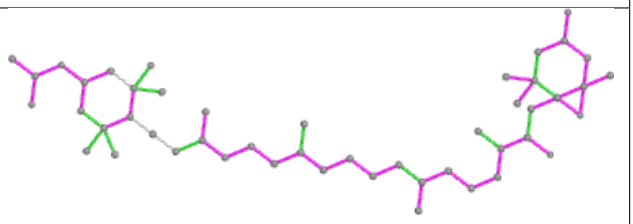

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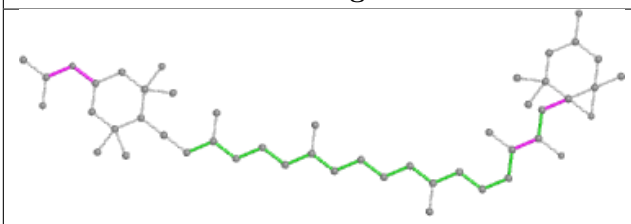

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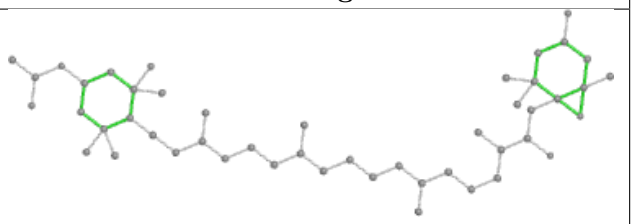
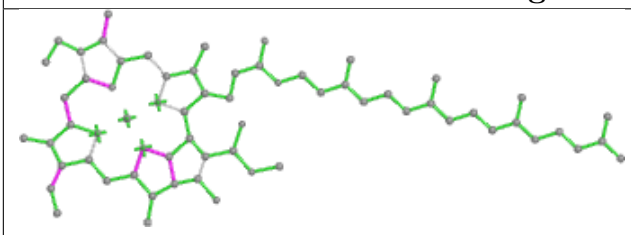


Rings

Ligand CLA 3 316



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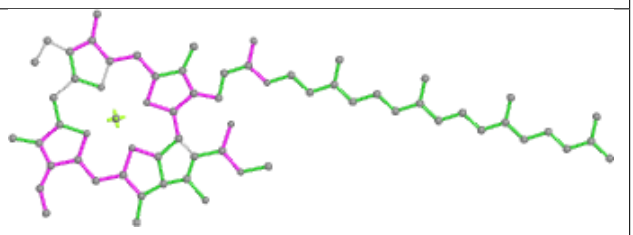

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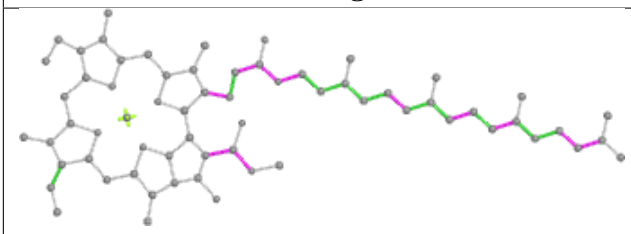

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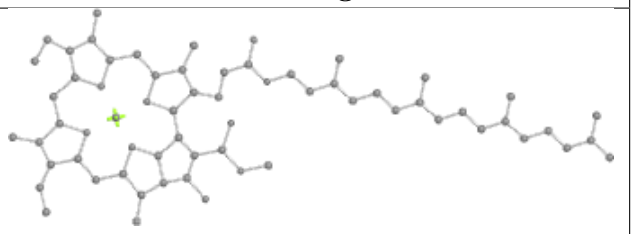
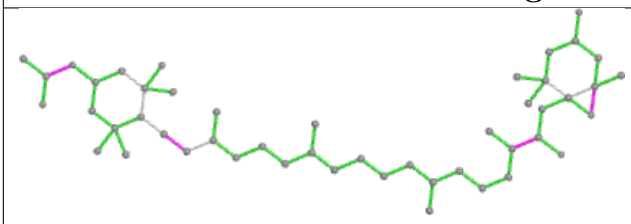


Rings

Ligand A86 12 305



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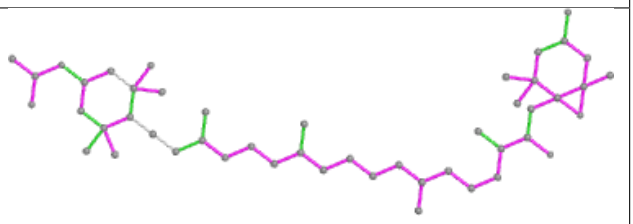

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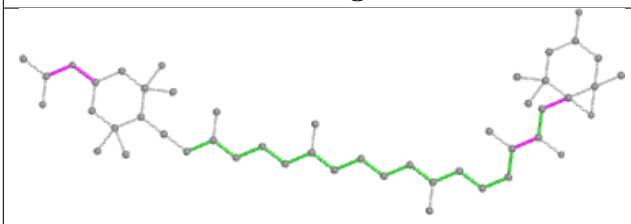

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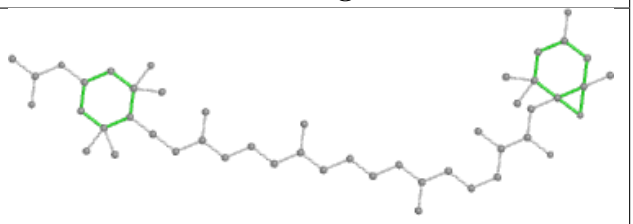
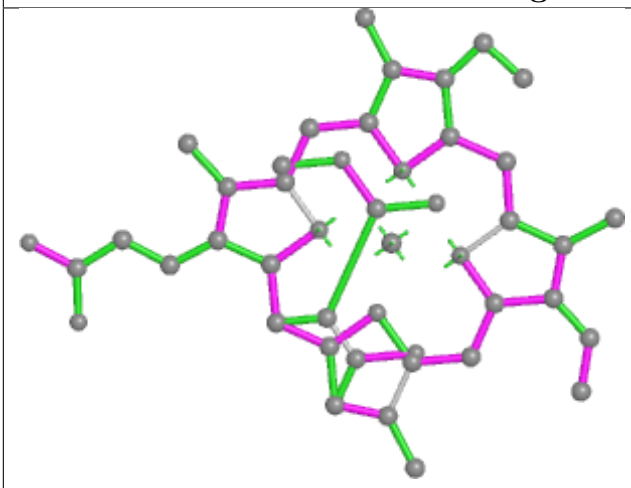


Rings

Ligand KC2 5 308



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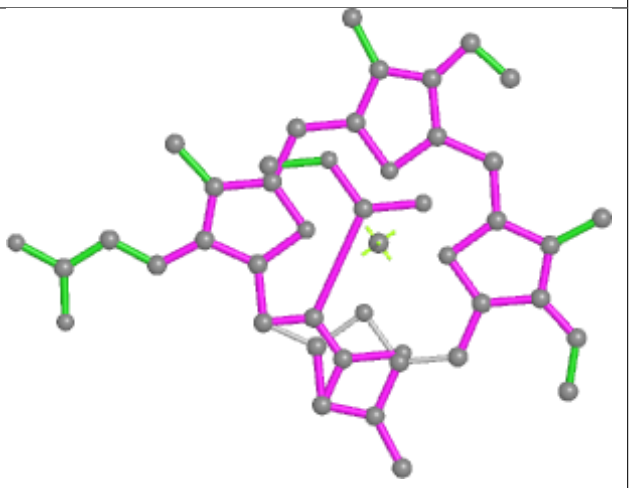

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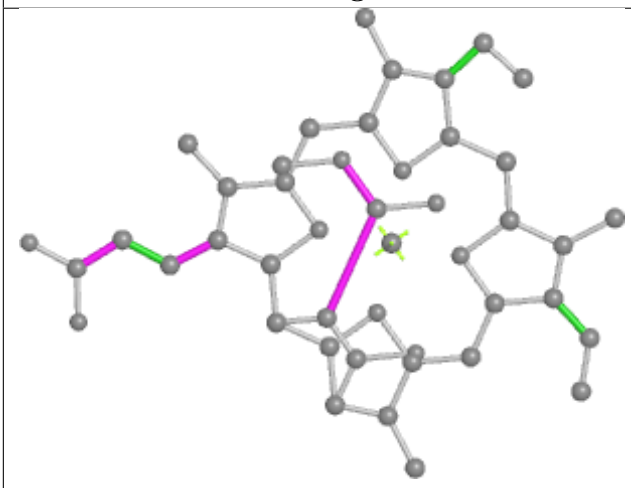

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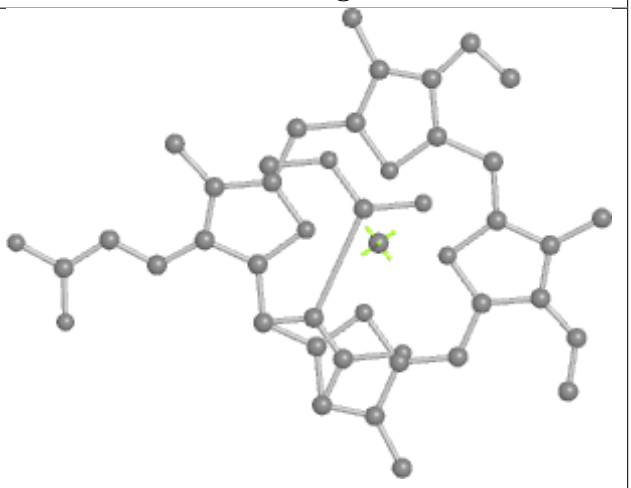
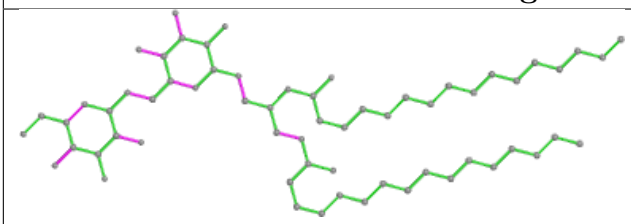


Rings

Ligand DGD C 519



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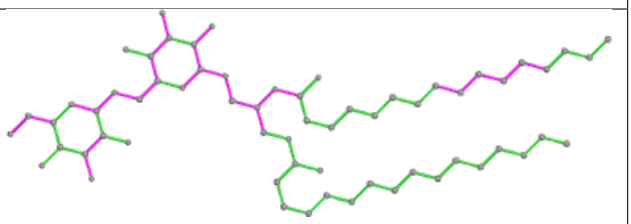

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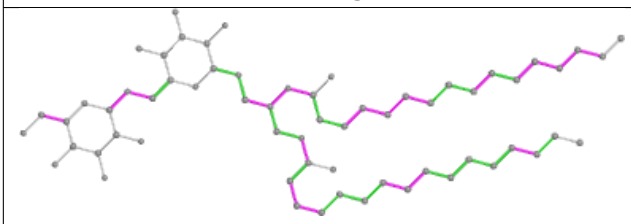

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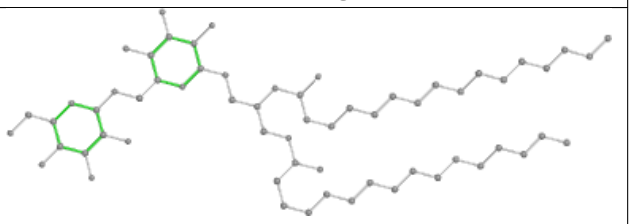
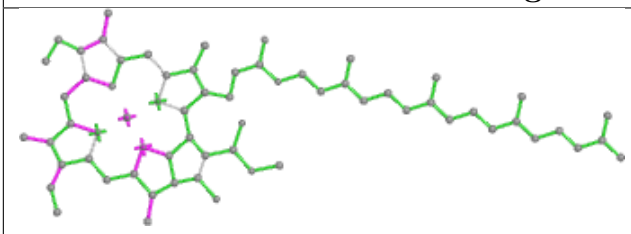


Rings

Ligand CLA C 503



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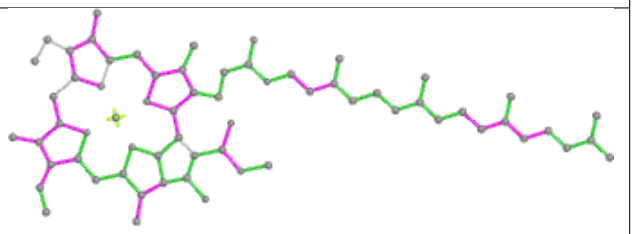
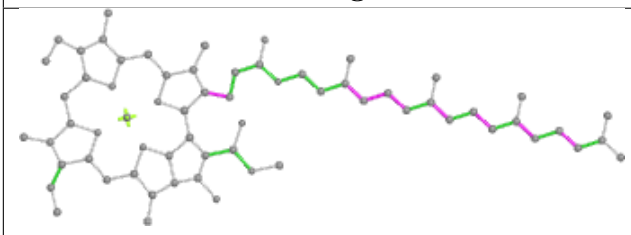


Bond angles



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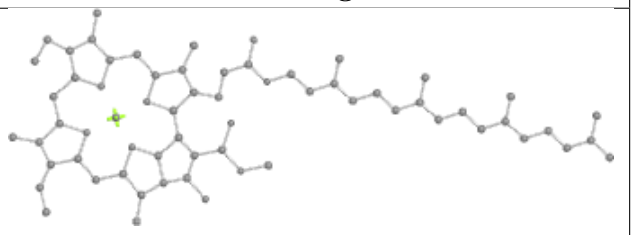
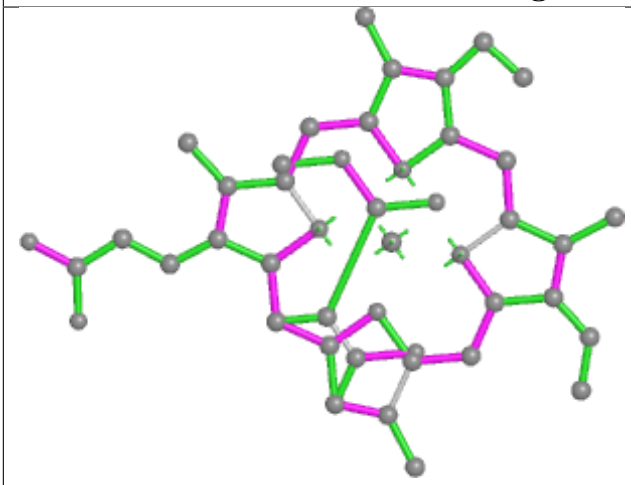


Rings

Ligand KC1 8 313



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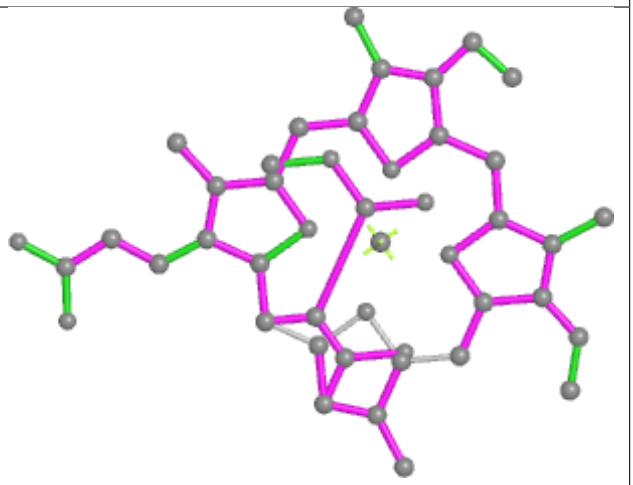
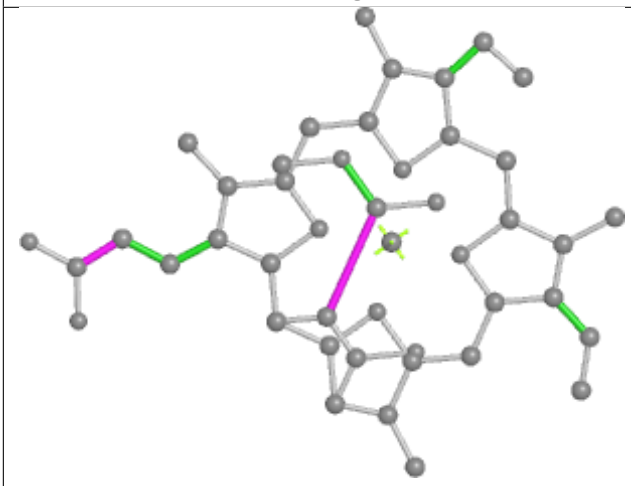
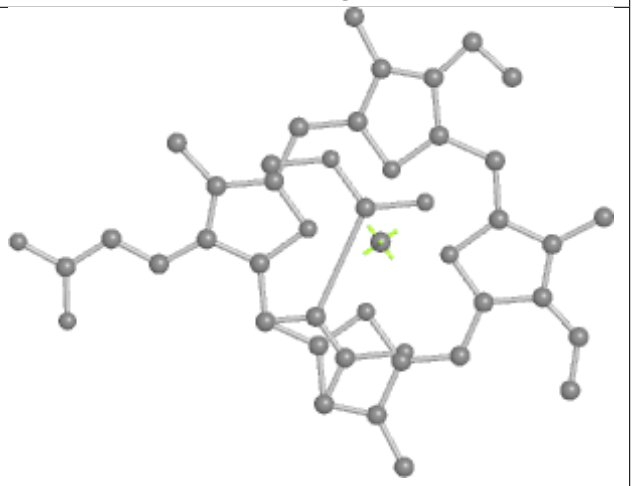


Bond angles

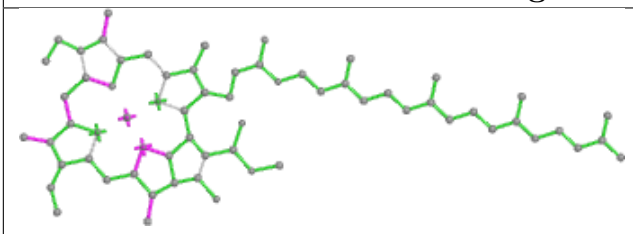


Torsions



Rings

Ligand CLA 3 313



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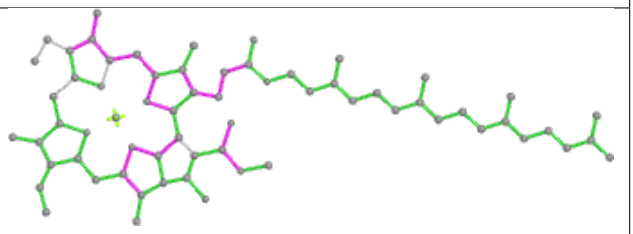
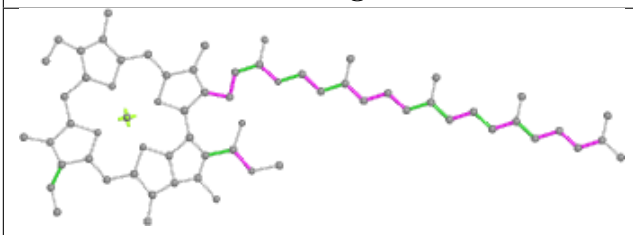


Bond angles



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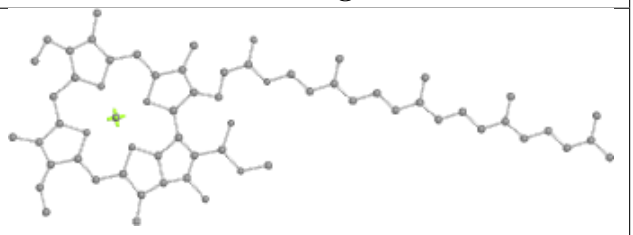
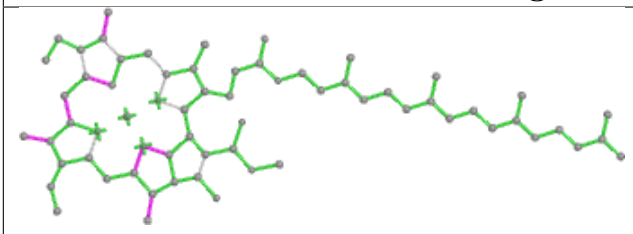


Rings

Ligand CLA 4 309



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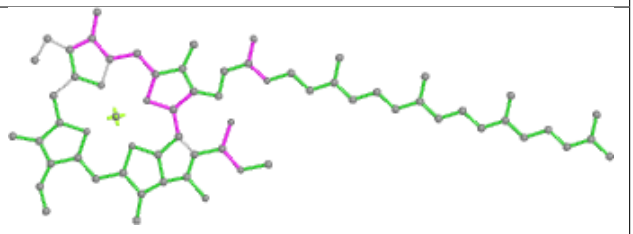

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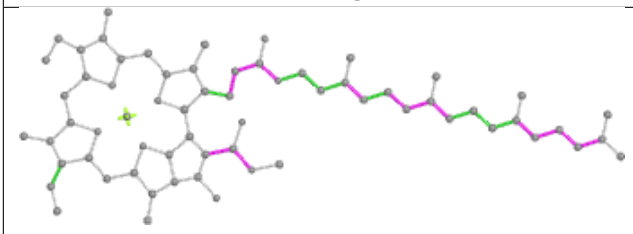
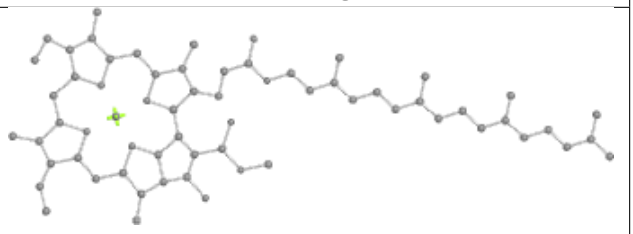
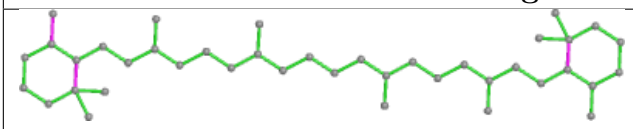


Torsions



Rings

Ligand BCR H 101



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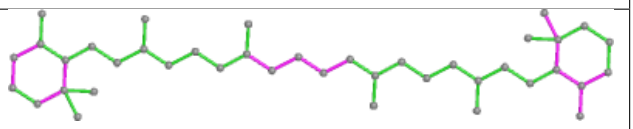

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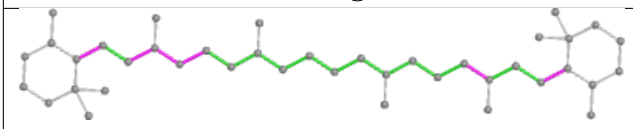
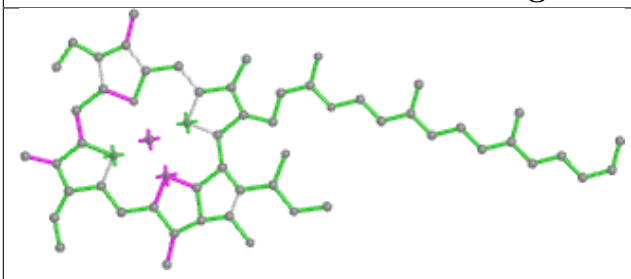


Torsions

Rings

Ligand CLA 0 309



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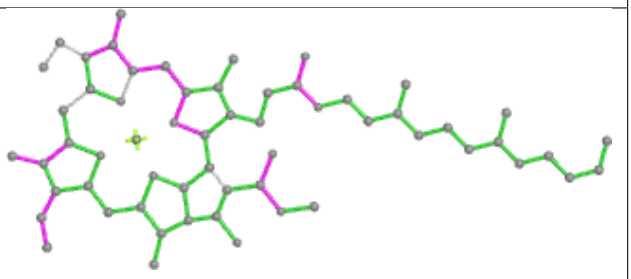

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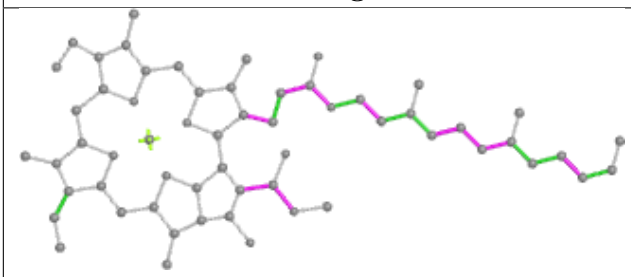

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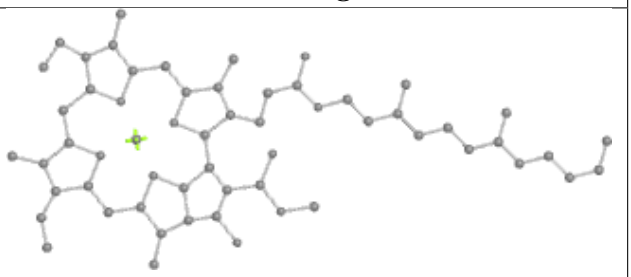

Rings

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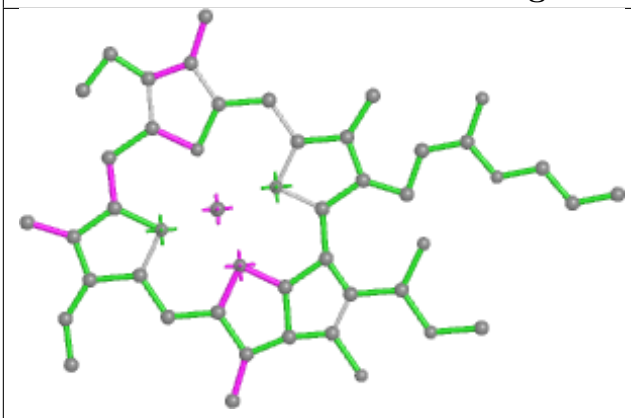

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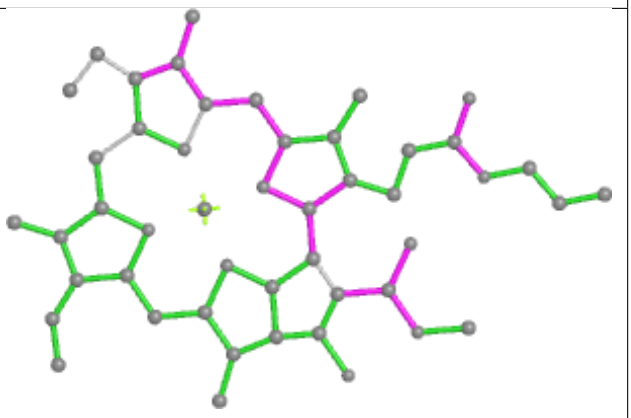

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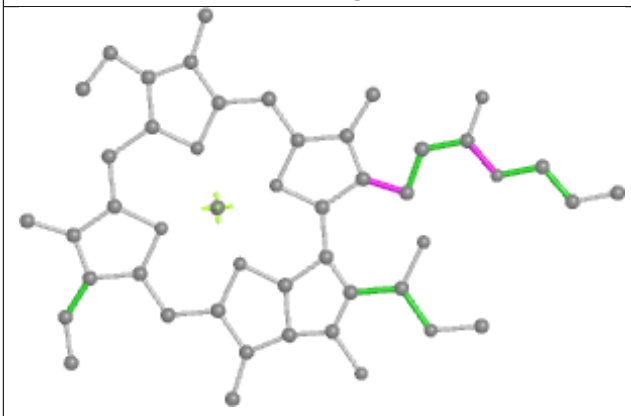

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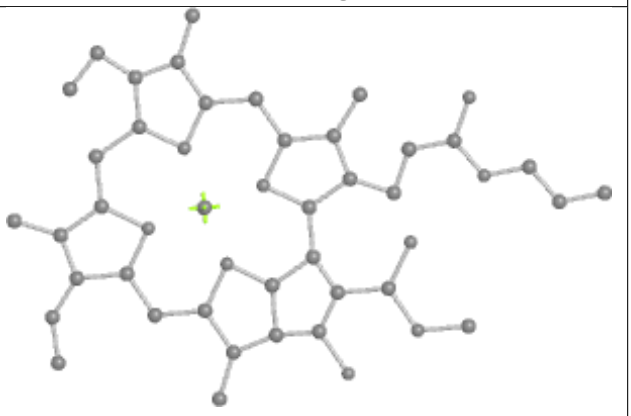
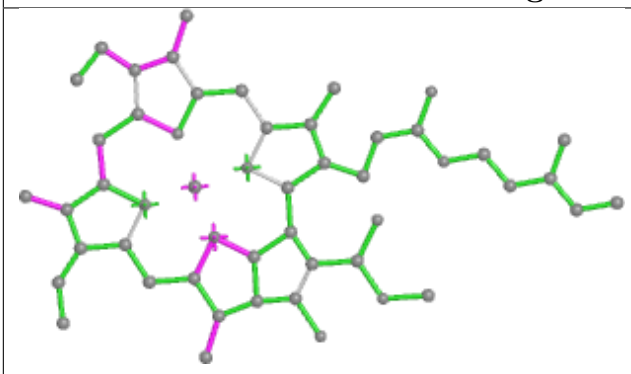


Rings

Ligand CLA Z 101



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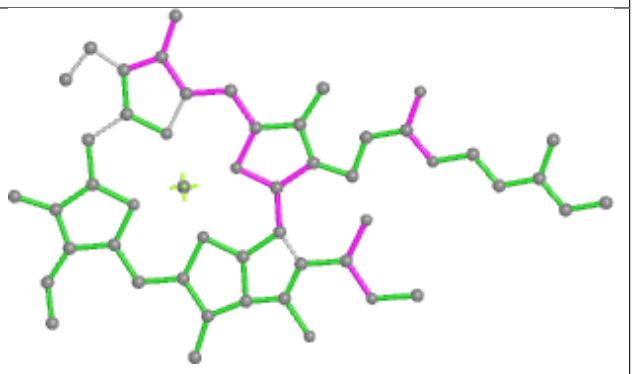

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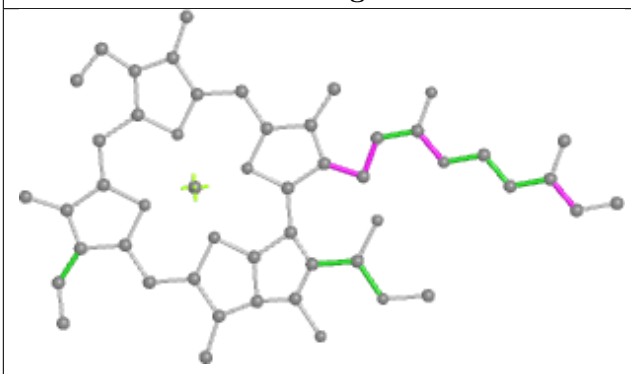

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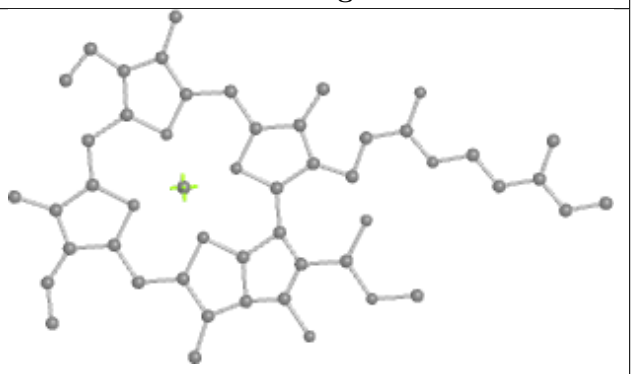
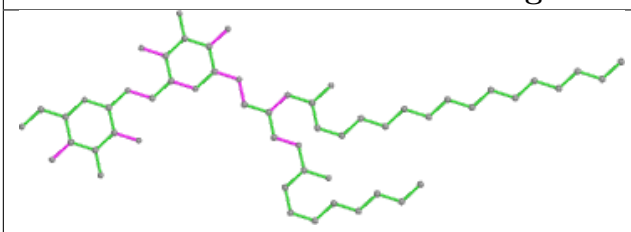


Rings

Ligand DGD c 518



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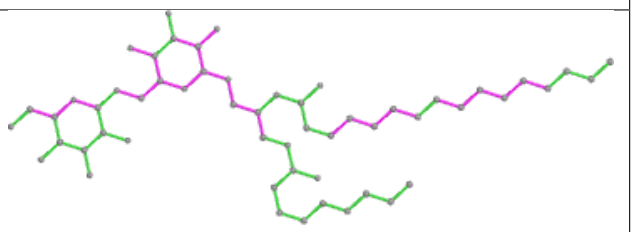

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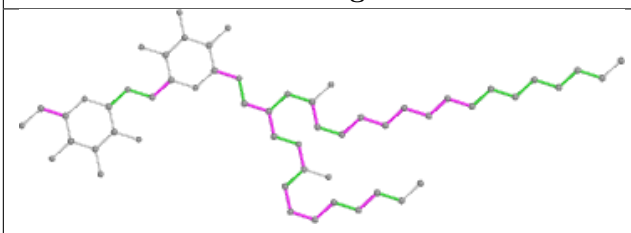

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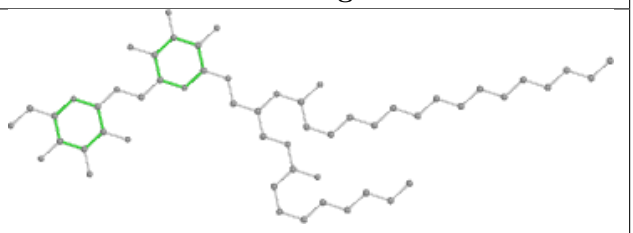
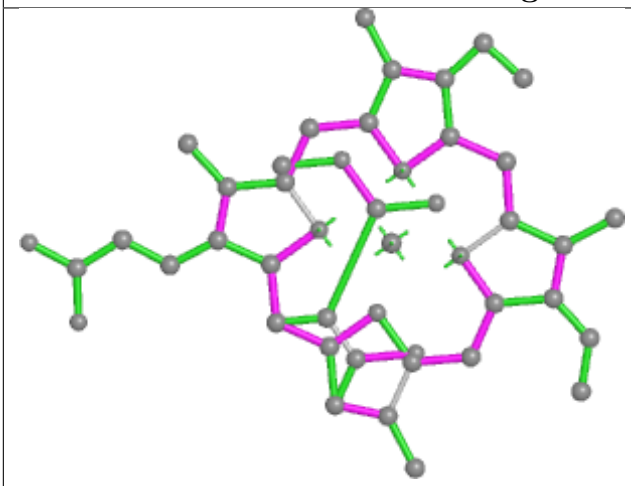


Rings

Ligand KC1 13 314



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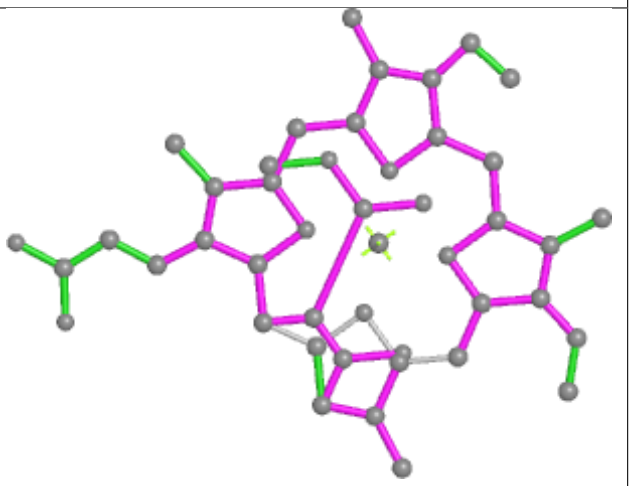

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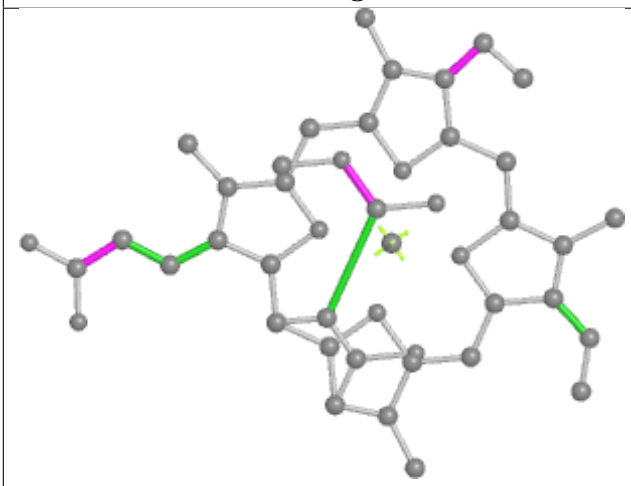

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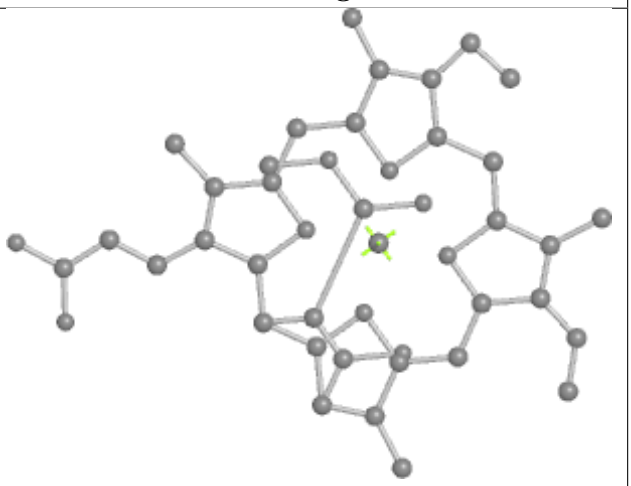
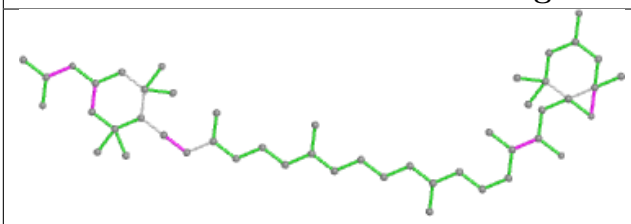


Rings

Ligand A86 4 306



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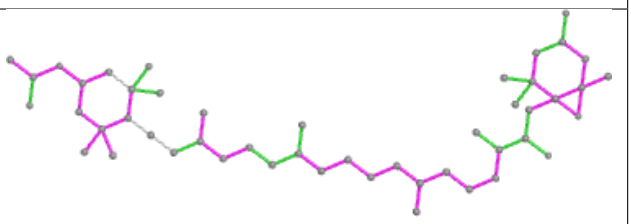

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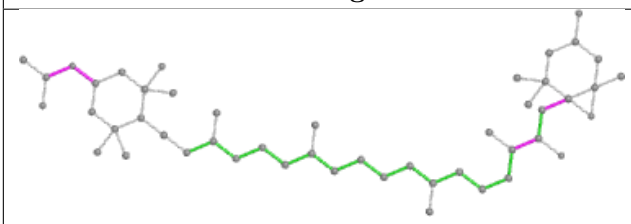

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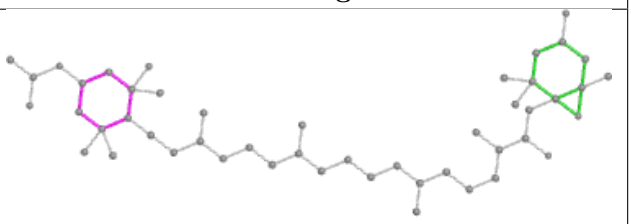
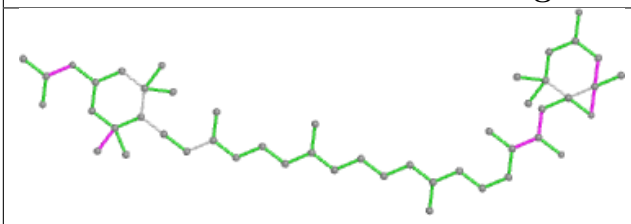


Rings

Ligand A86 7 304



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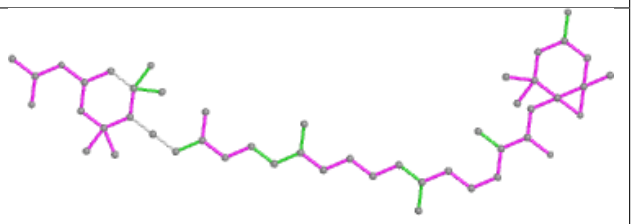

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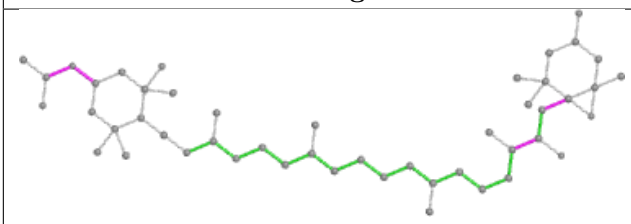

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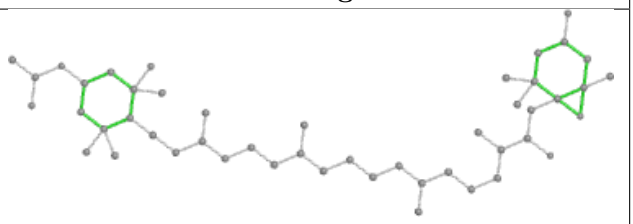
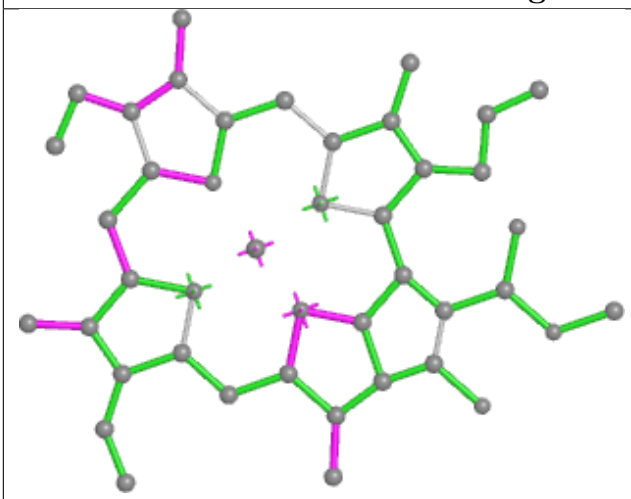


Rings

Ligand CLA 3 308



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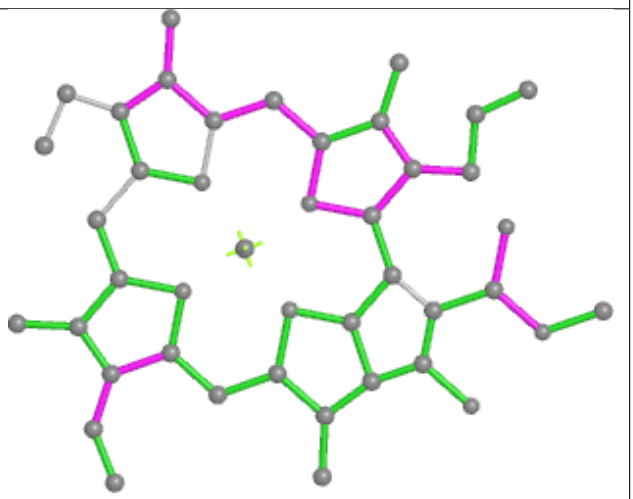

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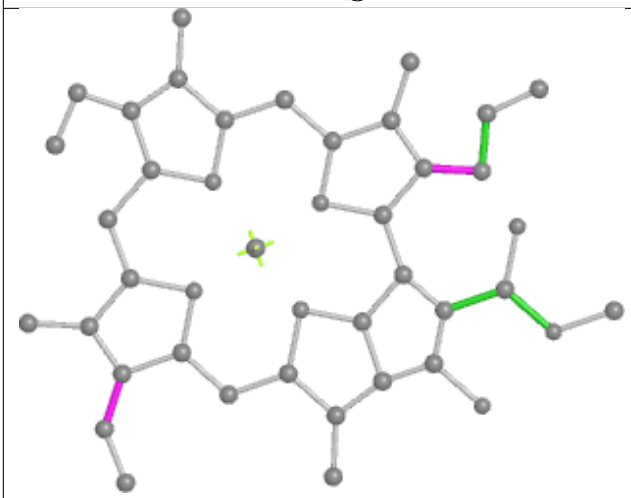

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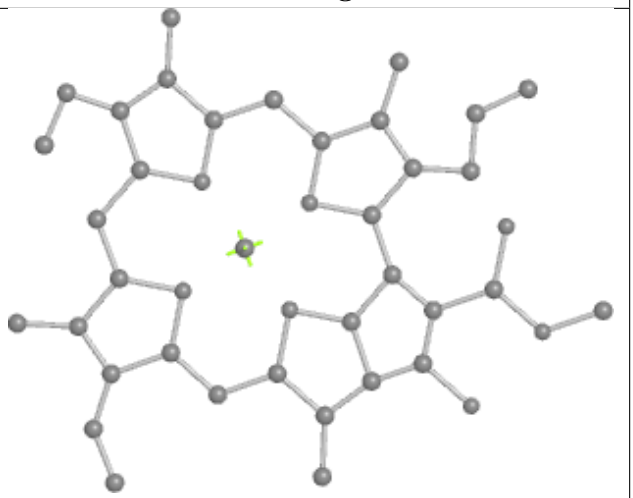
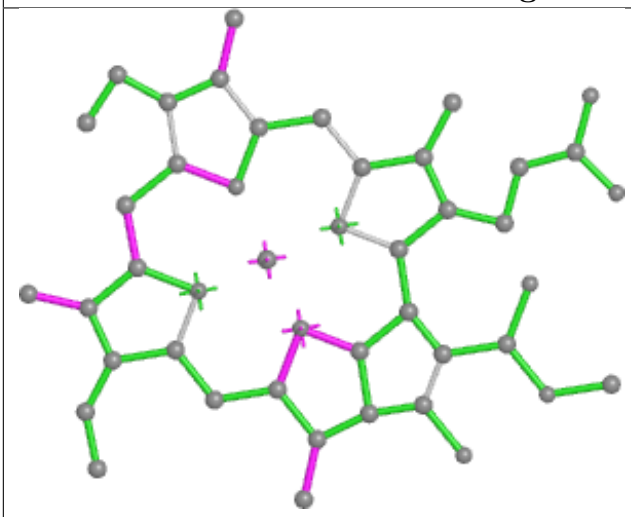


Rings

Ligand CLA 12 312



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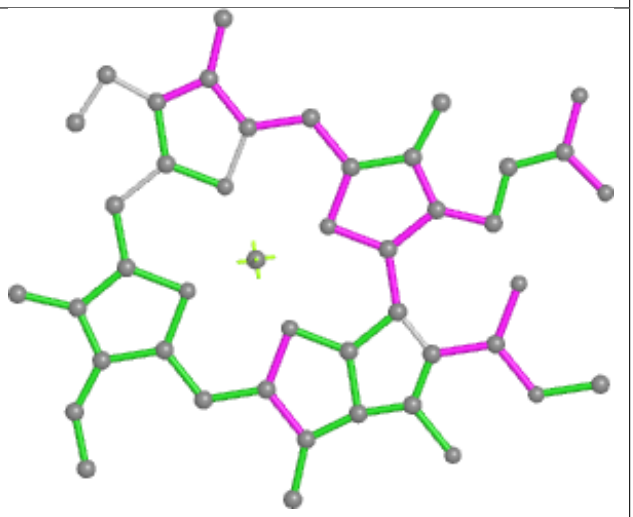

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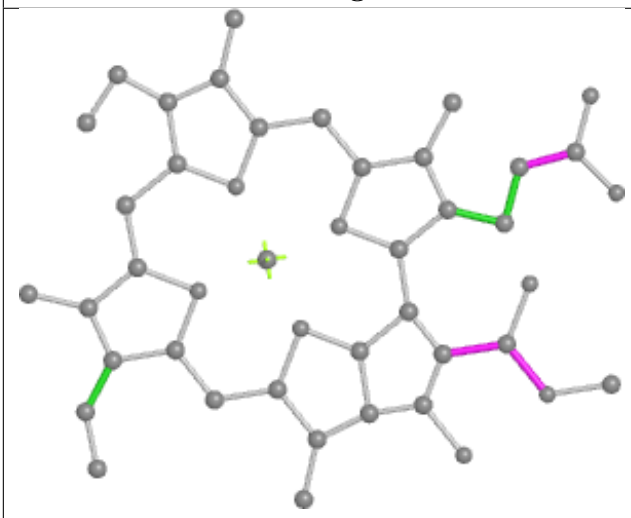

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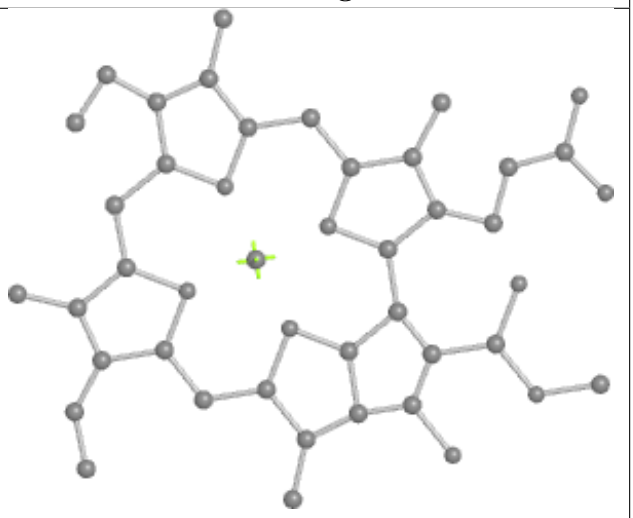
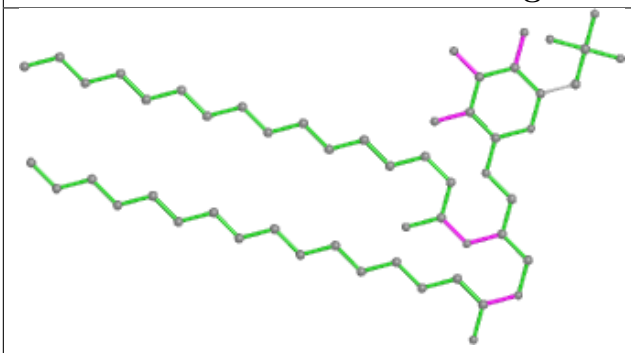


Rings

Ligand SQD A 408



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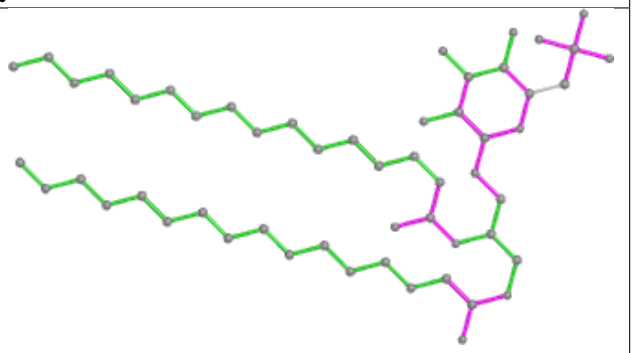

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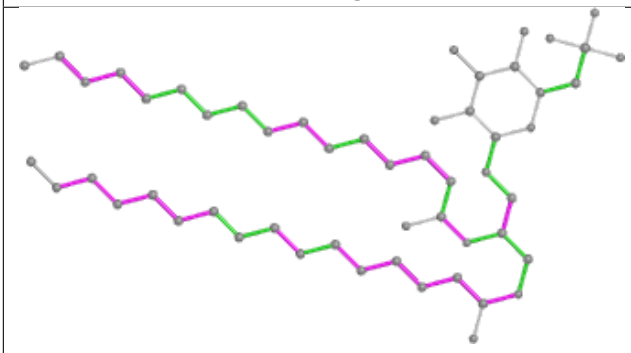

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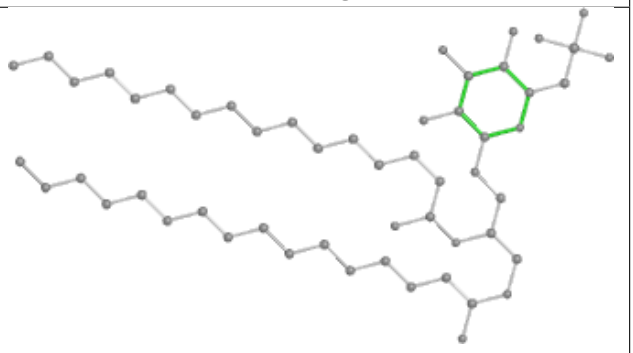
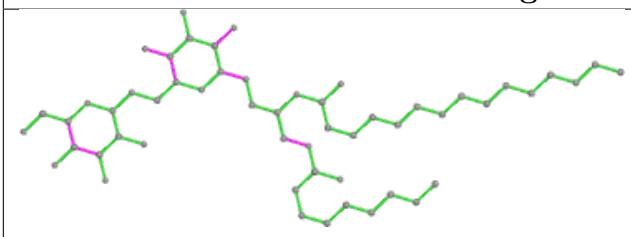


Rings

Ligand DGD B 621



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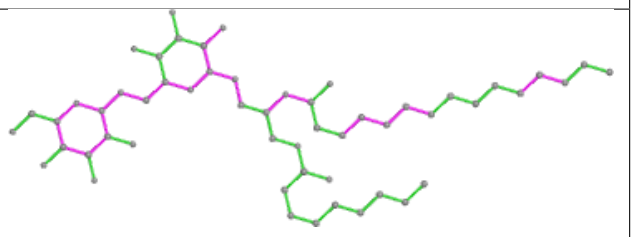
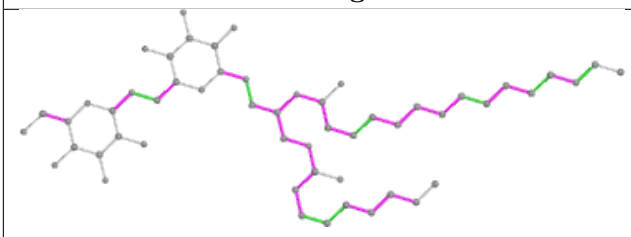


Bond angles



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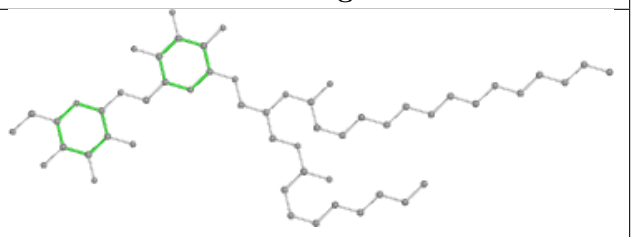
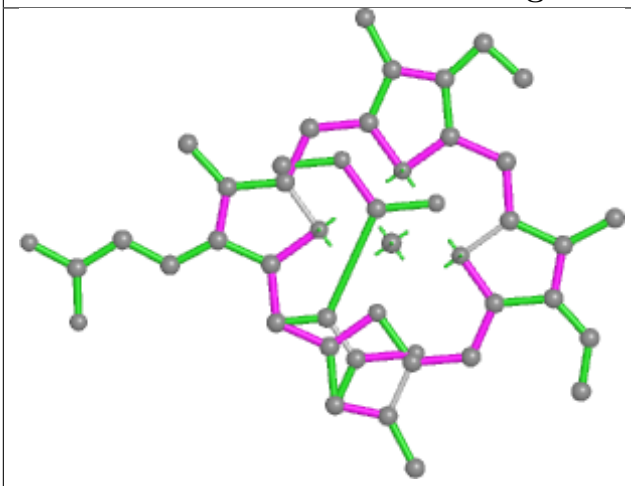


Rings

Ligand KC1 P 609



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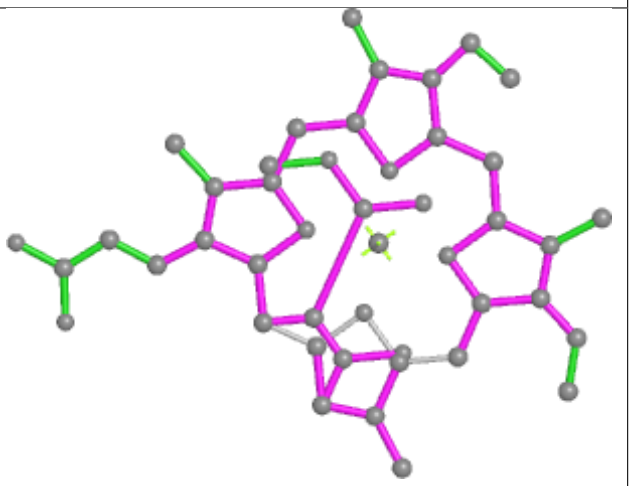
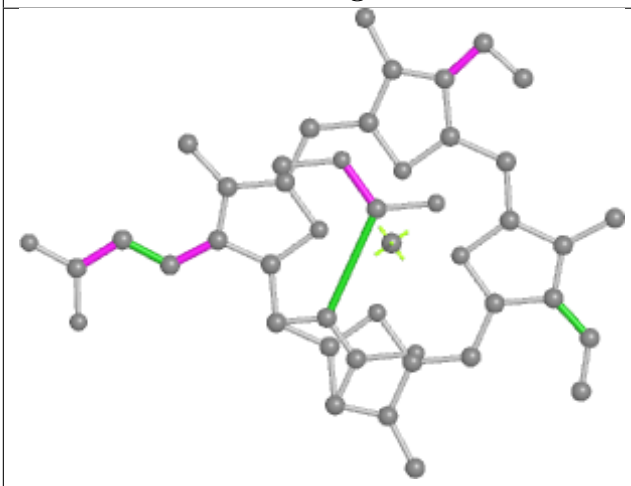


Bond angles



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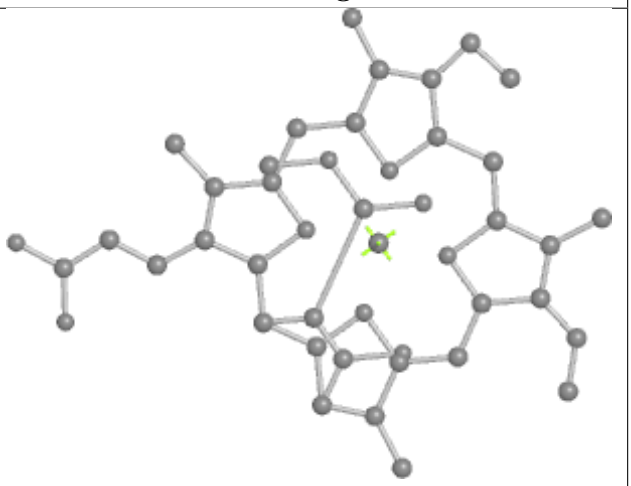
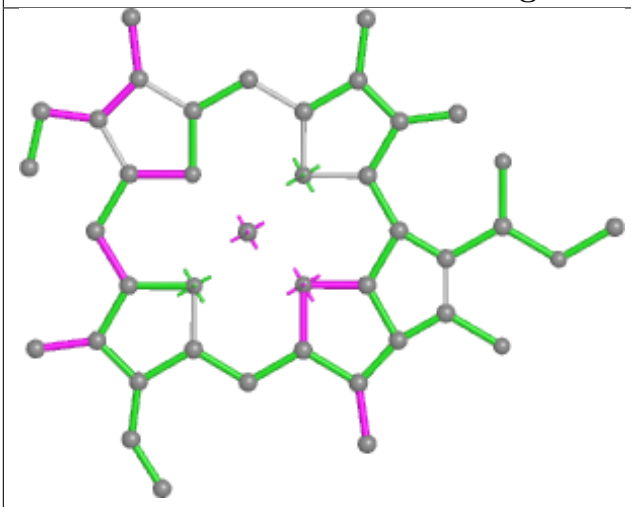
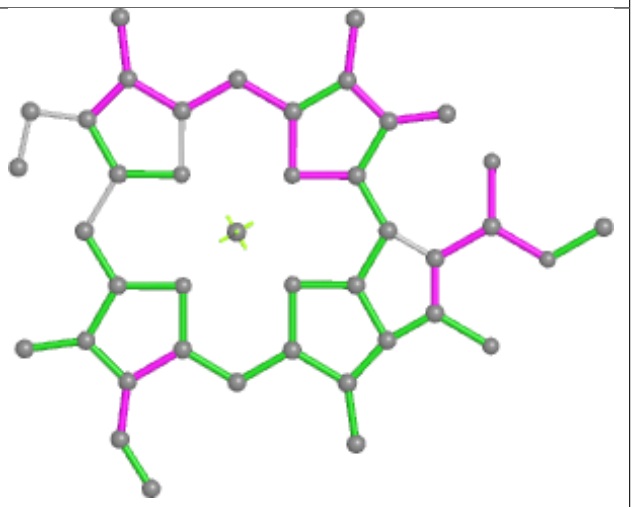


Rings

Ligand CLA 17 308



Bond lengths



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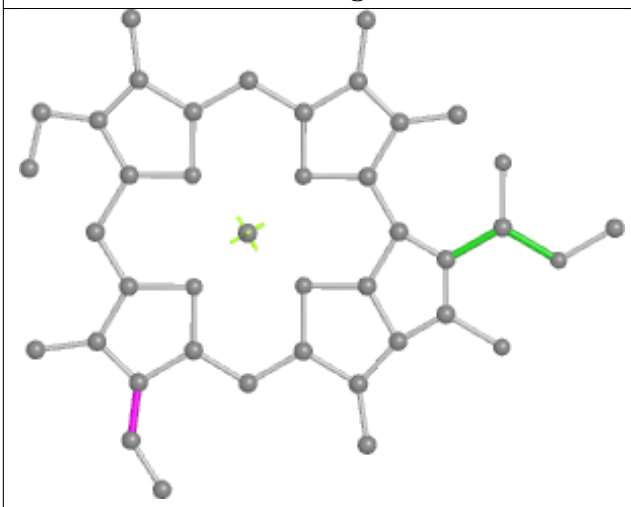
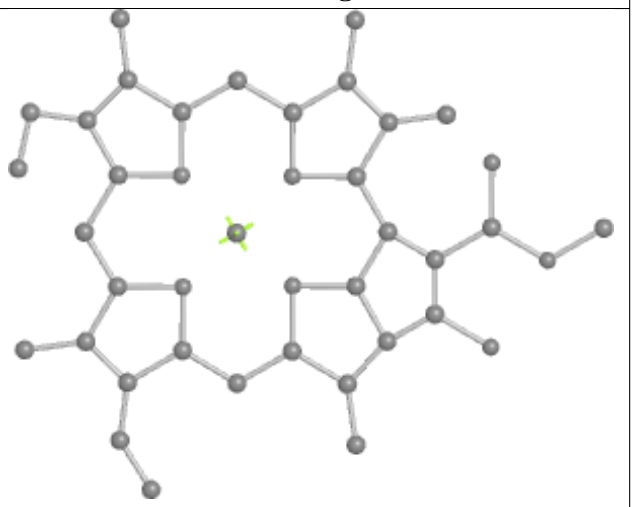
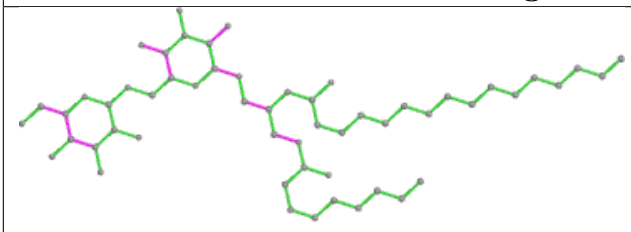


Torsions



Rings

Ligand DGD b 622



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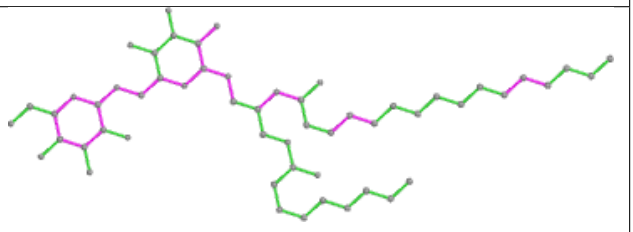

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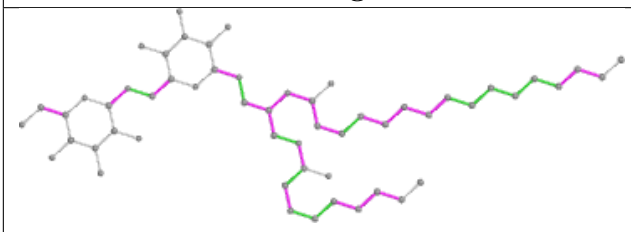

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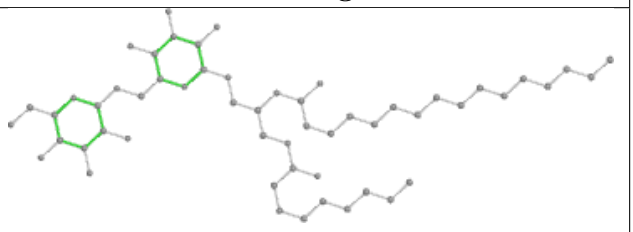
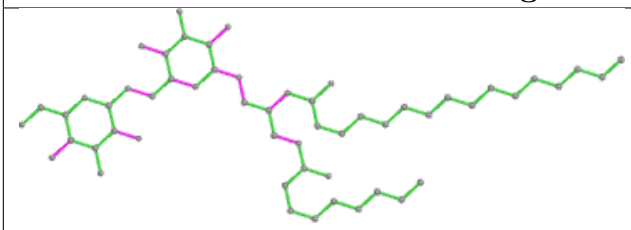


Rings

Ligand DGD C 518



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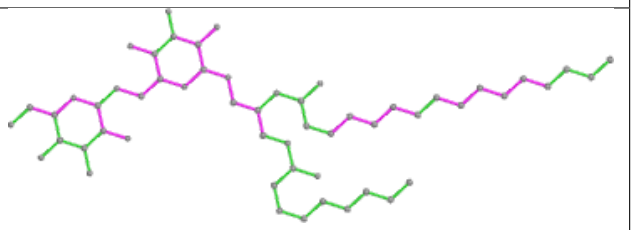

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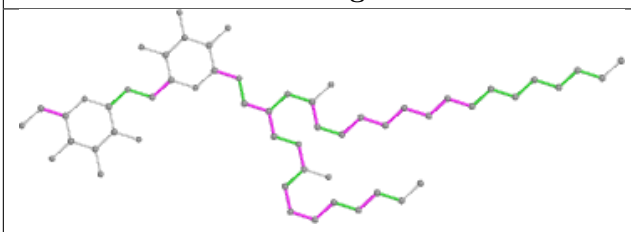

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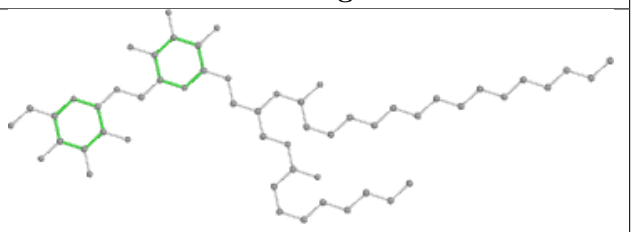
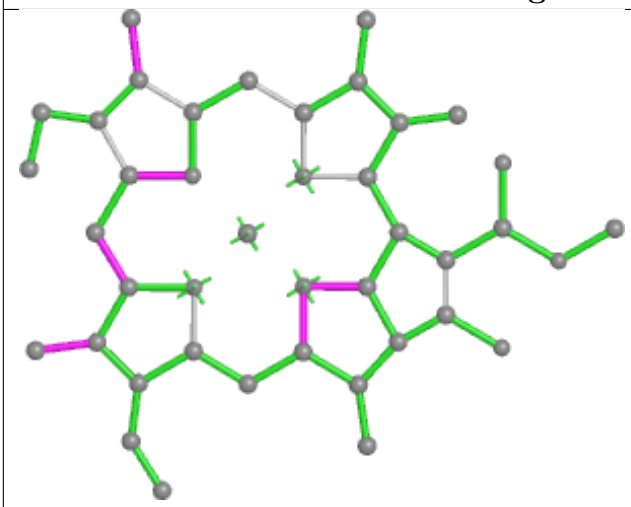


Rings

Ligand CLA 9 315



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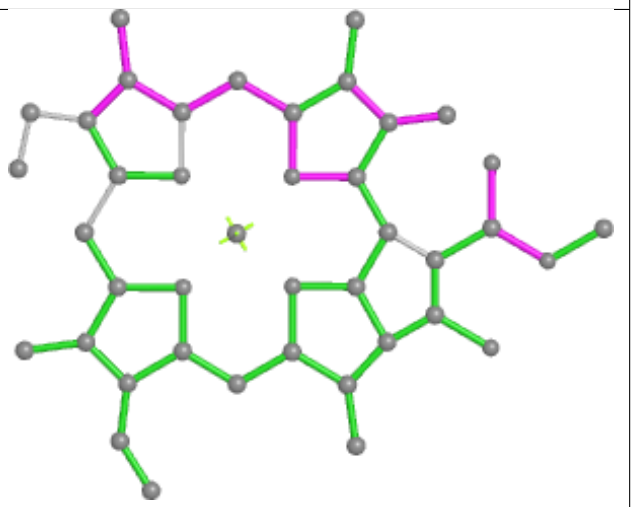

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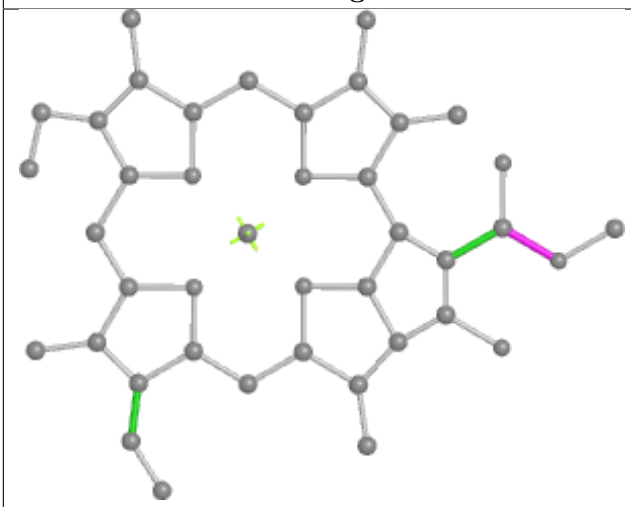

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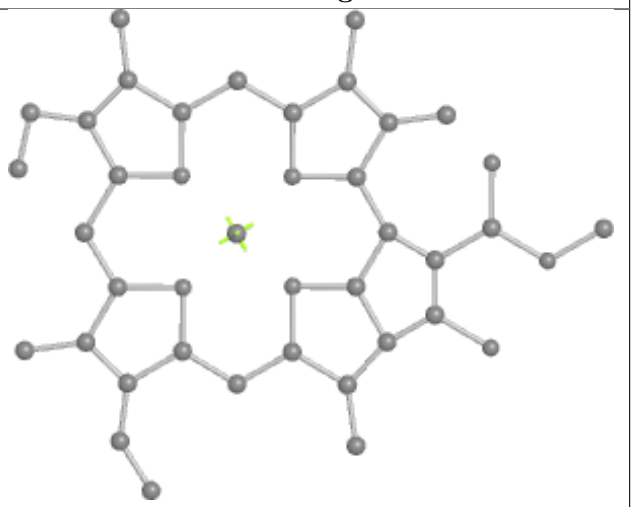
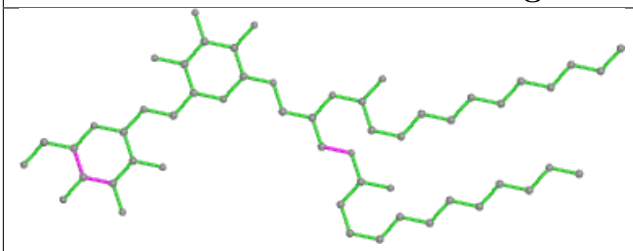


Rings

Ligand DGD 1 318



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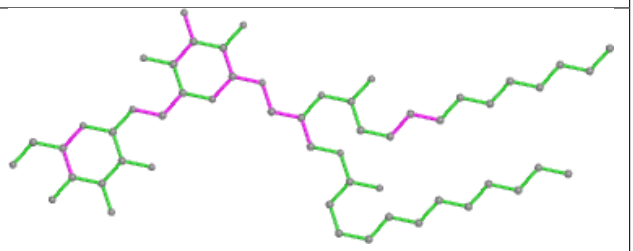

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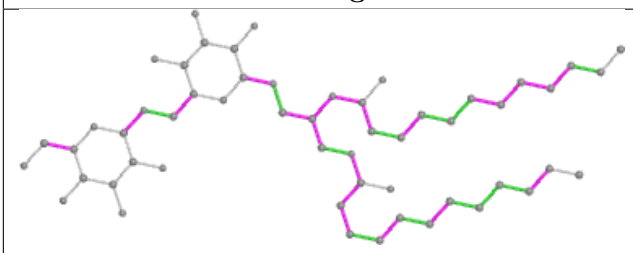

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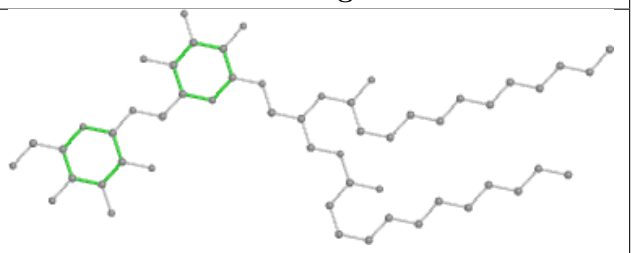
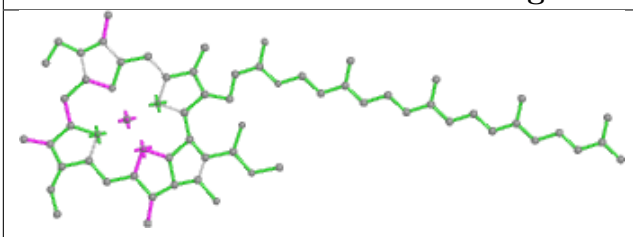


Rings

Ligand CLA b 615



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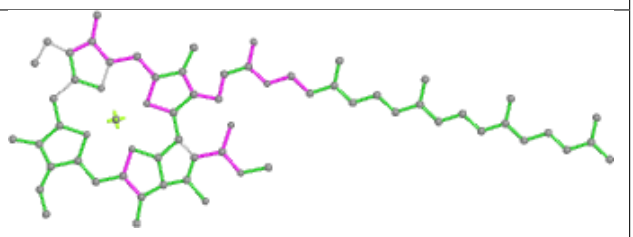

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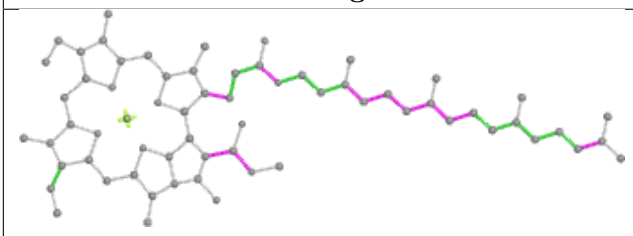

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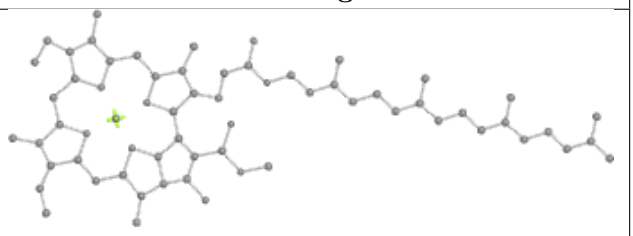
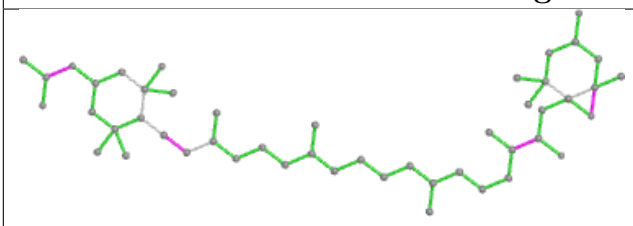


Rings

Ligand A86 6 301



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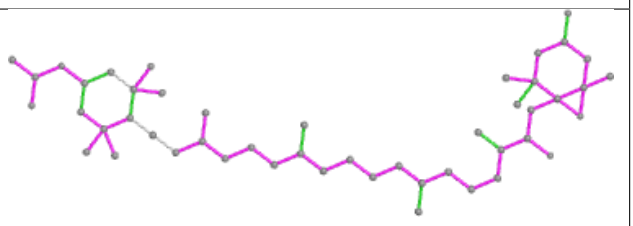

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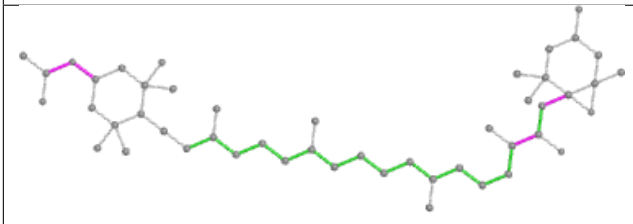

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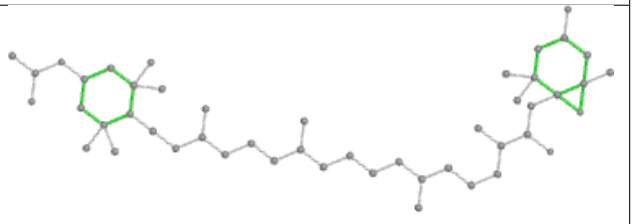
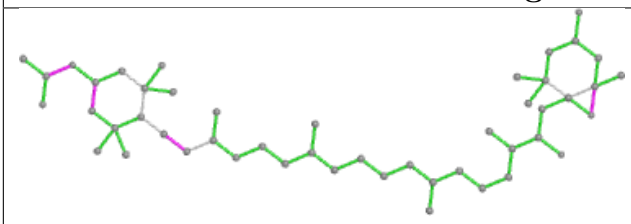


Rings

Ligand A86 17 306



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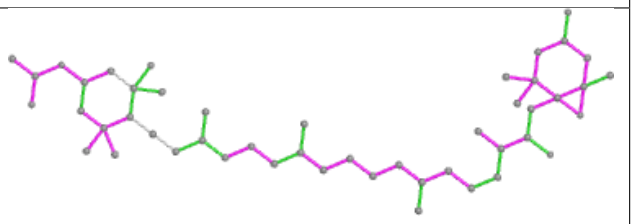

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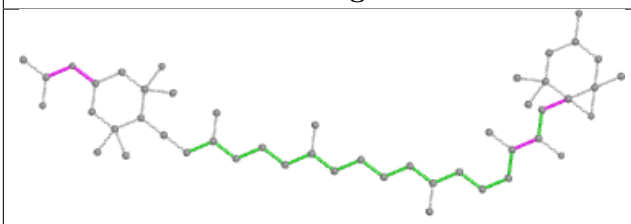

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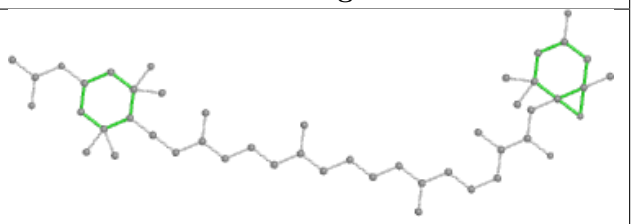
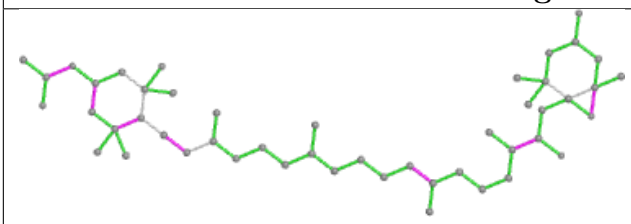


Rings

Ligand A86 5 305



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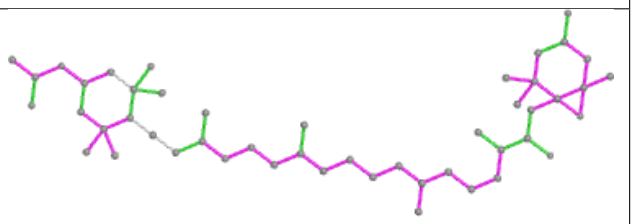

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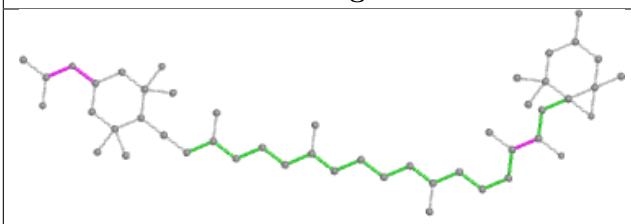

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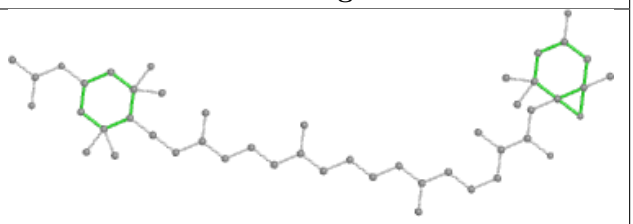
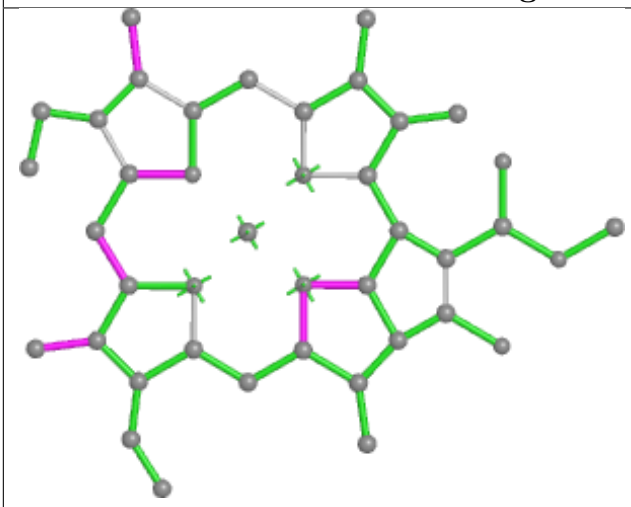


Rings

Ligand CLA 19 315



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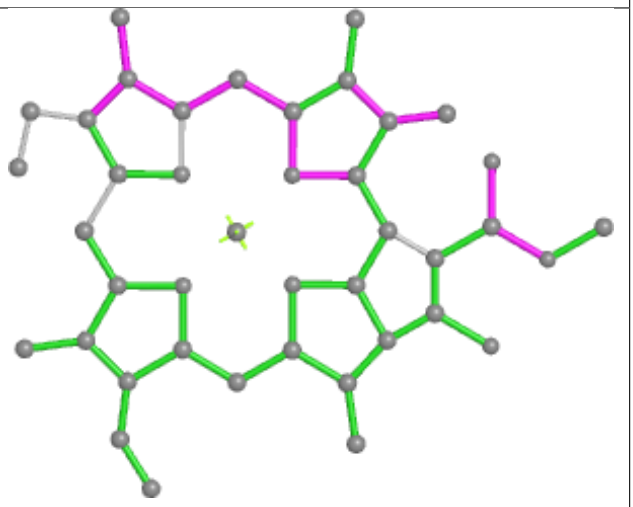

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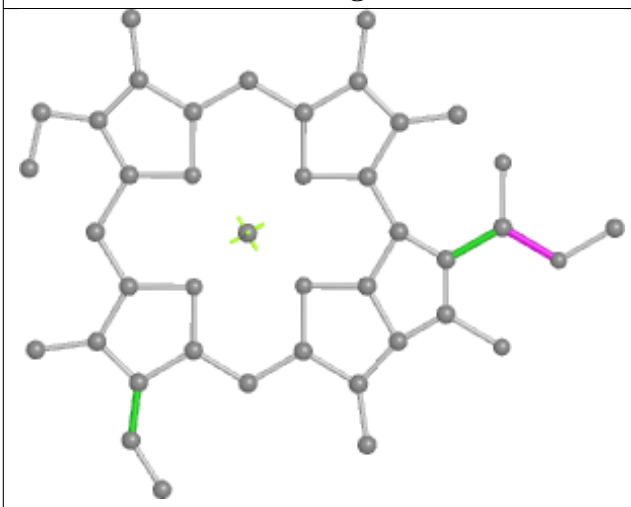

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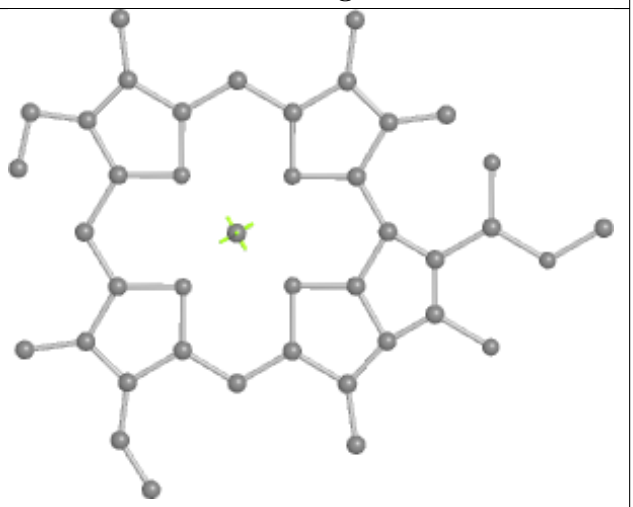
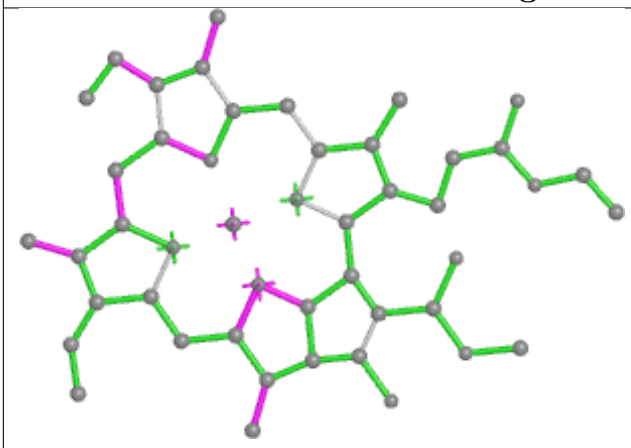


Rings

Ligand CLA 10 314



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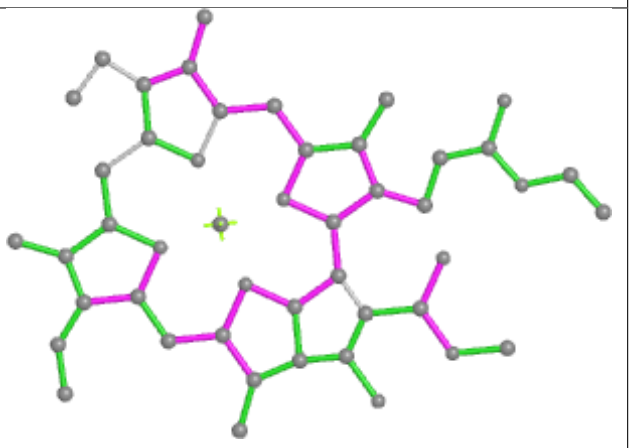

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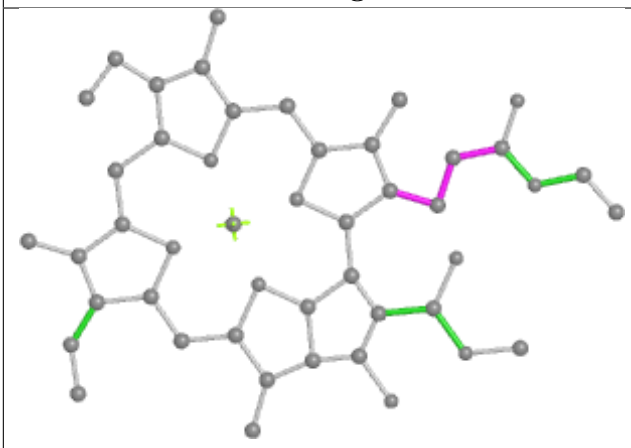

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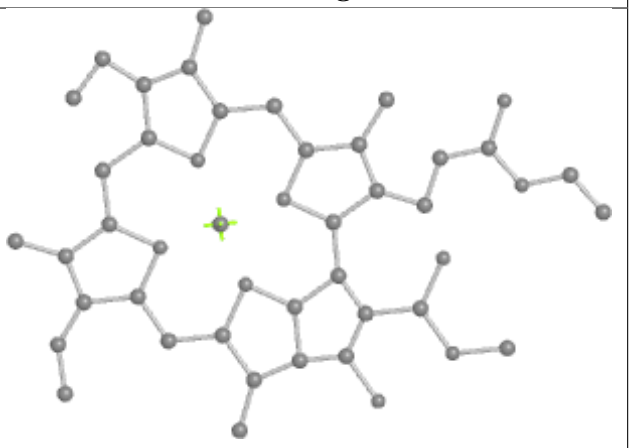
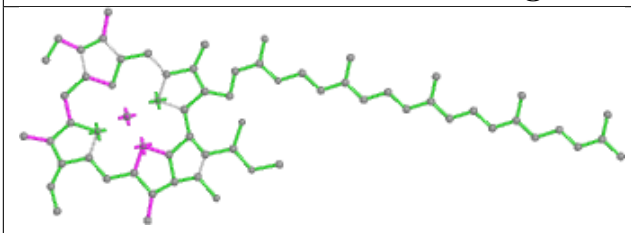


Rings

Ligand CLA C 511



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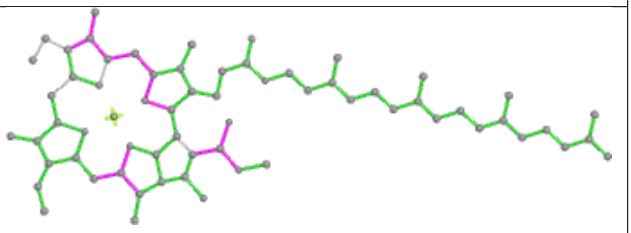

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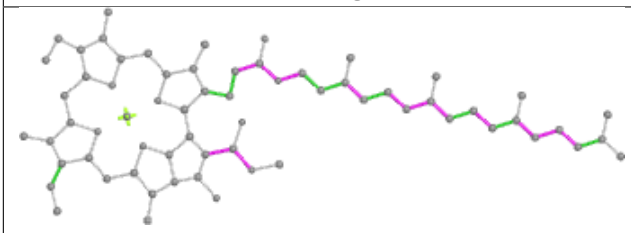

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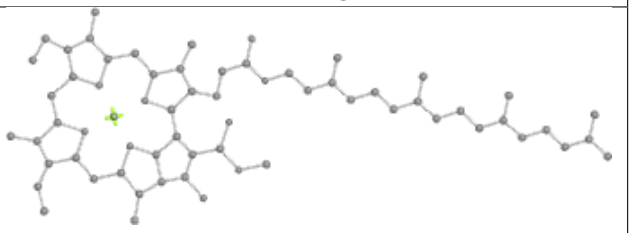
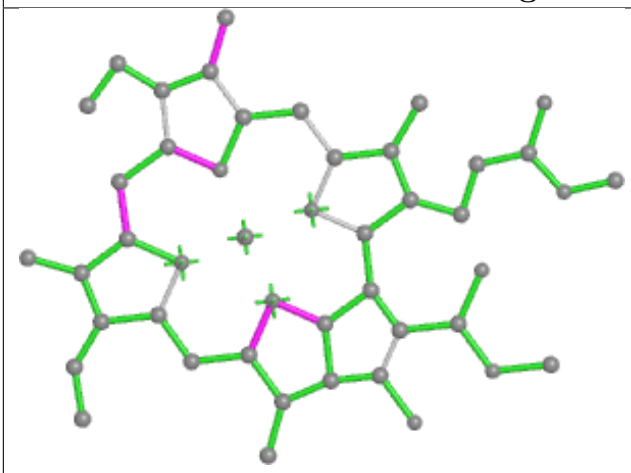


Rings

Ligand CLA 12 316



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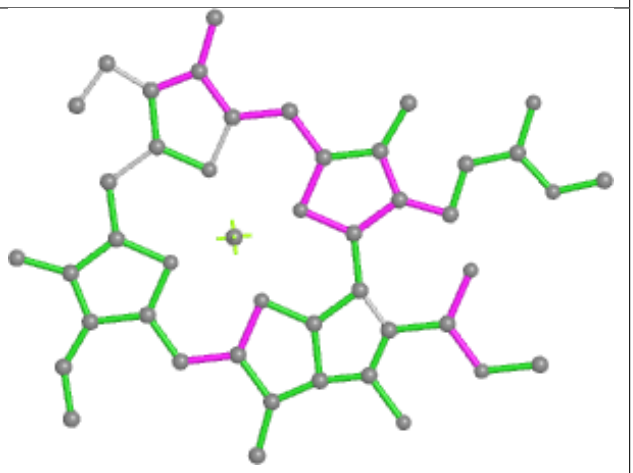

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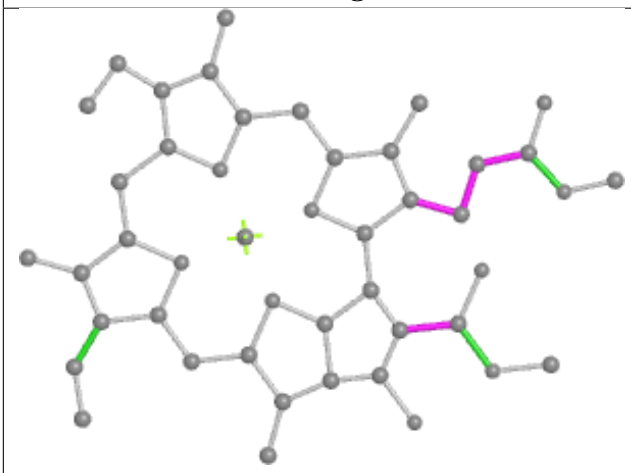

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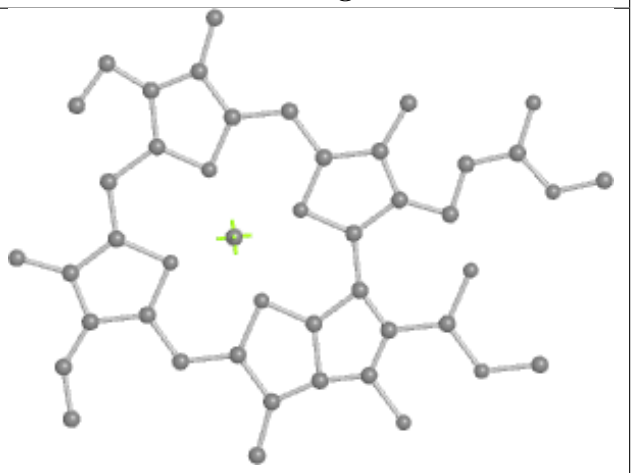
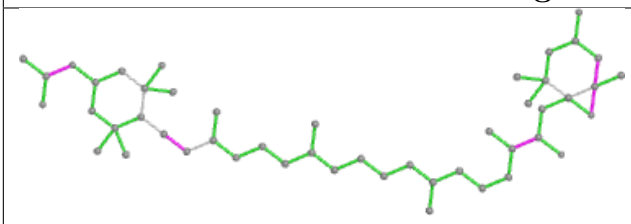


Rings

Ligand A86 7 306



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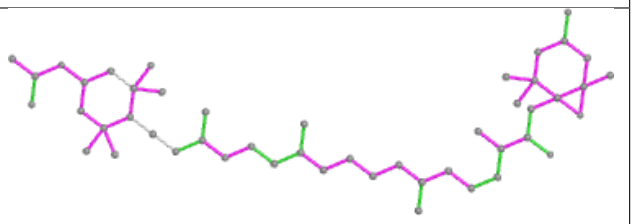
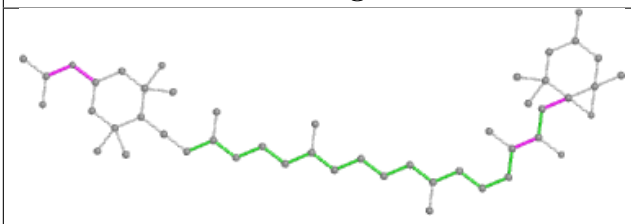
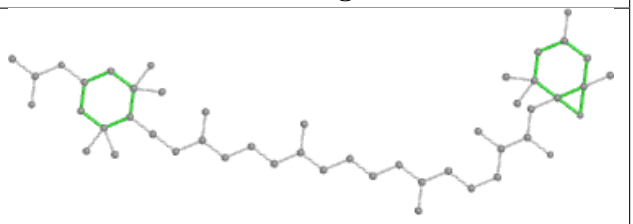


Bond angles

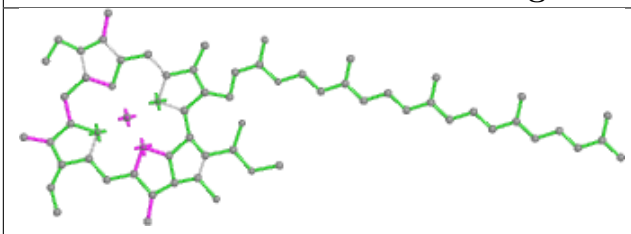


Torsions

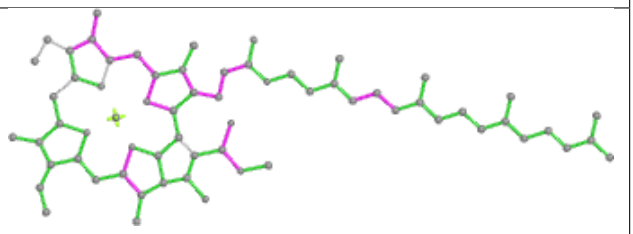


Rings

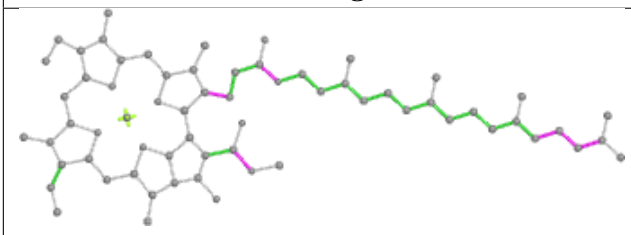
Ligand CLA a 403



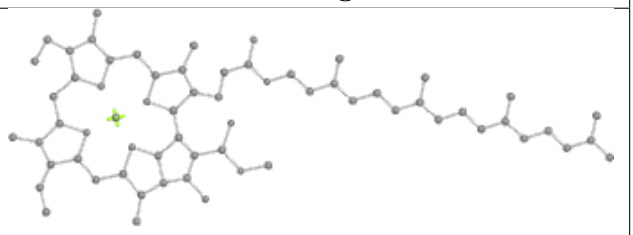
Bond lengths



Bond angles

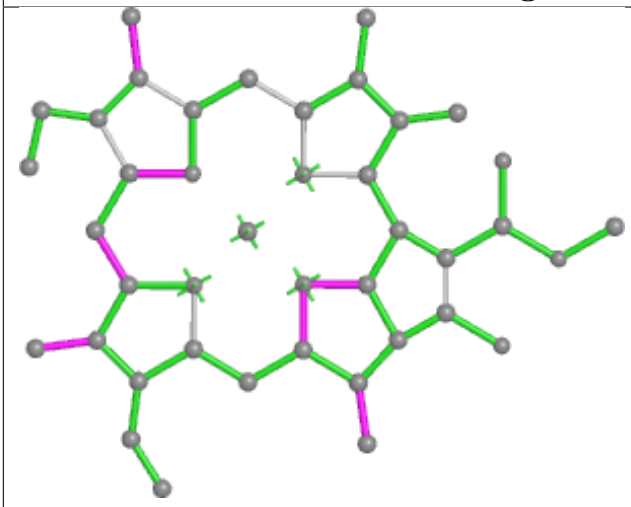


Torsions



Rings

Ligand CLA 11 316



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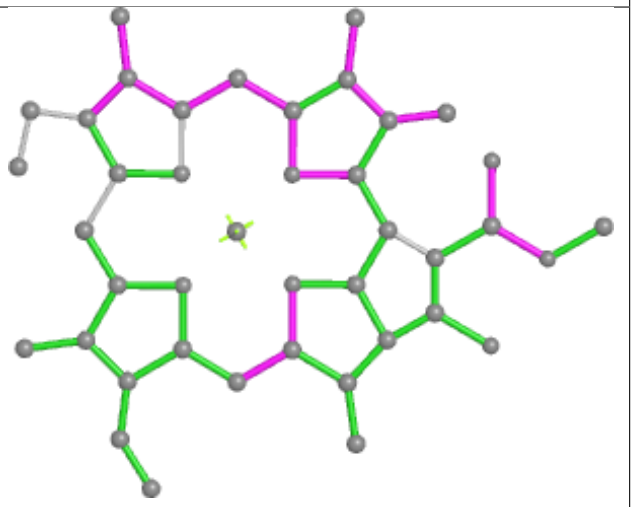

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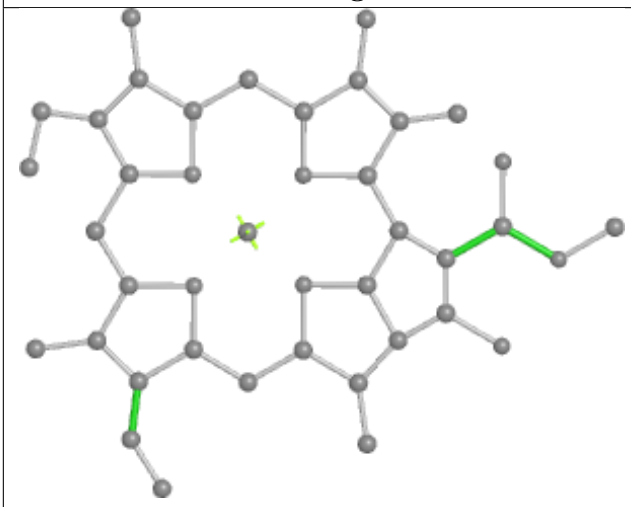

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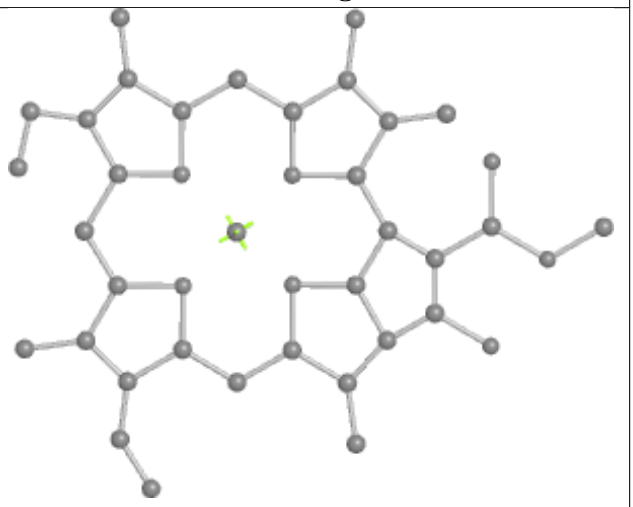
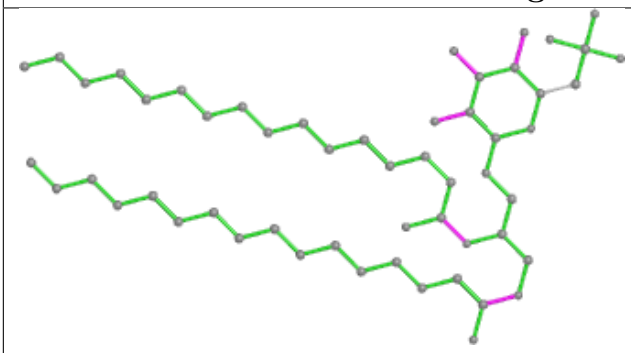


Rings

Ligand SQD b 601



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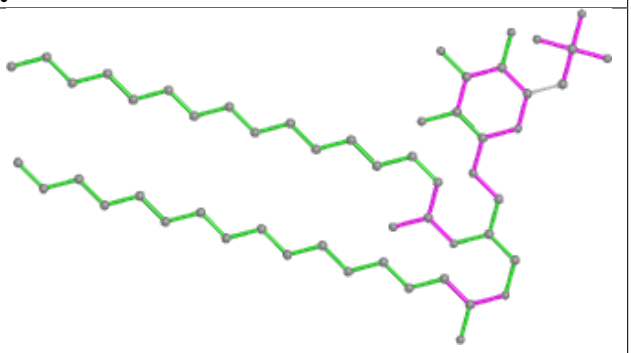

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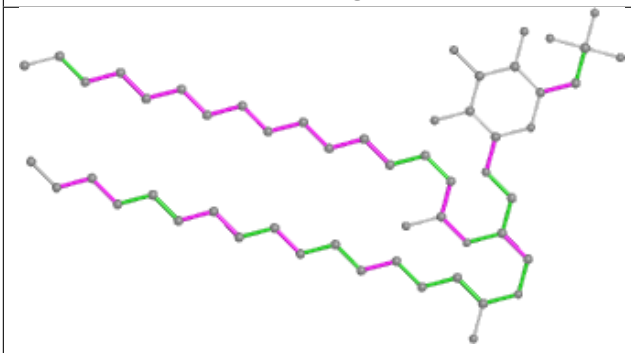

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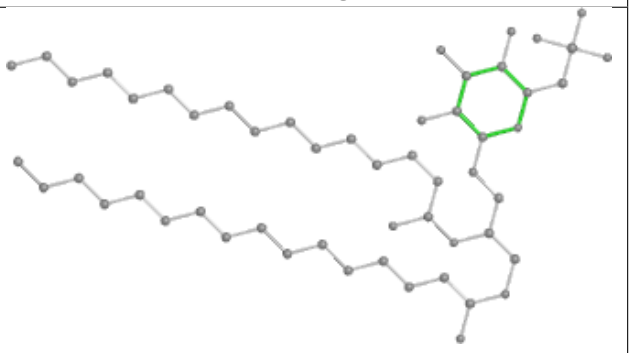
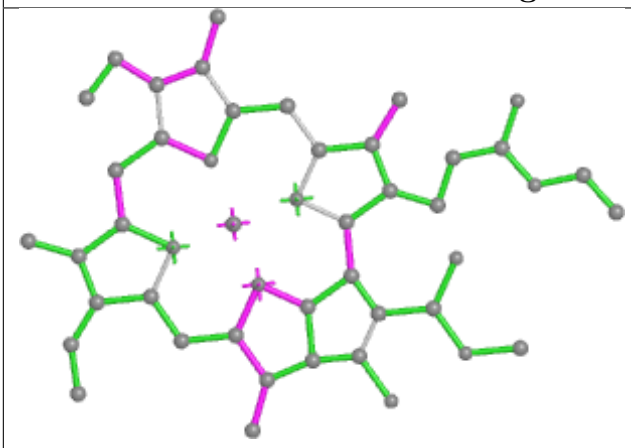


Rings

Ligand CLA 15 312



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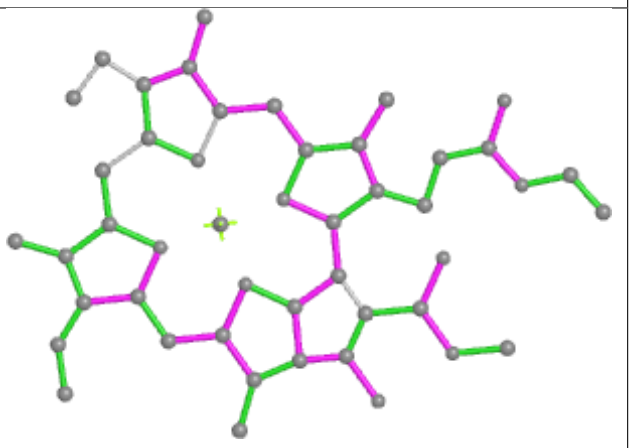

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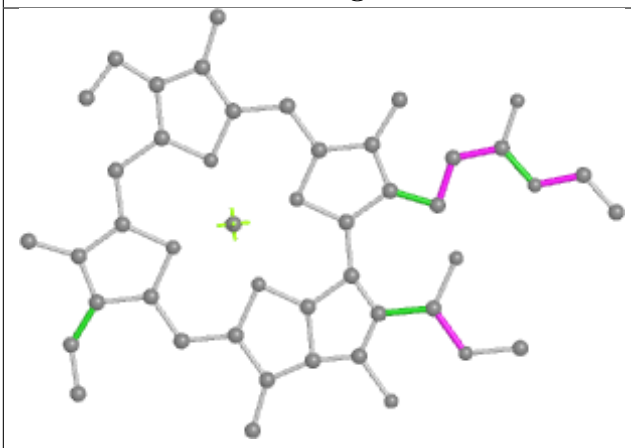

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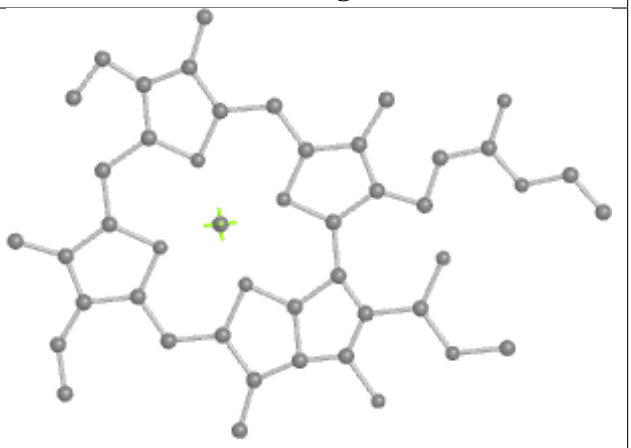
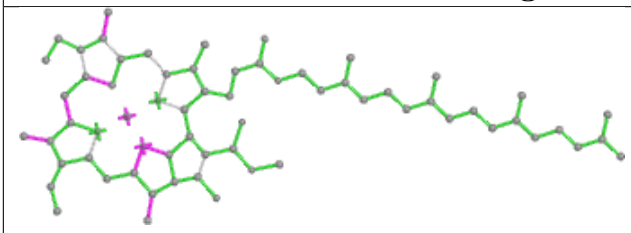


Rings

Ligand CLA 12 308



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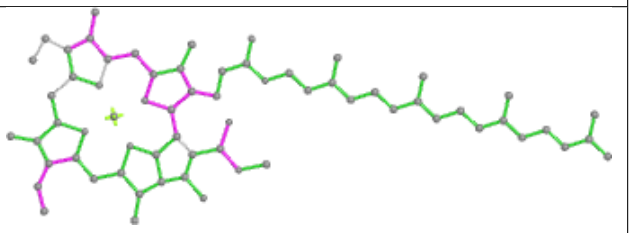

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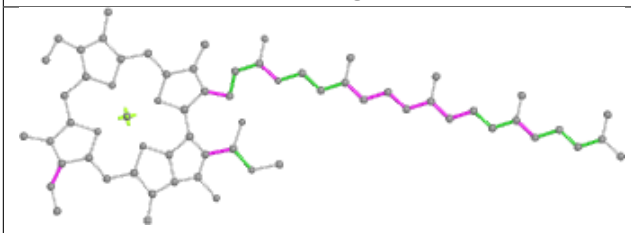

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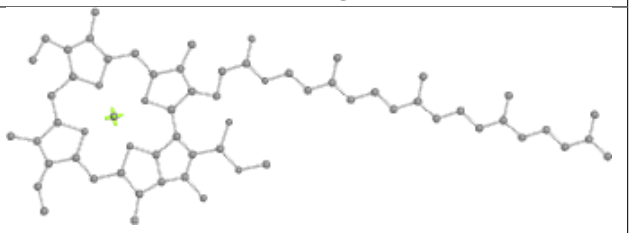
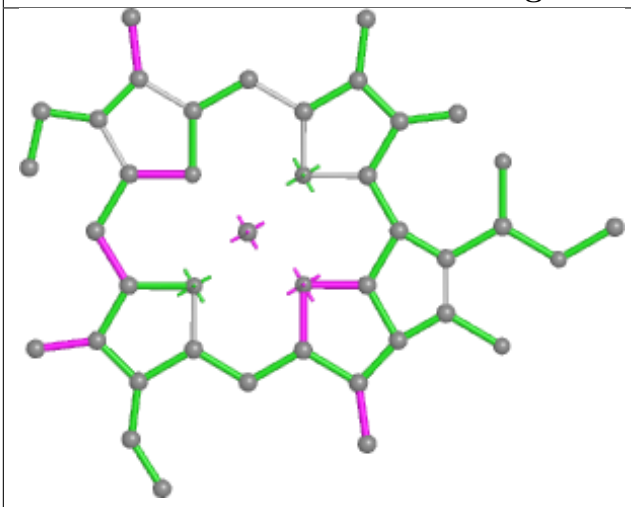


Rings

Ligand CLA P 610



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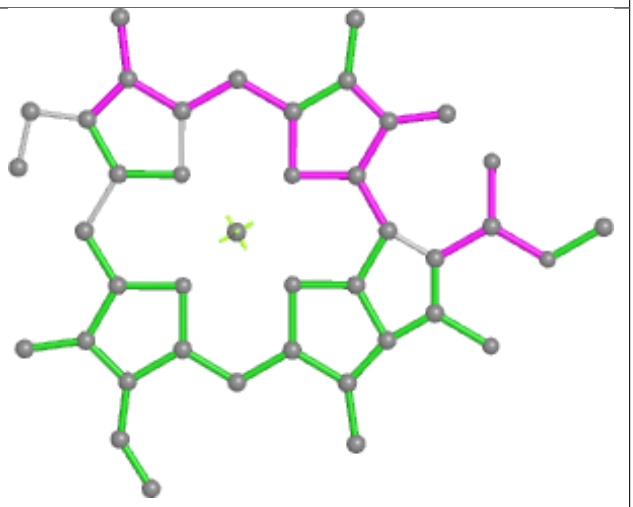

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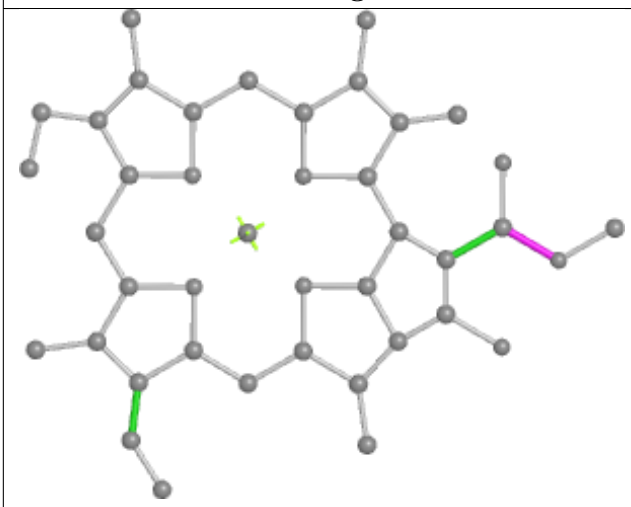

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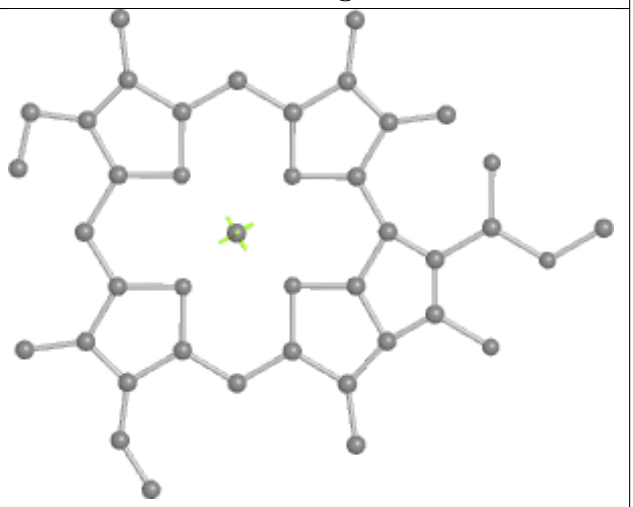
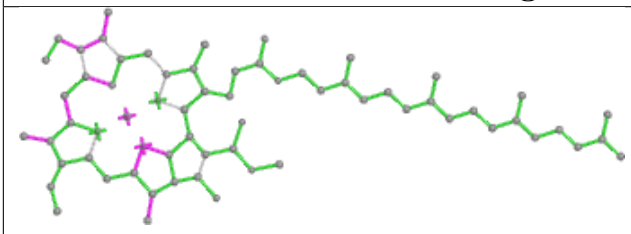


Rings

Ligand CLA 16 309



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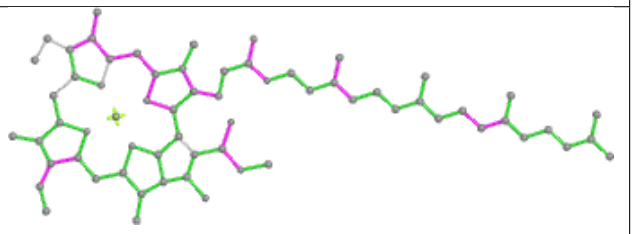

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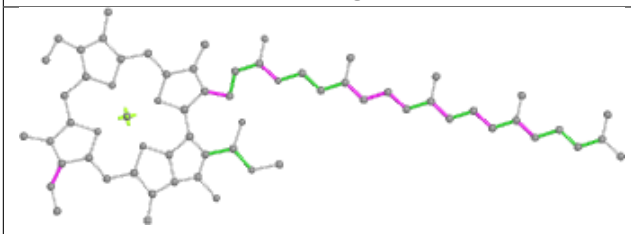

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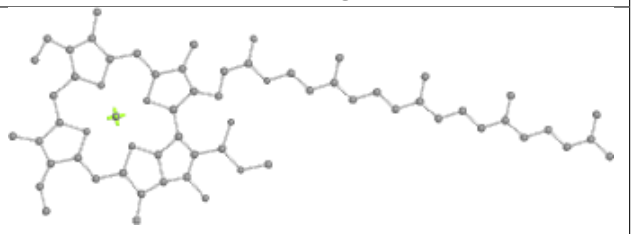
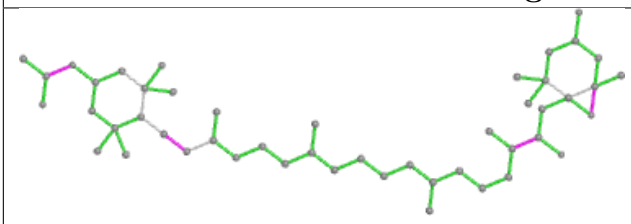


Rings

Ligand A86 16 302



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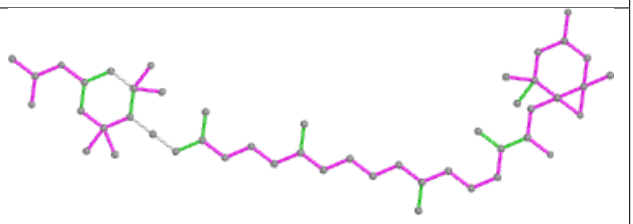

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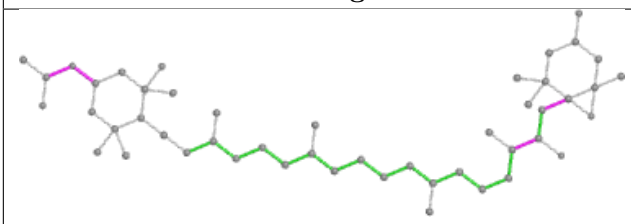

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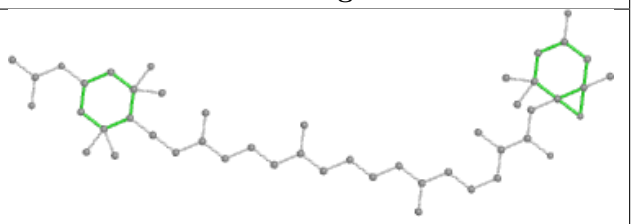
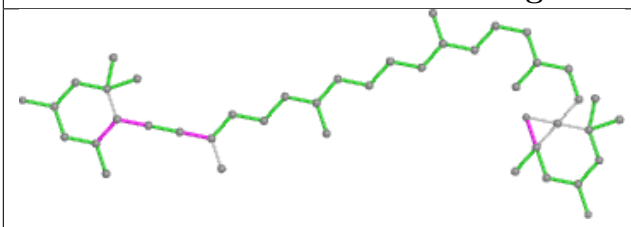


Rings

Ligand DD6 P 612



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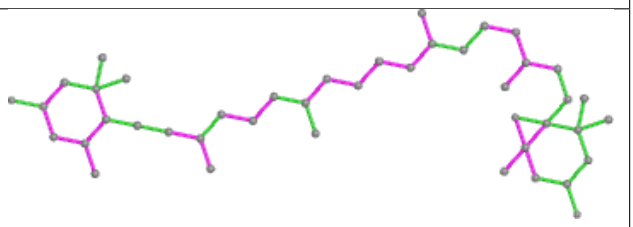

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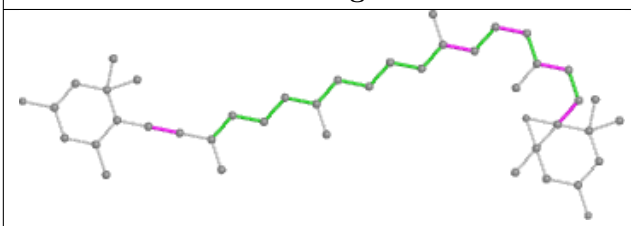

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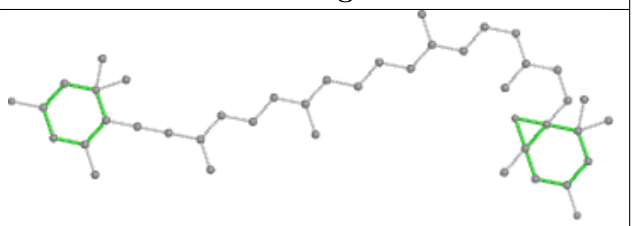
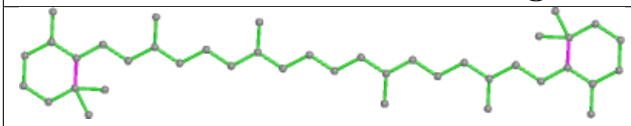


Rings

Ligand BCR c 515



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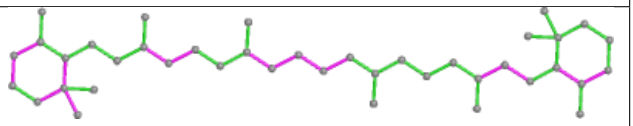

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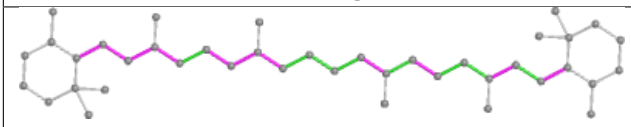

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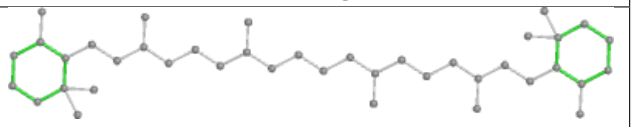
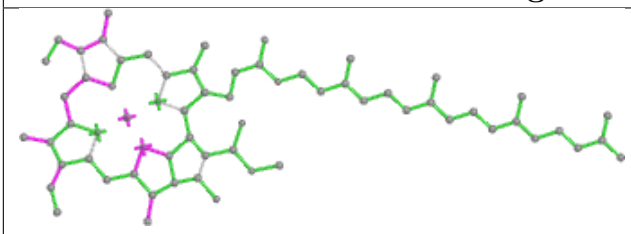


Rings

Ligand CLA b 606



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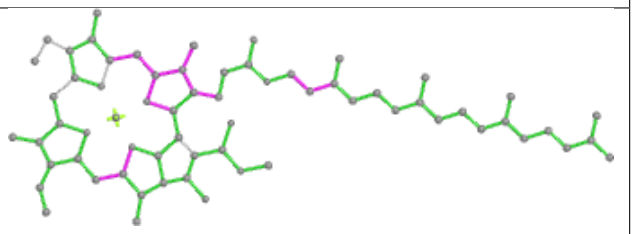

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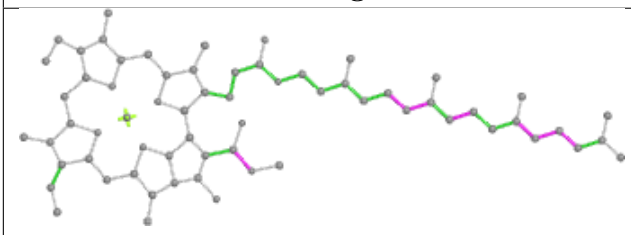

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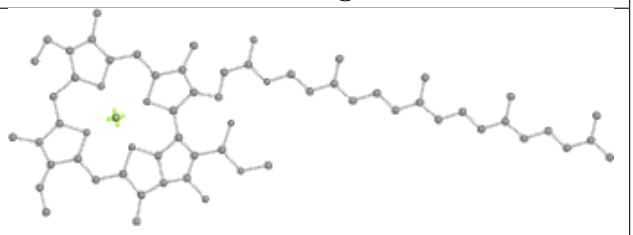
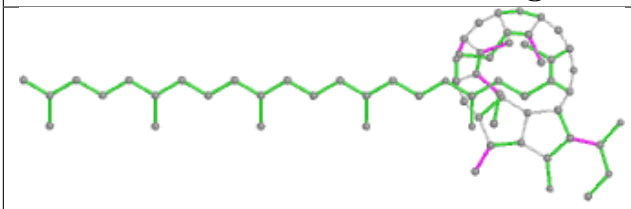


Rings

Ligand PHO a 405



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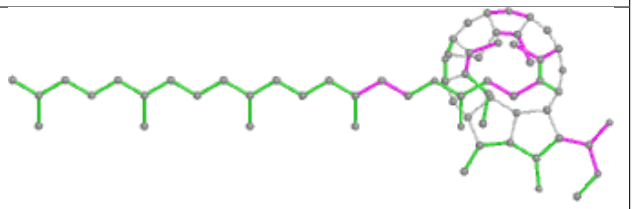
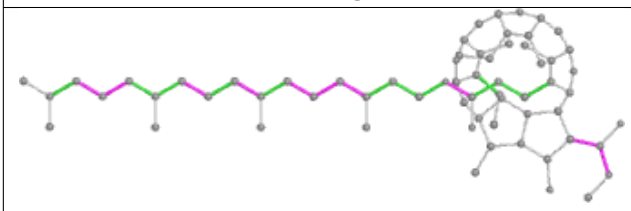
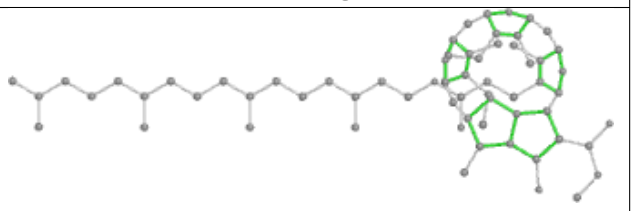


Bond angles

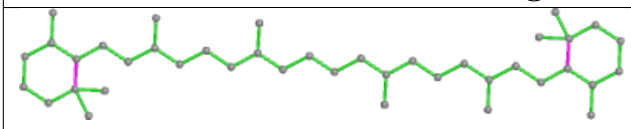


Torsions



Rings

Ligand BCR b 618



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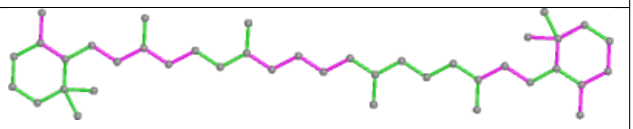
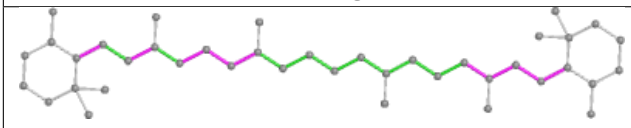


Bond angles



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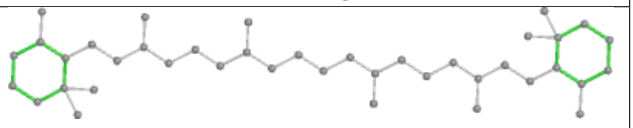
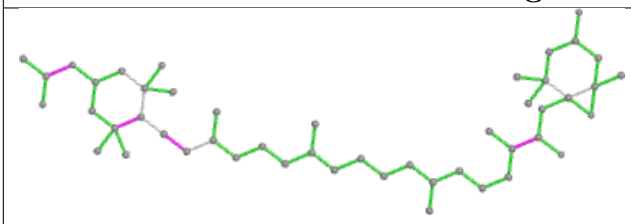


Rings

Ligand A86 18 305



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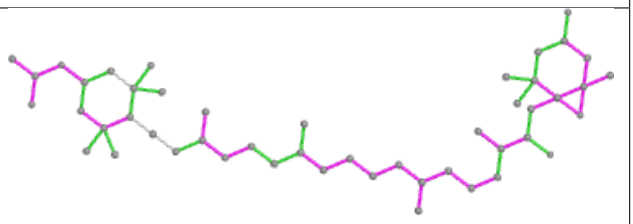
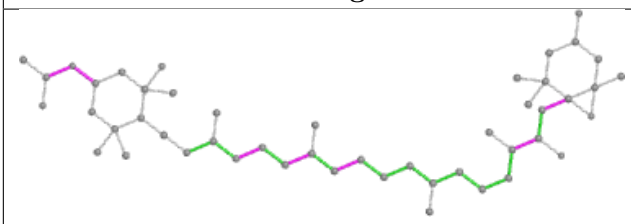


Bond angles



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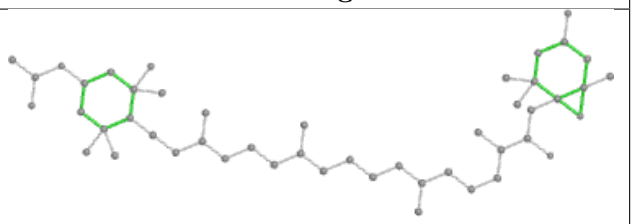
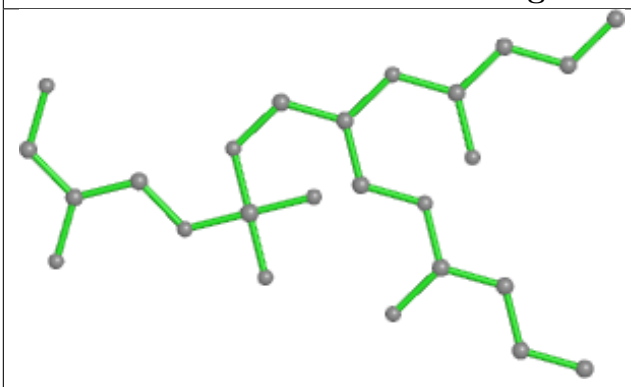
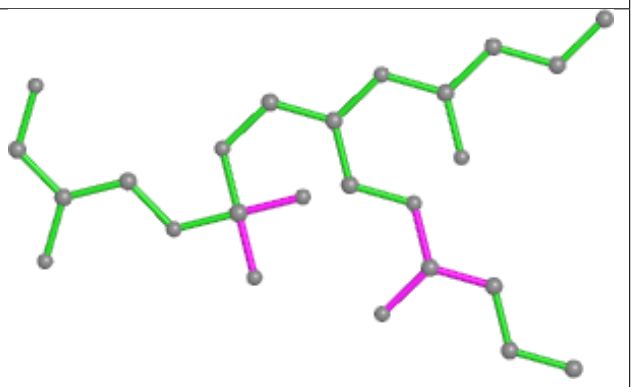


Rings

Ligand LHG z 102



Bond lengths



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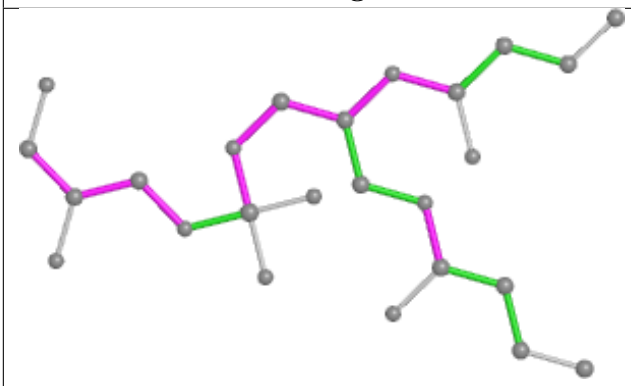
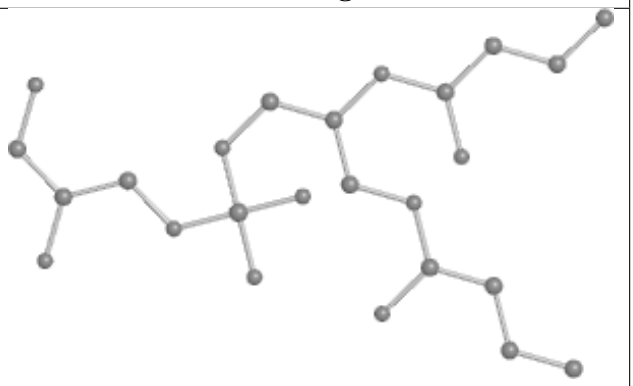
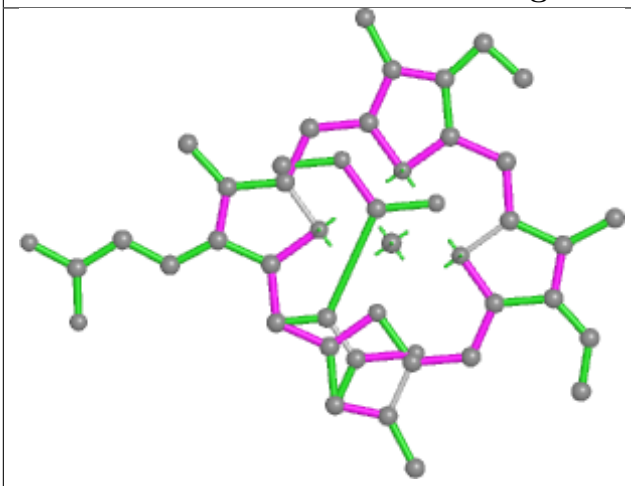


Torsions



Rings

Ligand KC1 7 314



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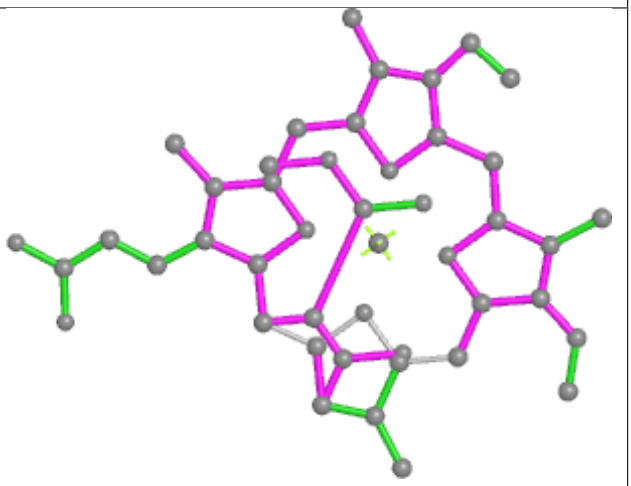

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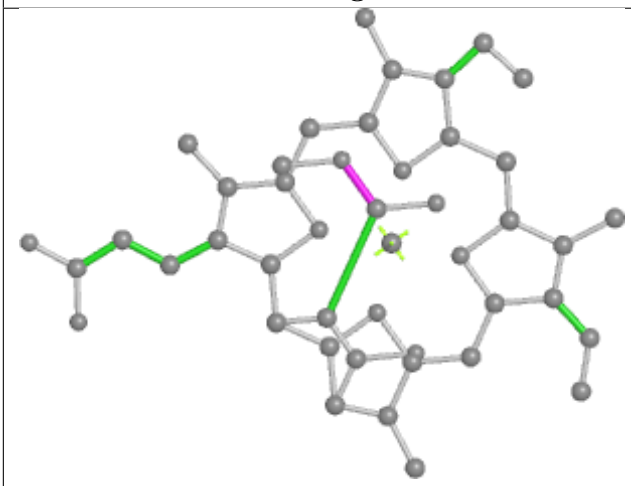

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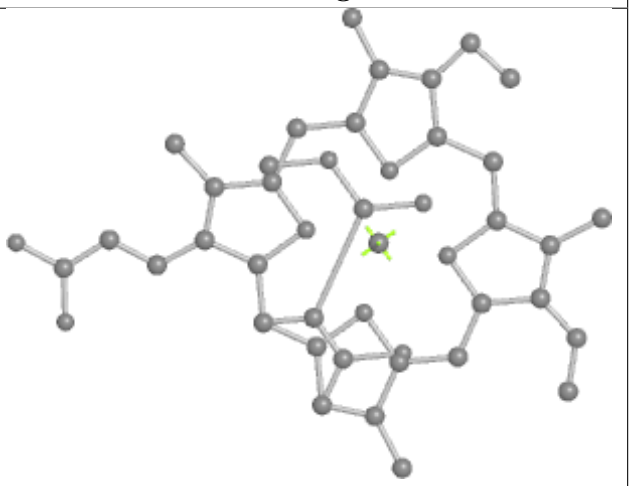
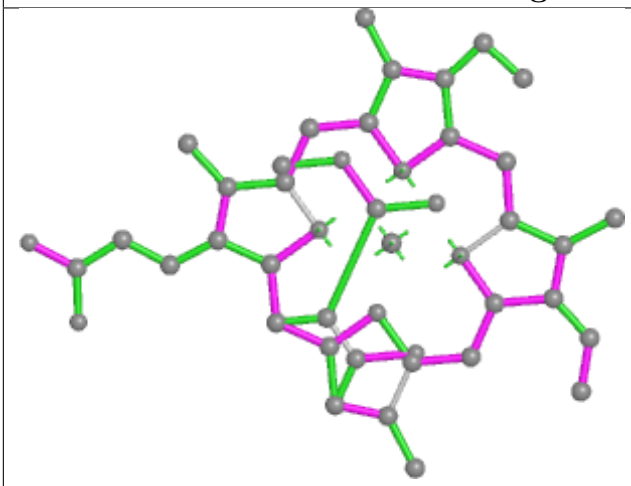


Rings

Ligand KC2 5 310



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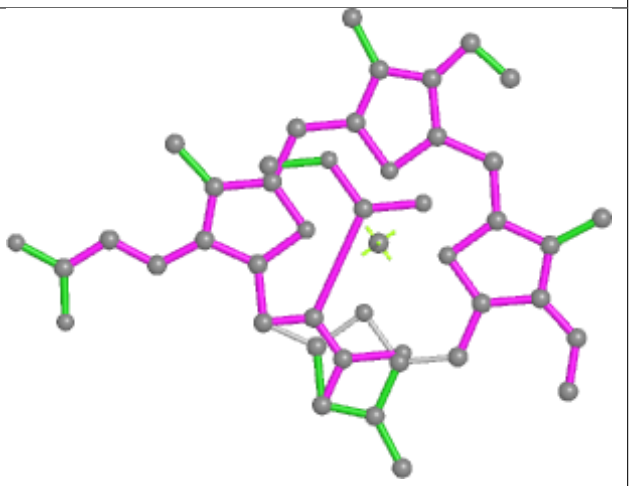

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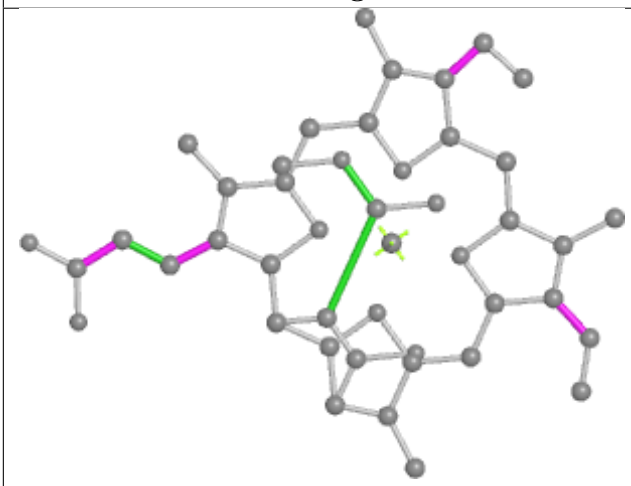

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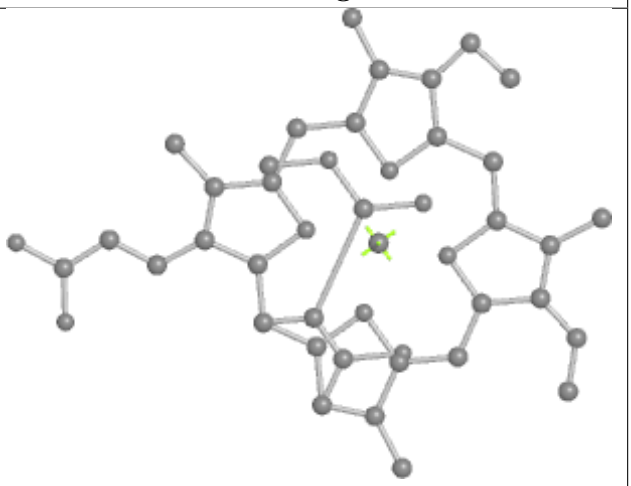
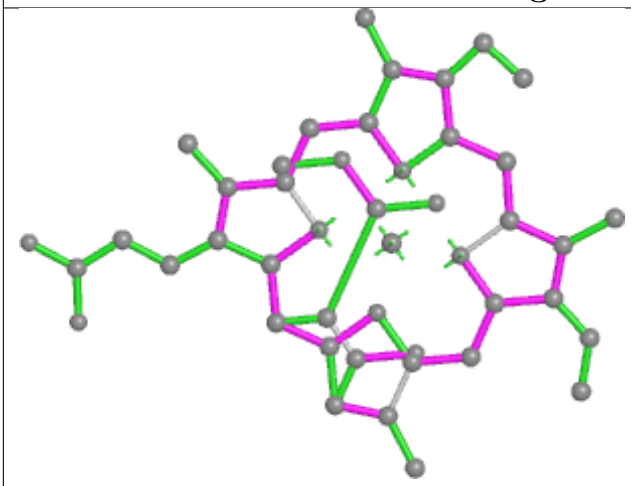


Rings

Ligand KC1 9 314



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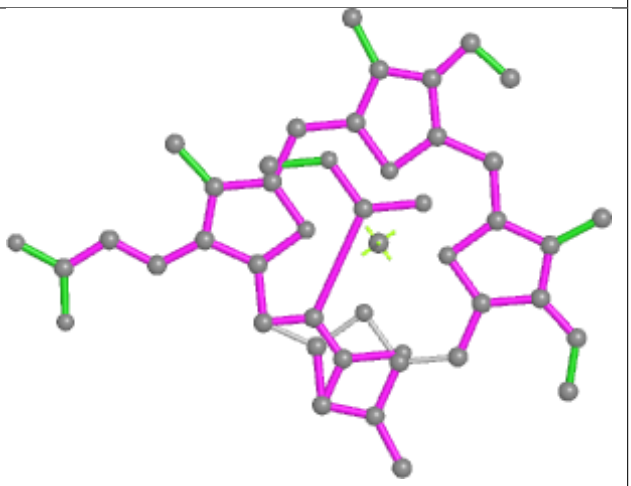

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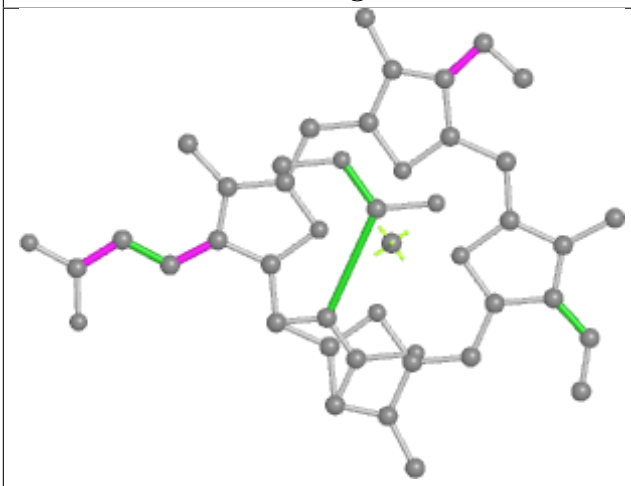

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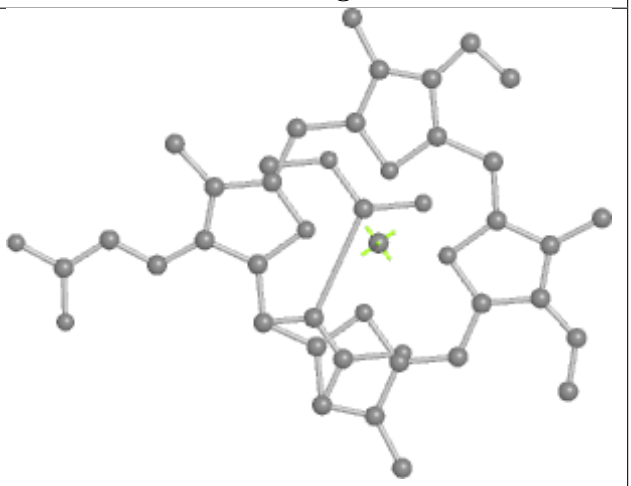
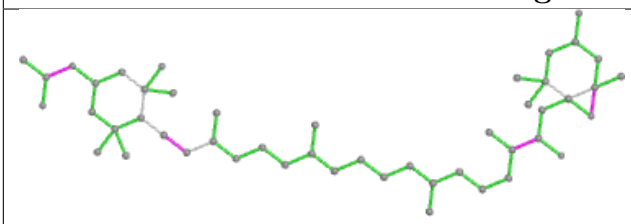


Rings

Ligand A86 3 303



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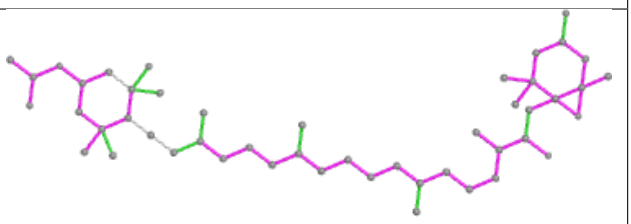

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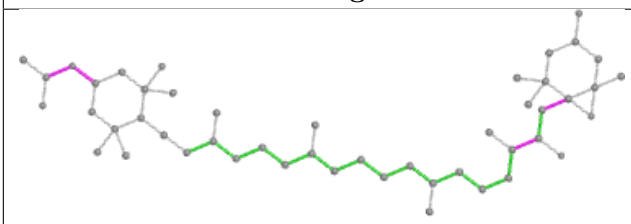

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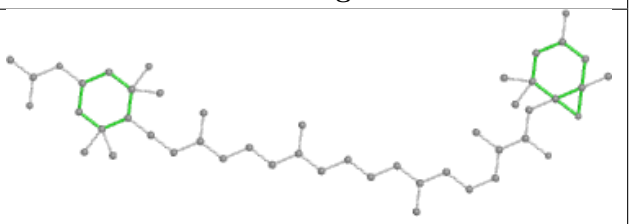
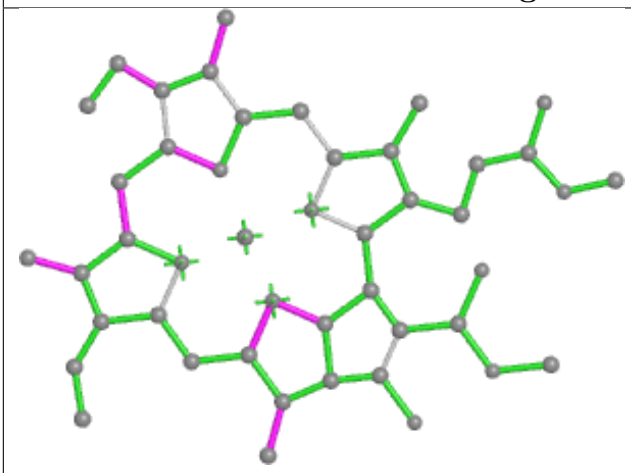


Rings

Ligand CLA 10 316



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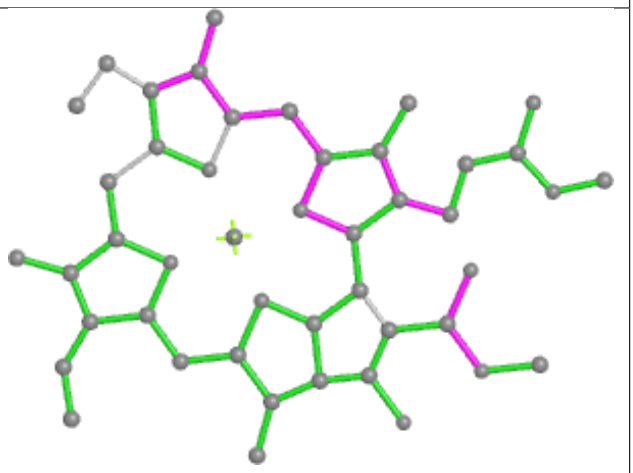

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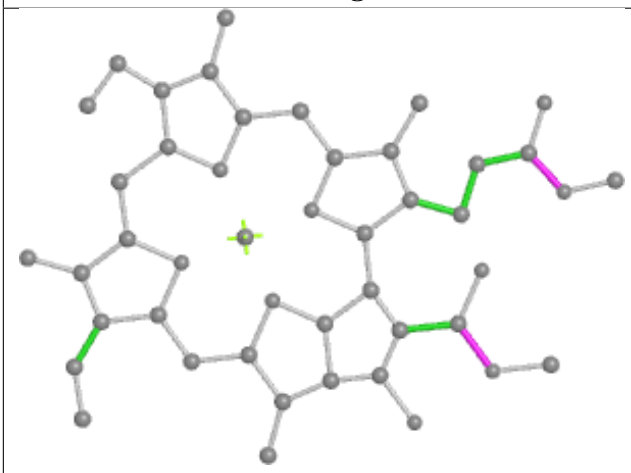

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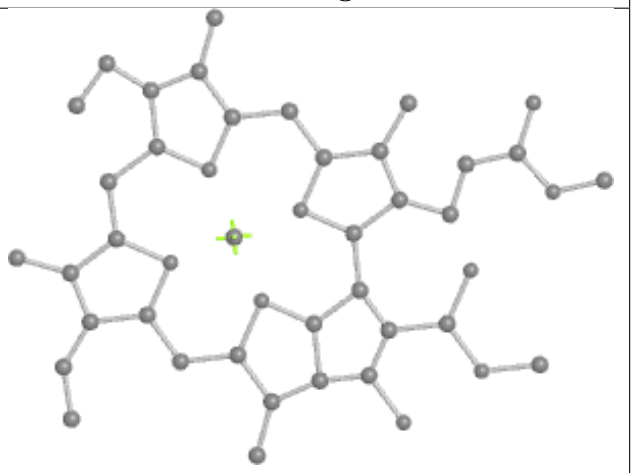
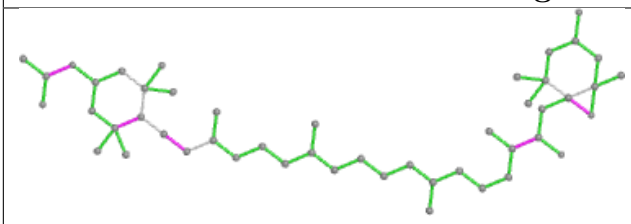


Rings

Ligand A86 0 304



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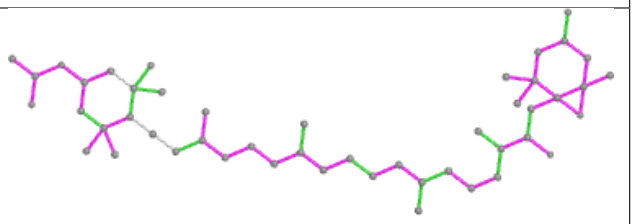

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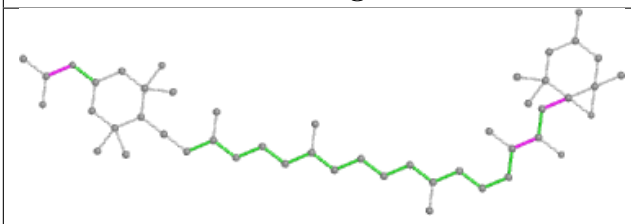

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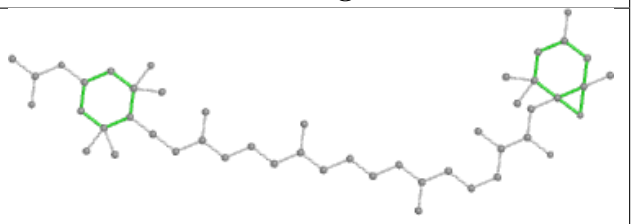
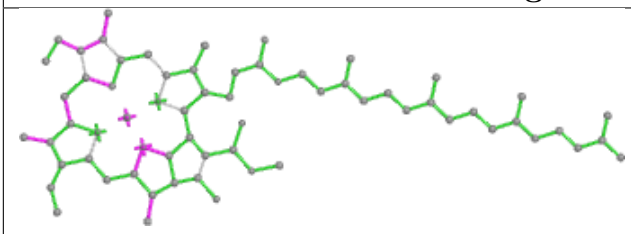


Rings

Ligand CLA P 601



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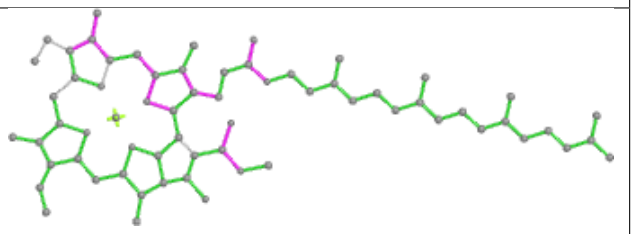

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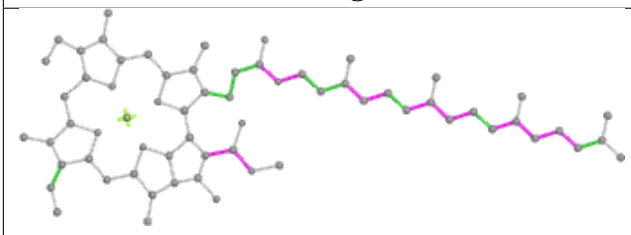

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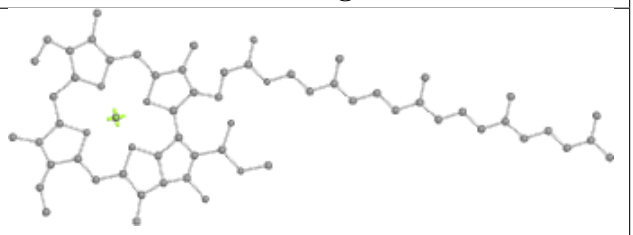
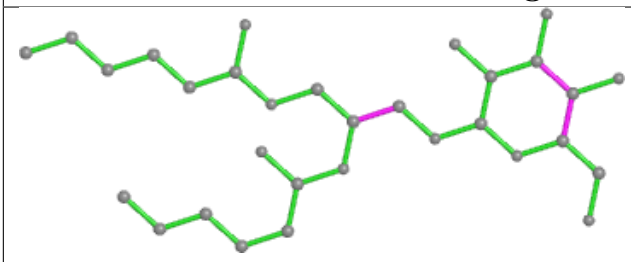


Rings

Ligand LMG 0 317



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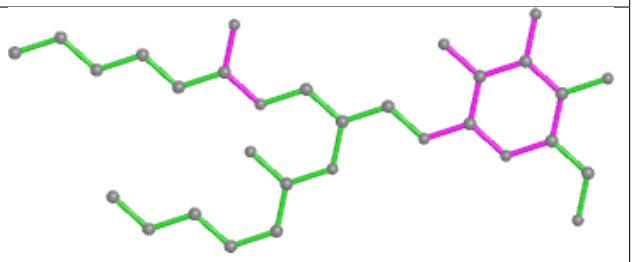

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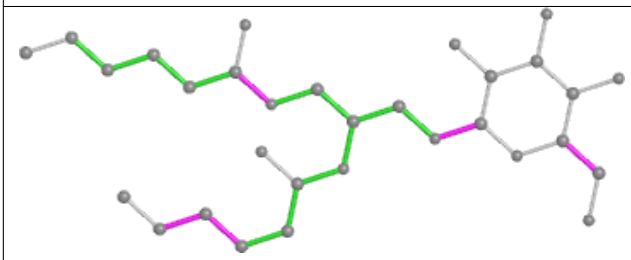

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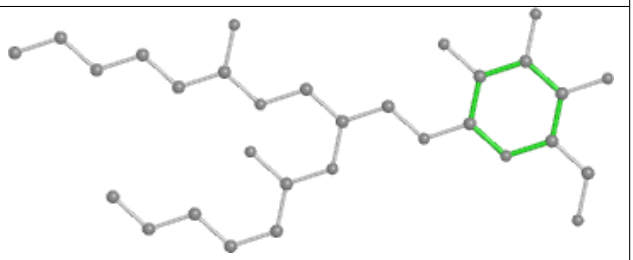
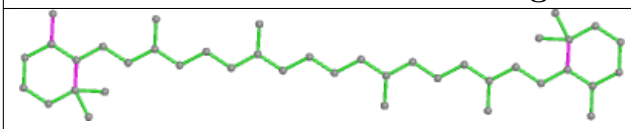


Rings

Ligand BCR f 101



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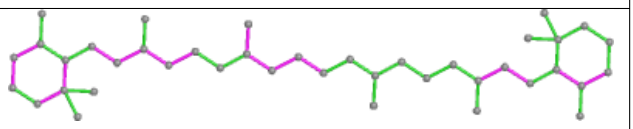

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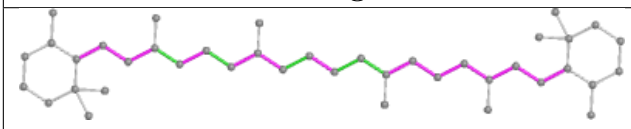

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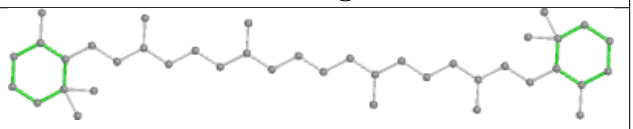
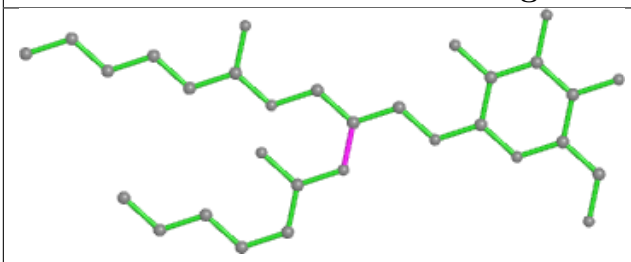


Rings

Ligand LMG P 614



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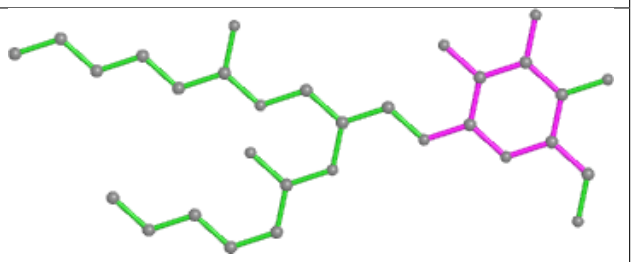

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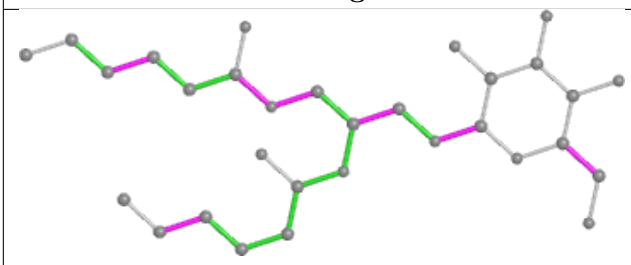

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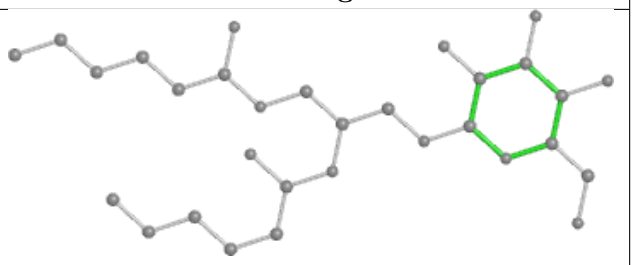
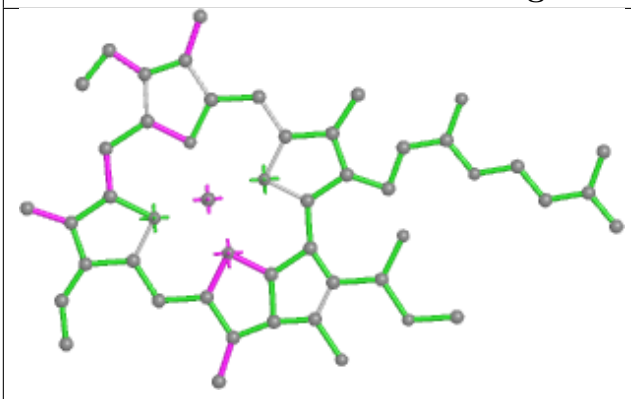


Rings

Ligand CLA p 603



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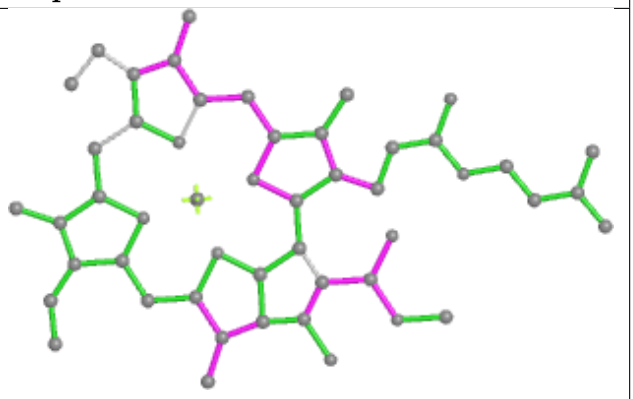
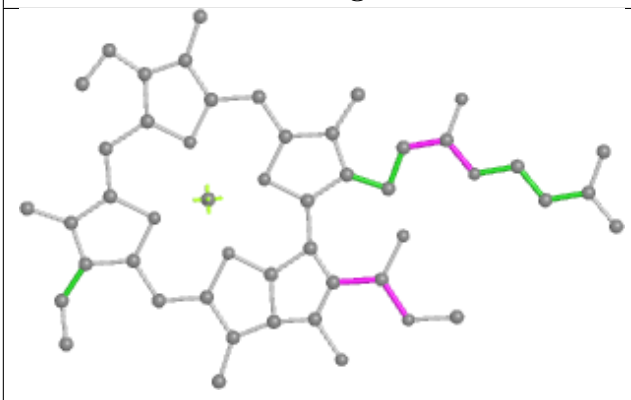


Bond angles



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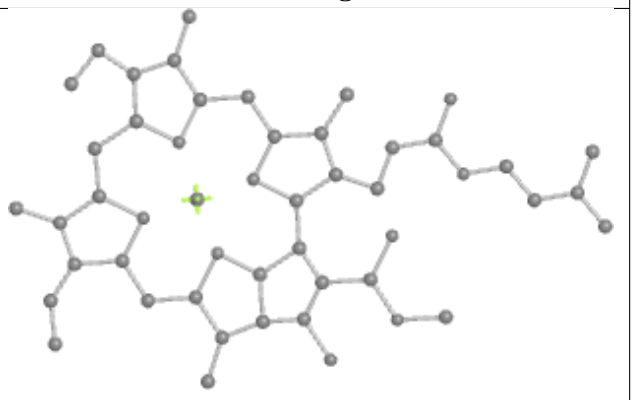
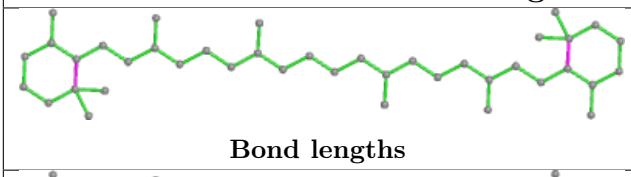


Rings

Ligand BCR c 517



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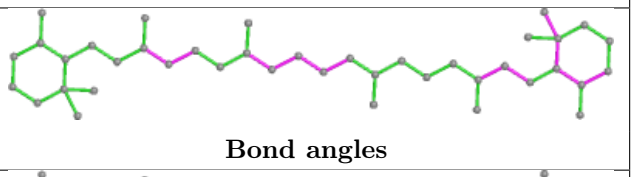
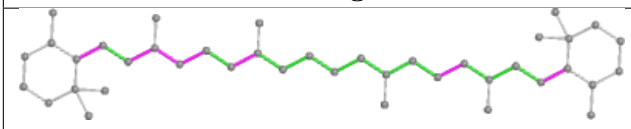


Bond angles



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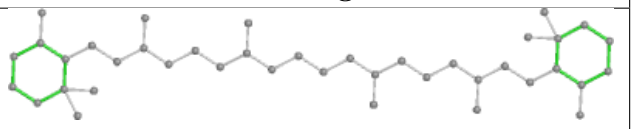
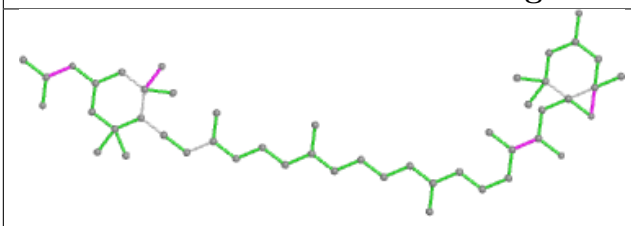


Rings

Ligand A86 12 303



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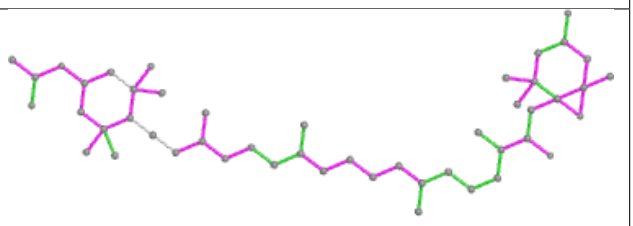
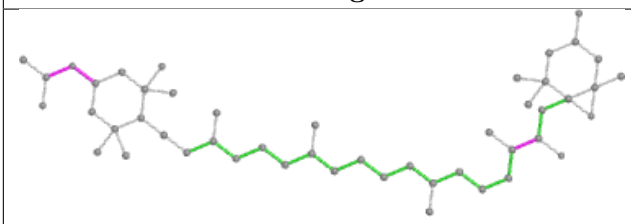
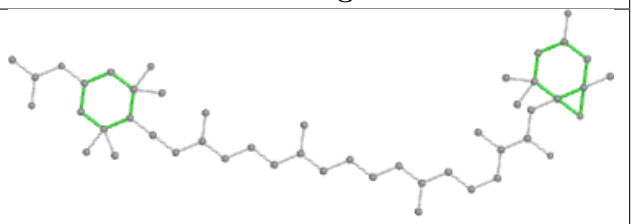


Bond angles

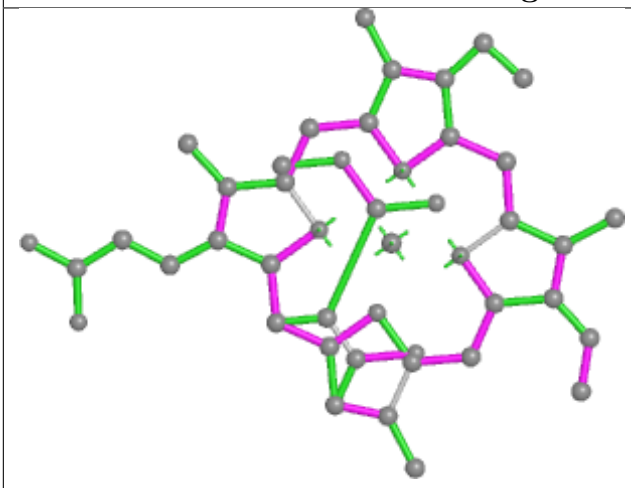


Torsions



Rings

Ligand KC2 14 310



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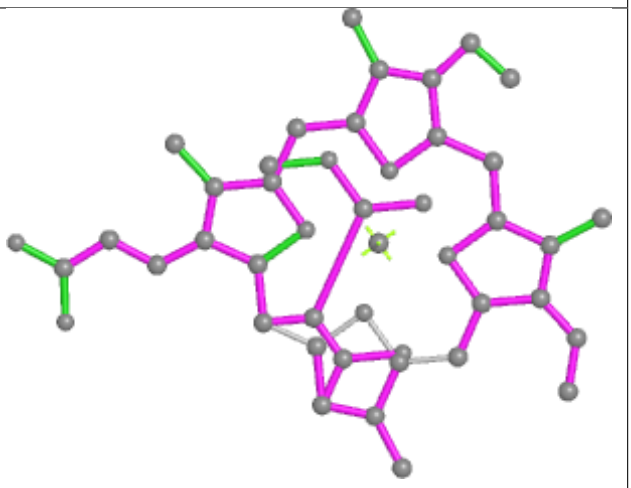
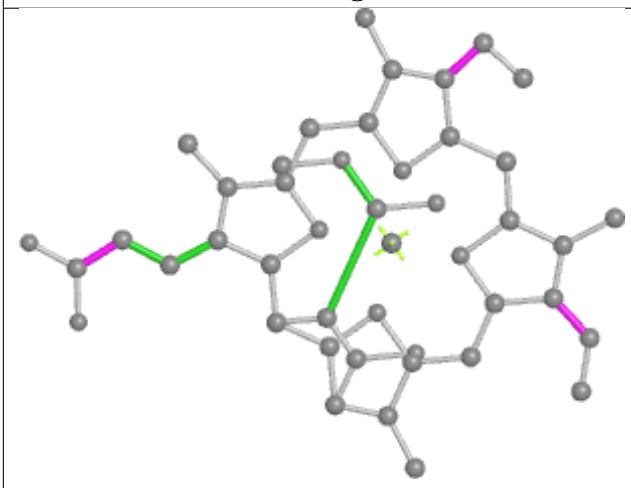
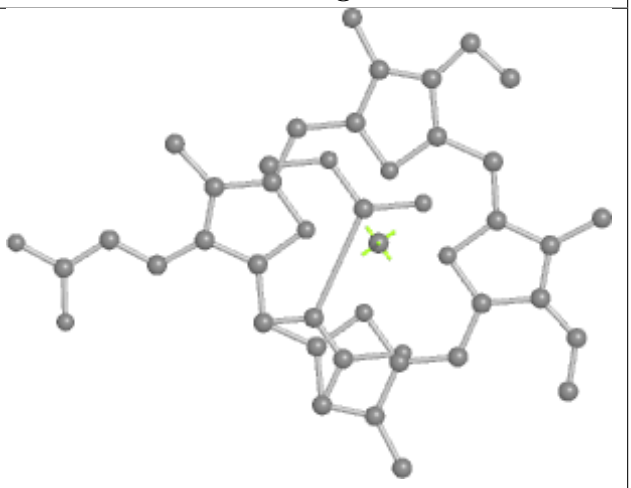


Bond angles

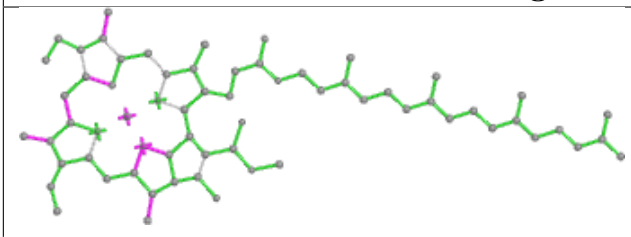


Torsions



Rings

Ligand CLA c 502



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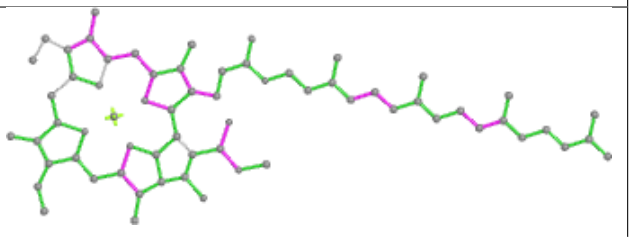

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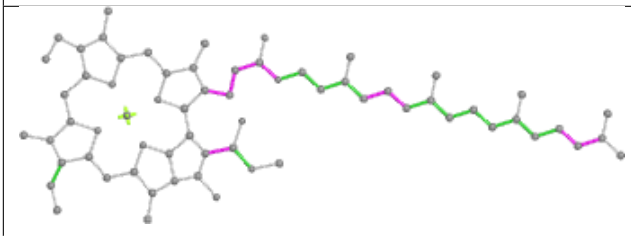

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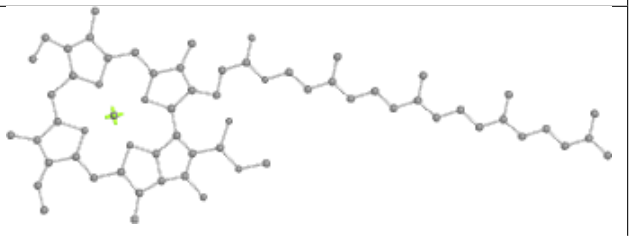
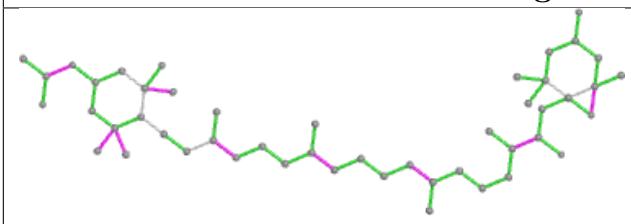


Rings

Ligand A86 4 305



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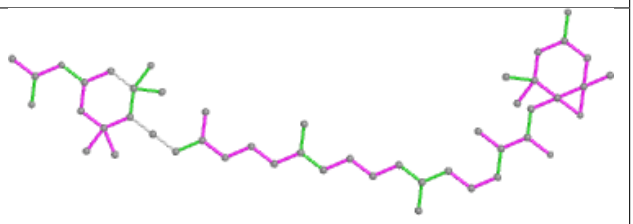

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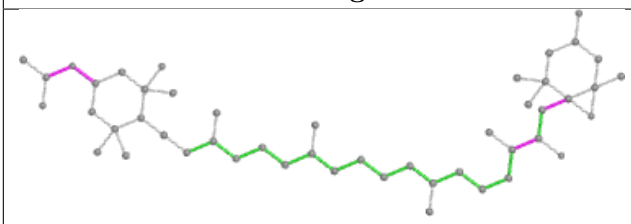

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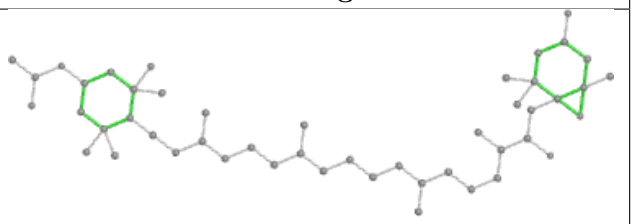
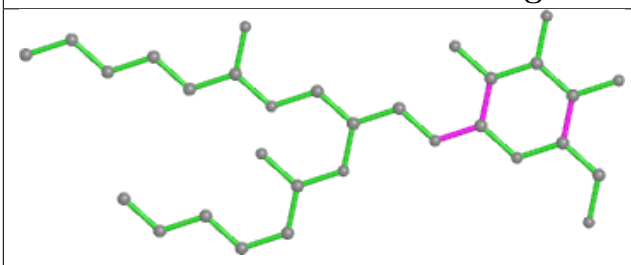


Rings

Ligand LMG c 522



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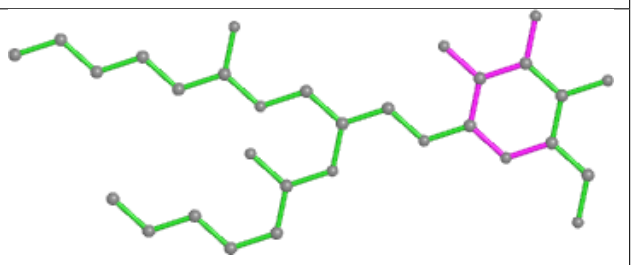
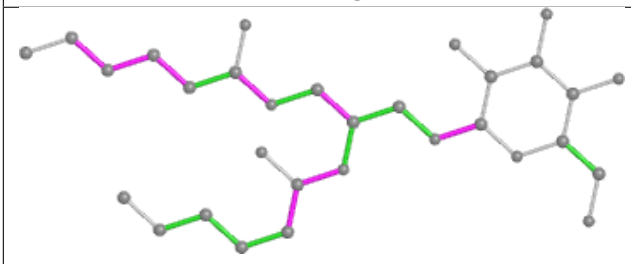


Bond angles



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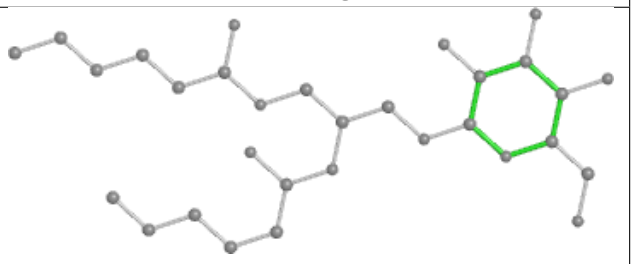
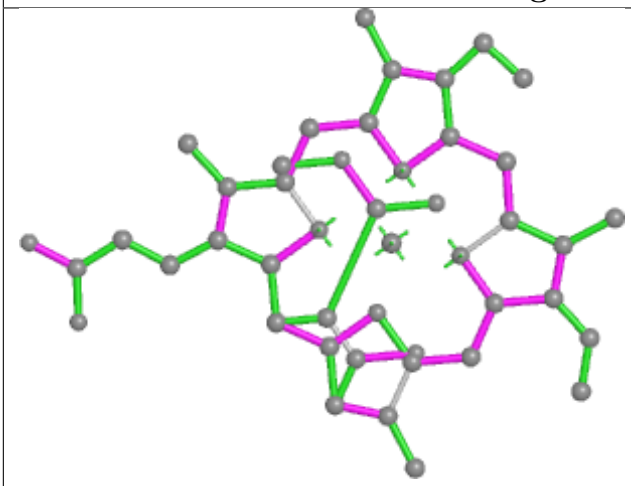


Rings

Ligand KC1 4 313



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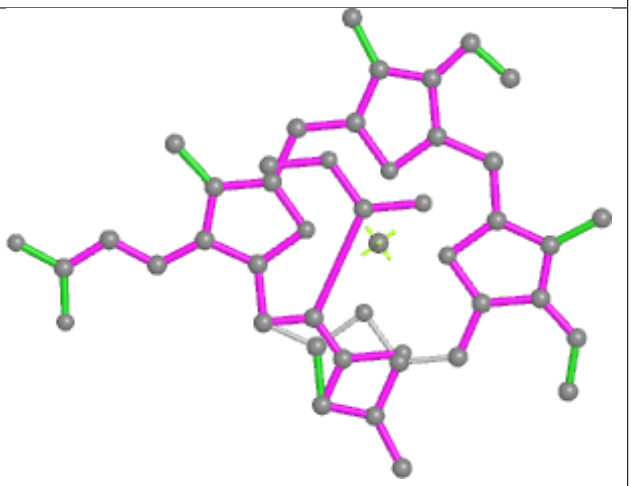
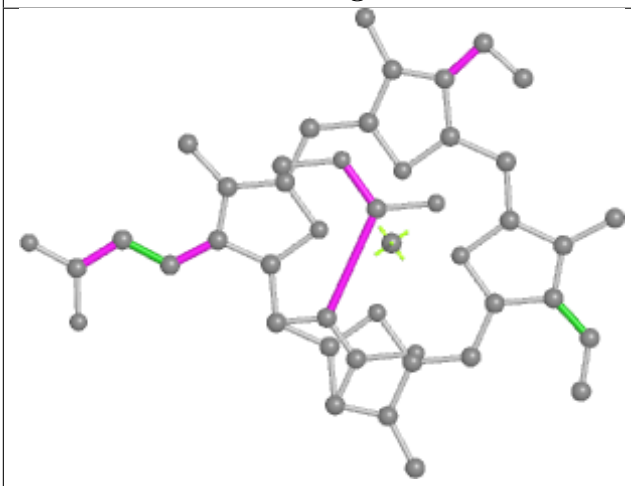


Bond angles



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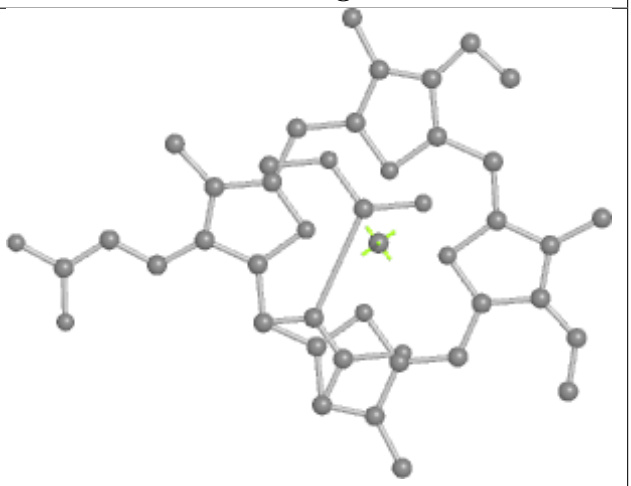
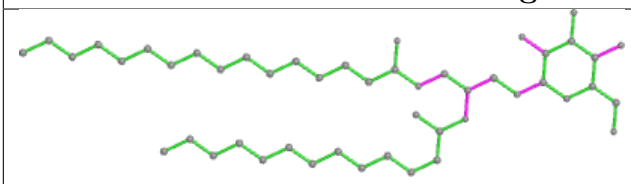


Rings

Ligand LMG w 201



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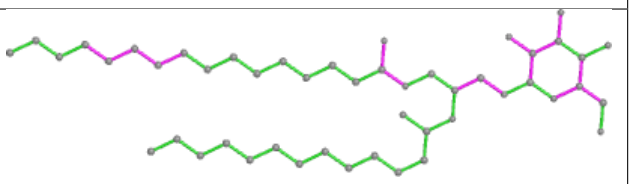

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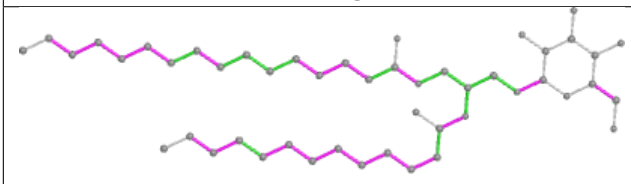

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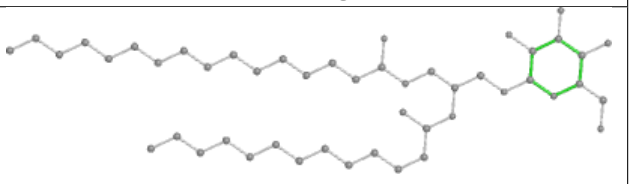
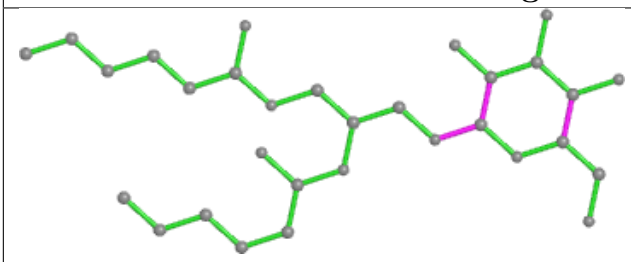


Rings

Ligand LMG Z 102



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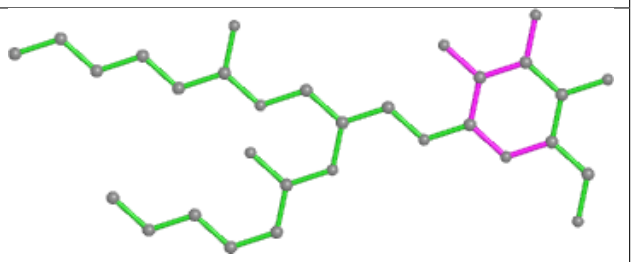

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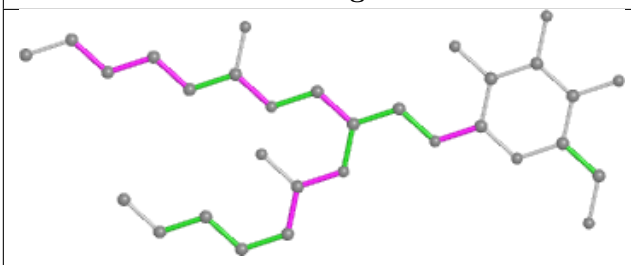

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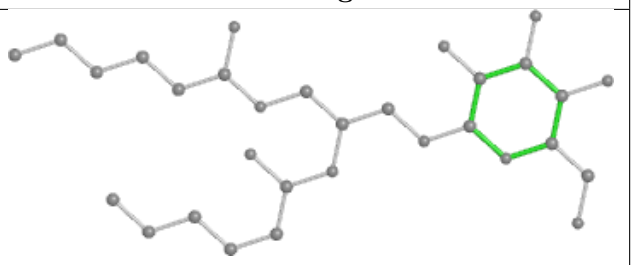
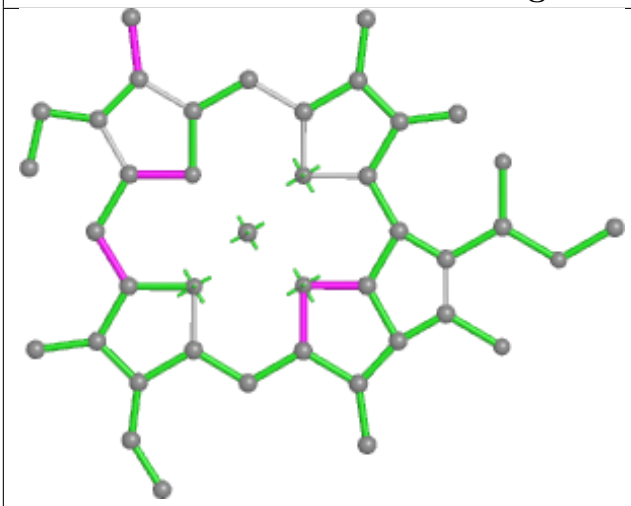


Rings

Ligand CLA 3 310



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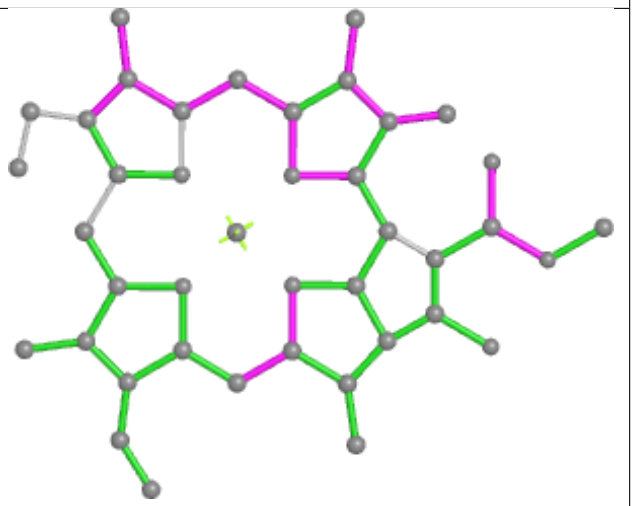

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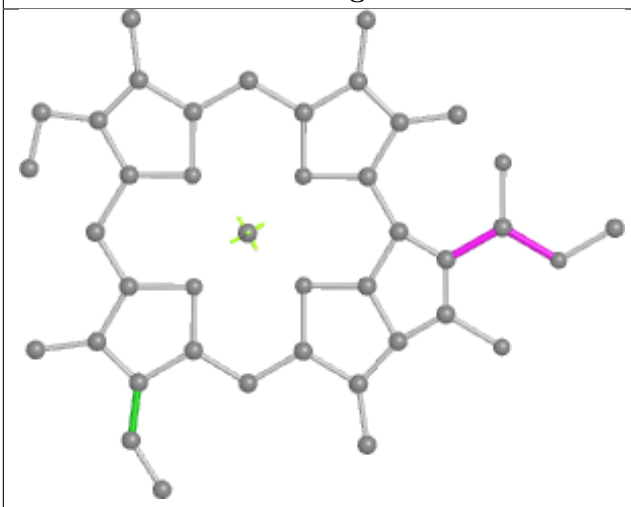

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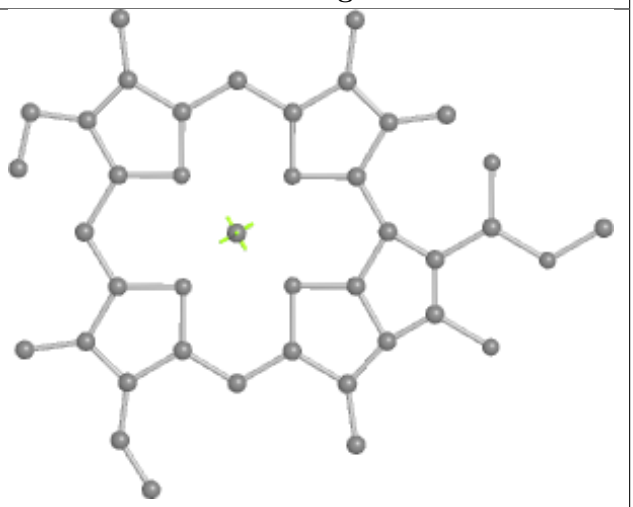
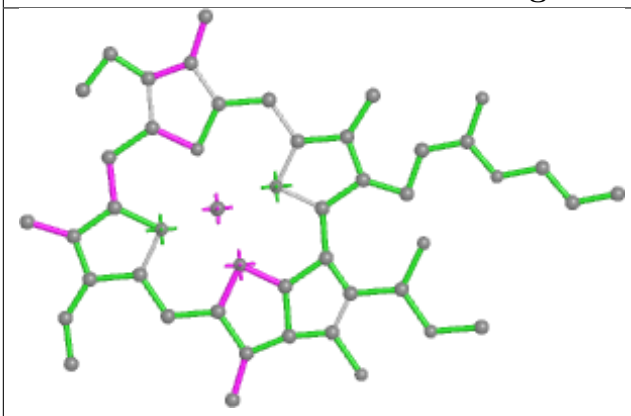


Rings

Ligand CLA z 103



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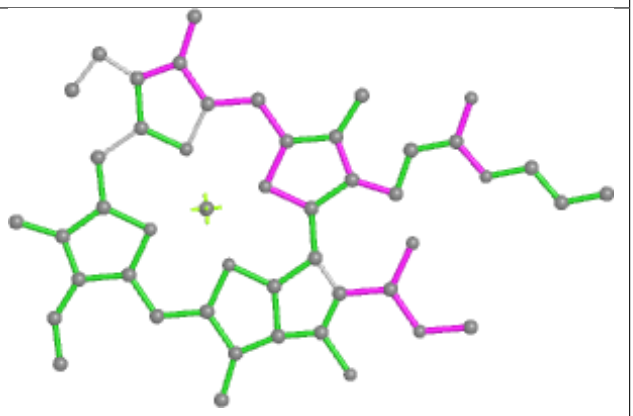

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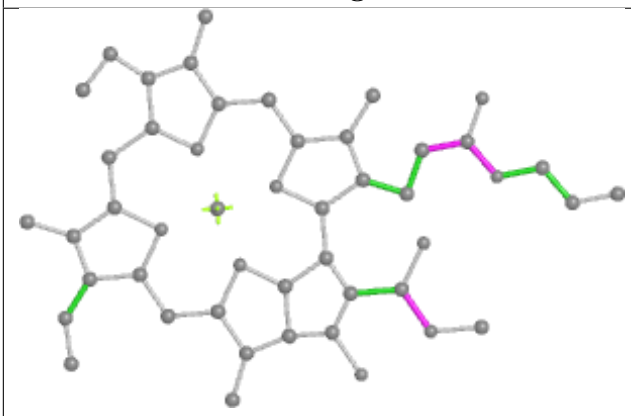

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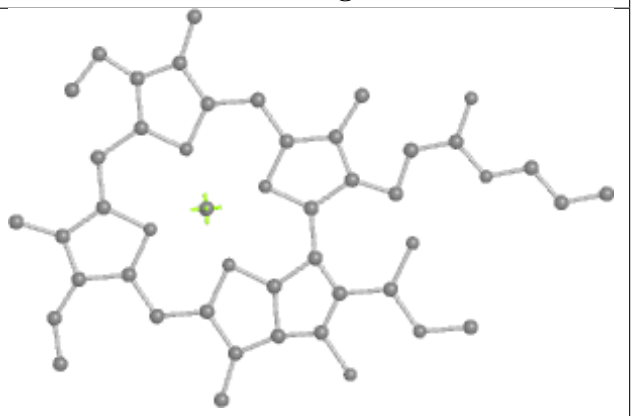
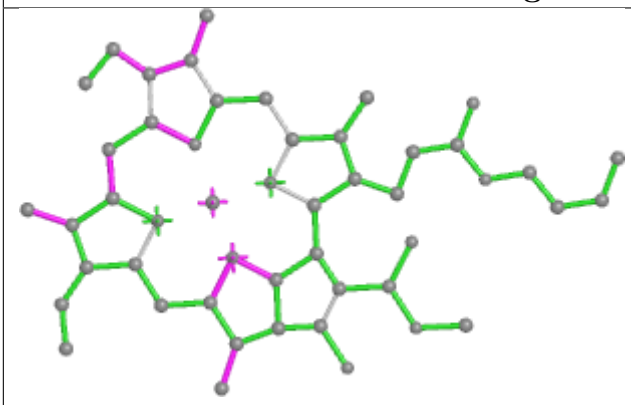


Rings

Ligand CLA A 404



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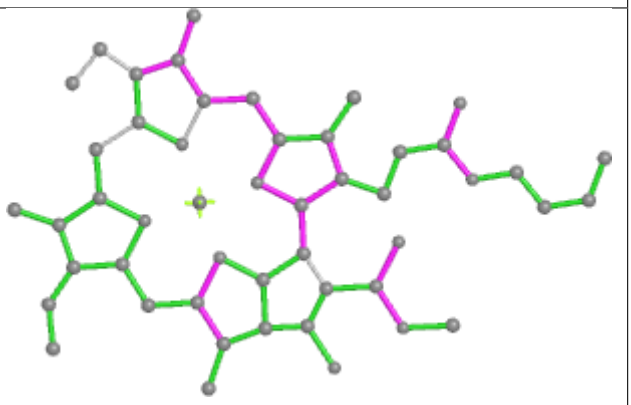

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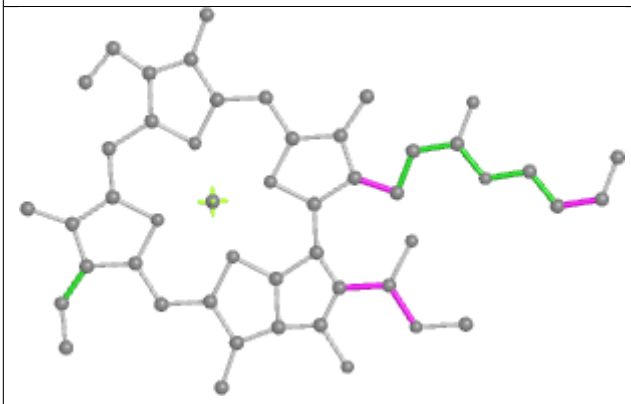

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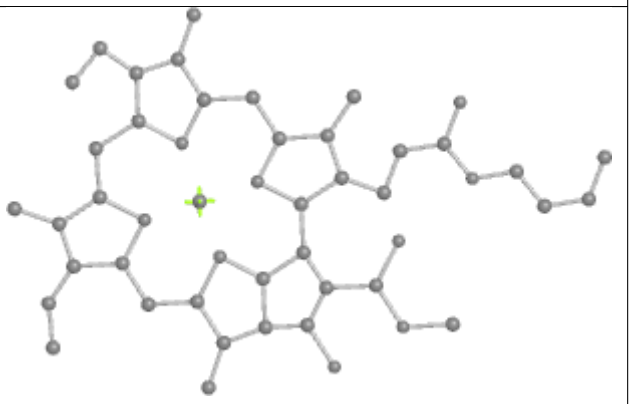
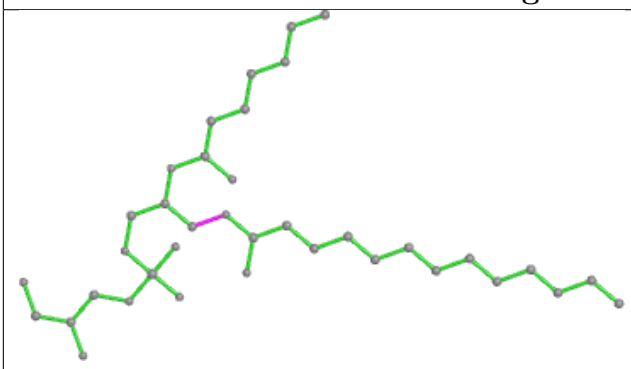


Rings

Ligand LHG A 410



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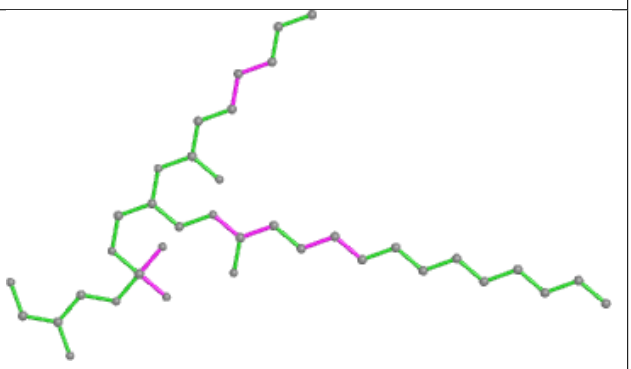

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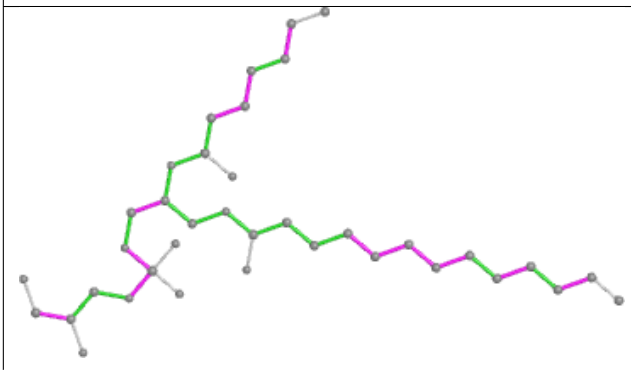

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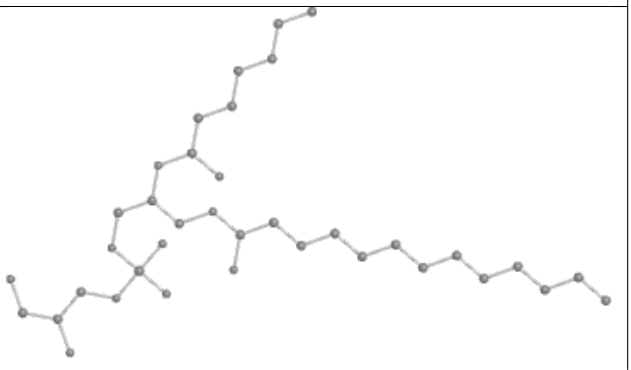
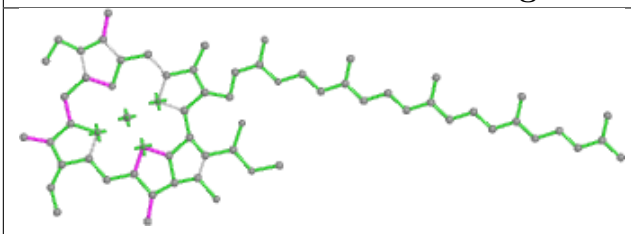


Rings

Ligand CLA 19 313



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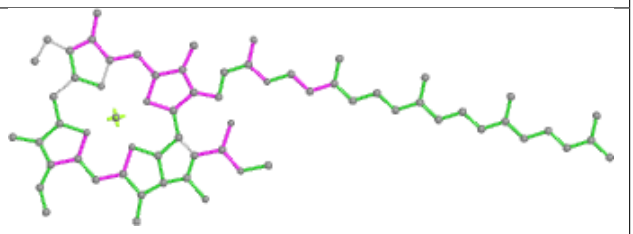
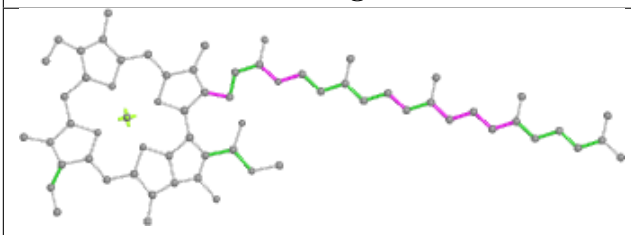


Bond angles



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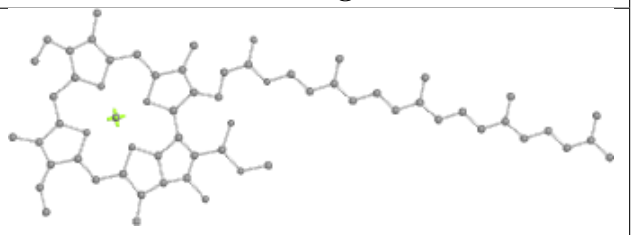
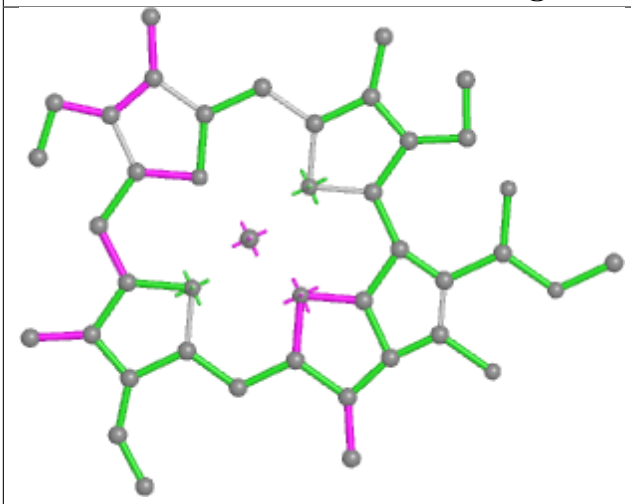


Rings

Ligand CLA 6 314



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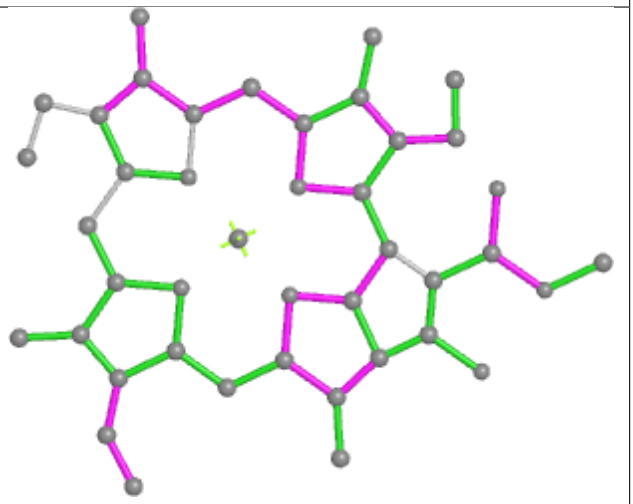
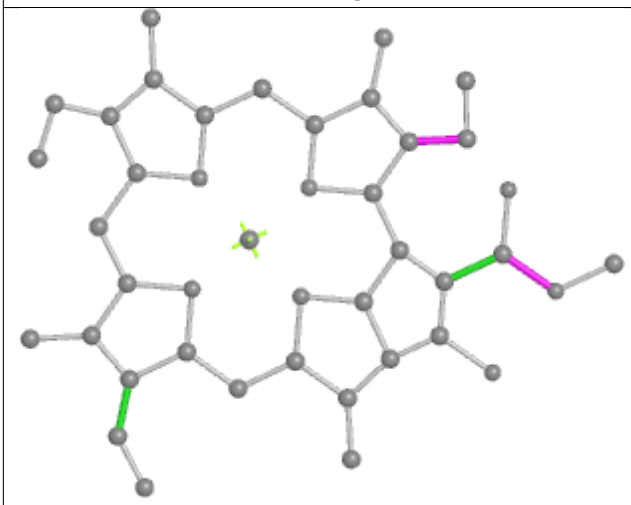


Bond angles



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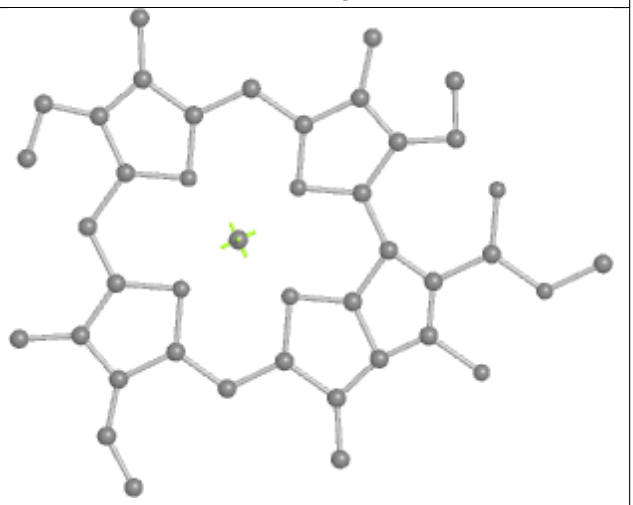
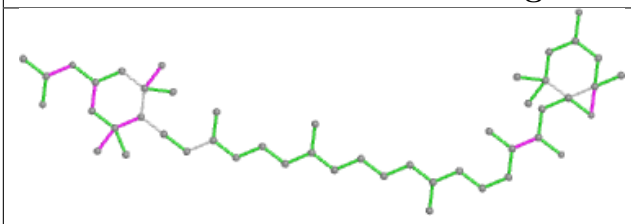


Rings

Ligand A86 15 301



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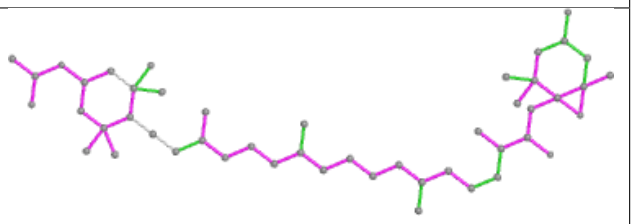
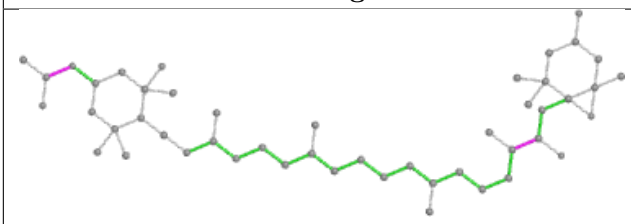


Bond angles



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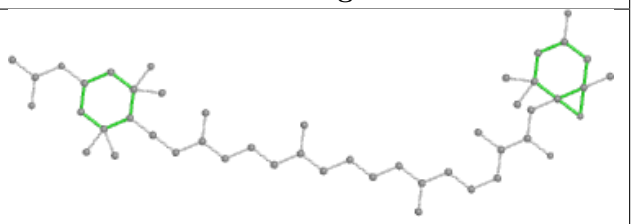
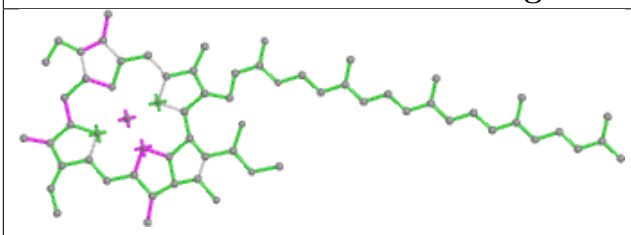
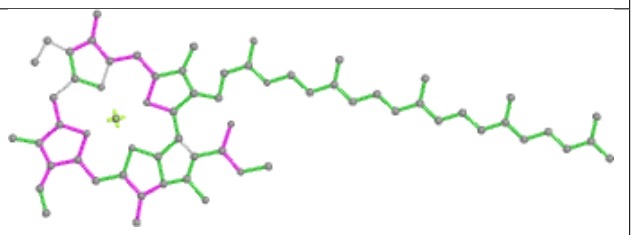


Rings

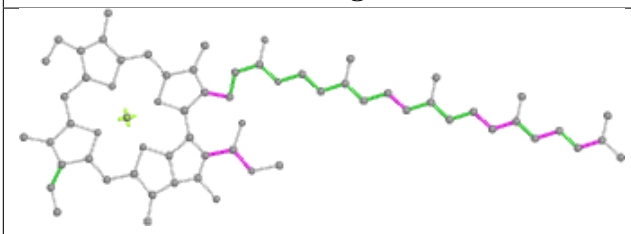
Ligand CLA C 509



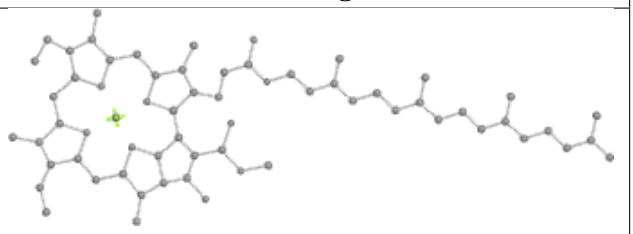
Bond lengths



Bond angles

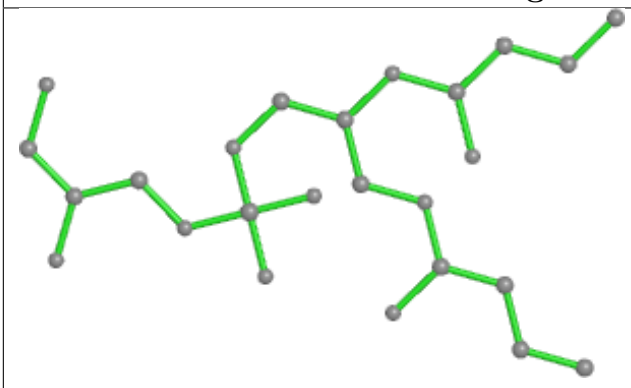


Torsions



Rings

Ligand LHG 5 317



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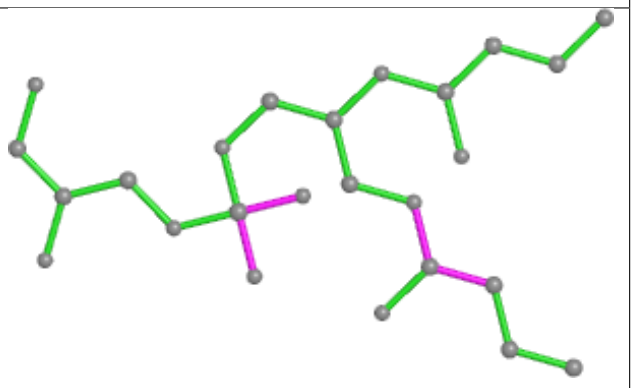
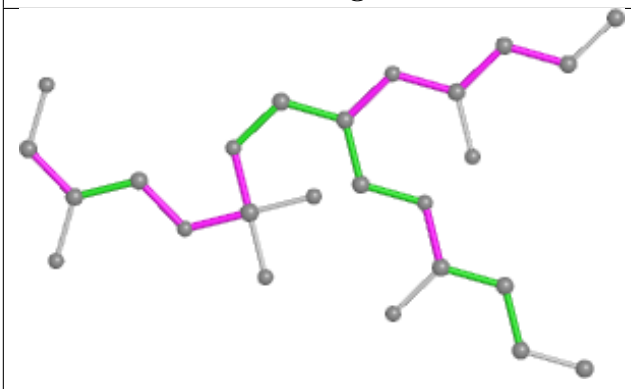


Bond angles



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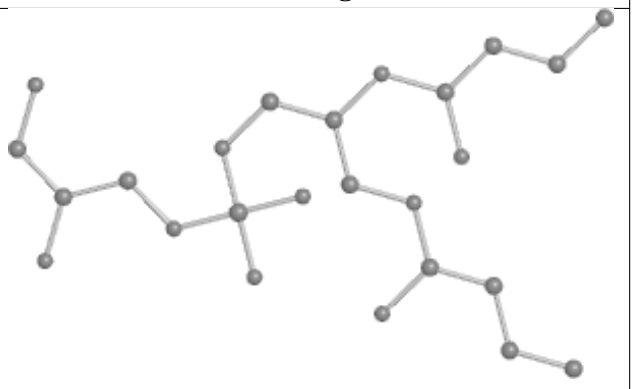
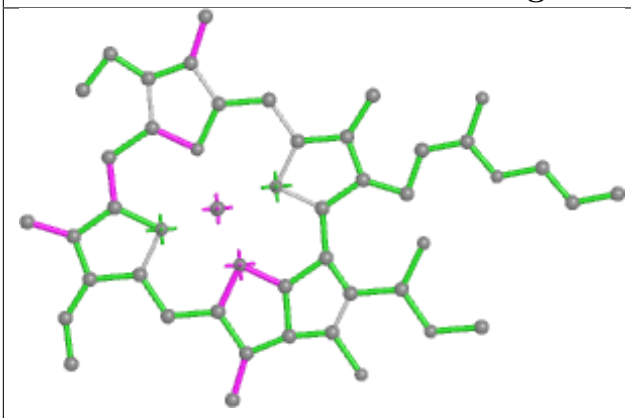


Rings

Ligand CLA p 604



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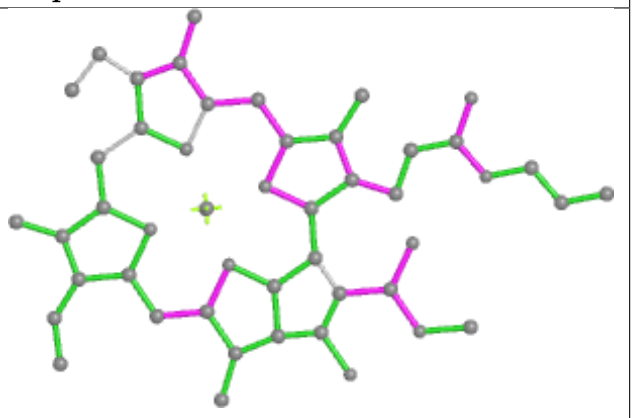

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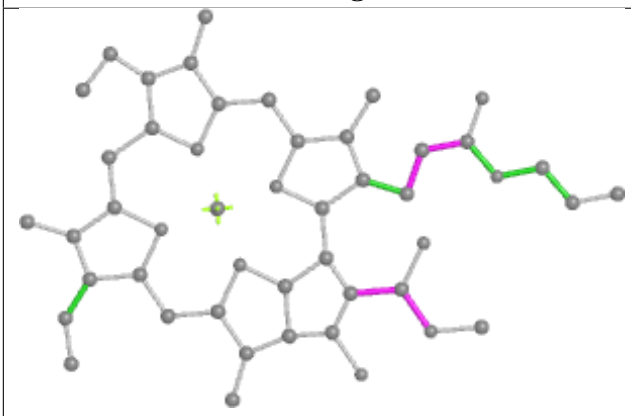

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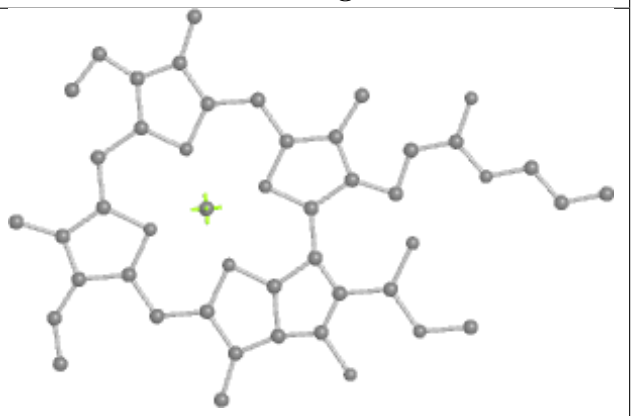
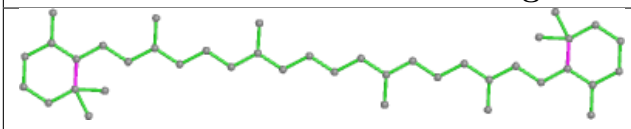


Rings

Ligand BCR C 515



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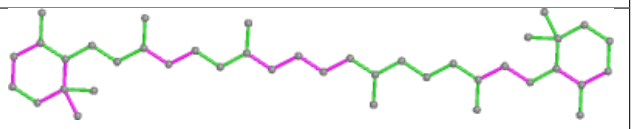

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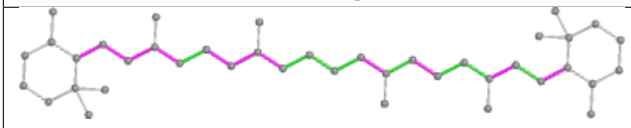
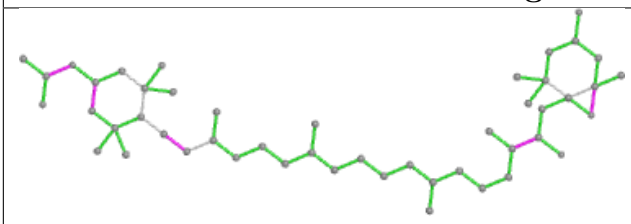


Torsions

Rings

Ligand A86 13 301



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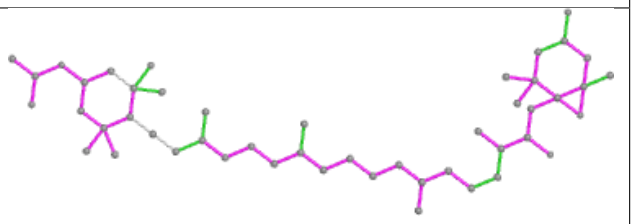

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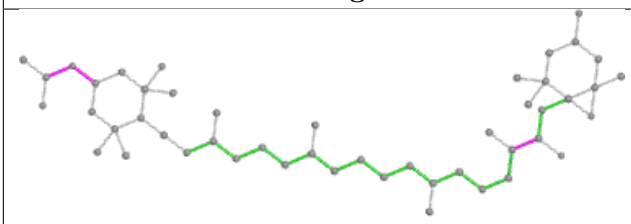

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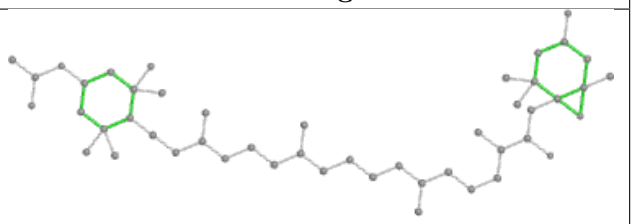
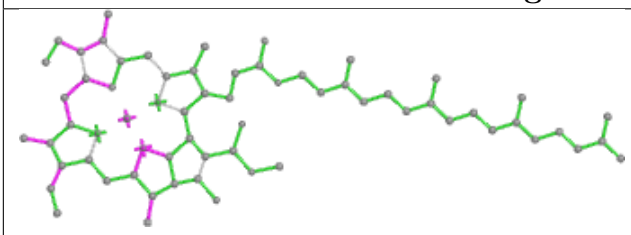


Rings

Ligand CLA B 606



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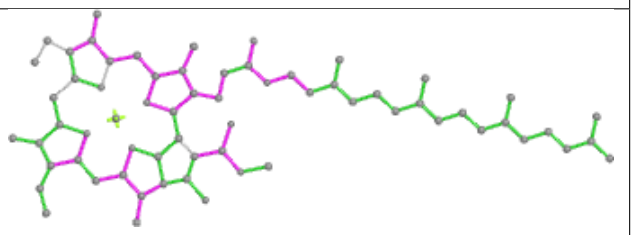

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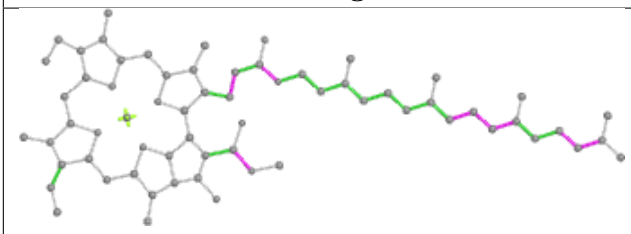

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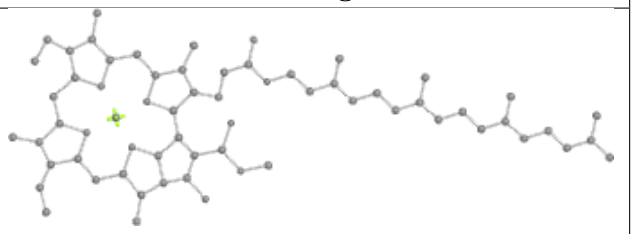
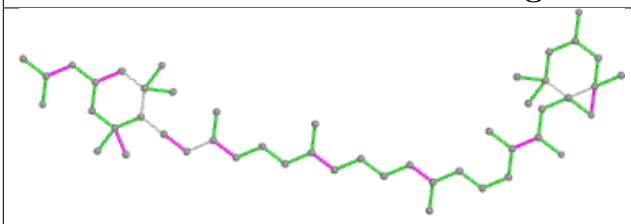


Rings

Ligand A86 12 306



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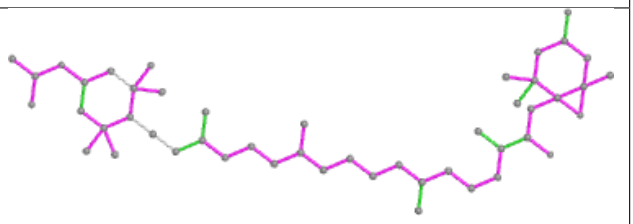

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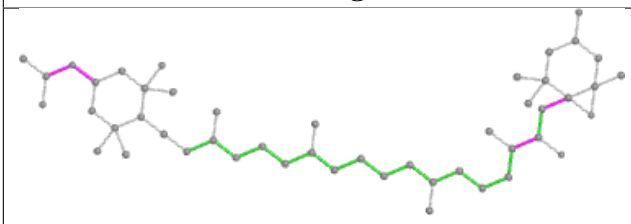

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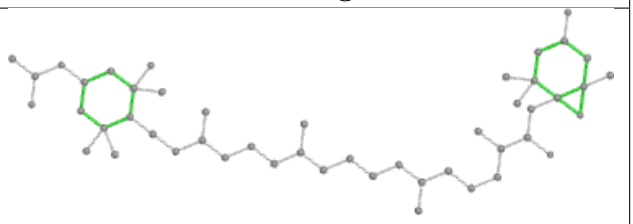
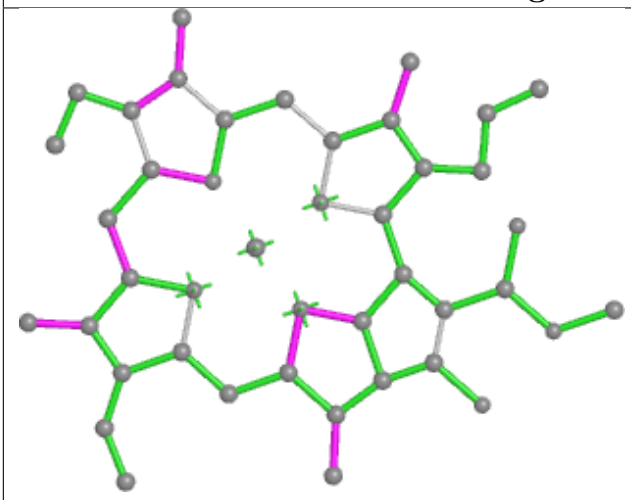


Rings

Ligand CLA 4 315



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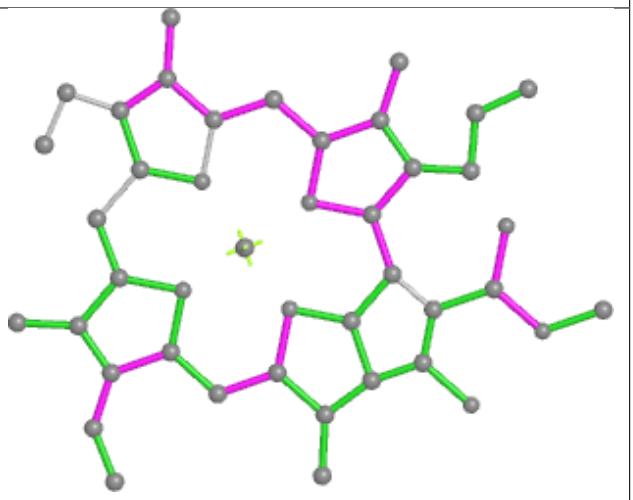

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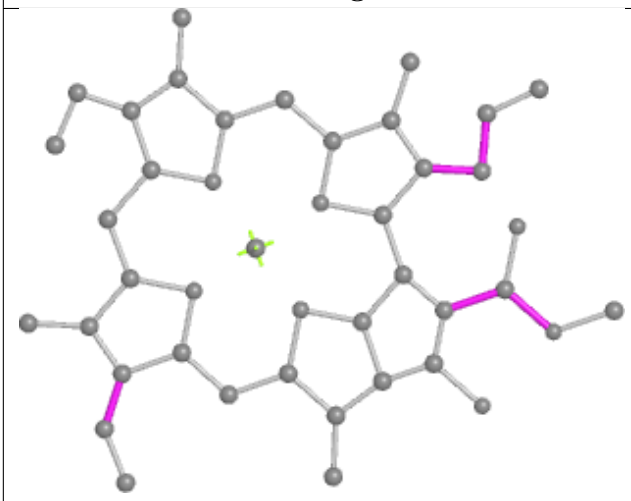

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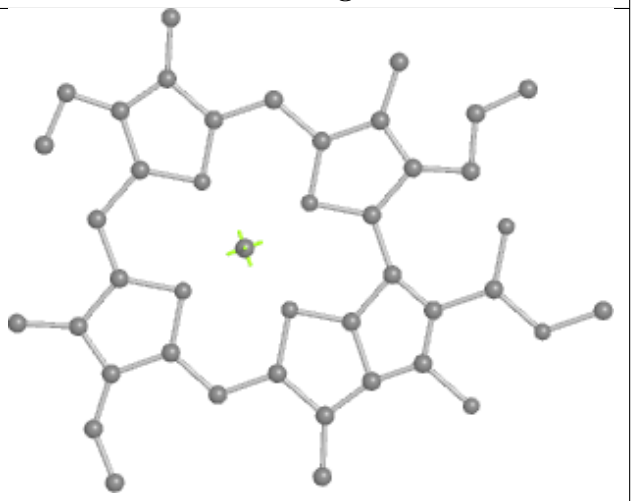
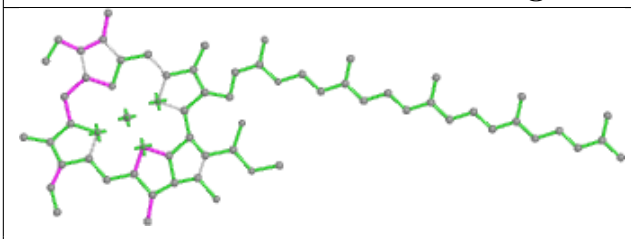


Rings

Ligand CLA b 604



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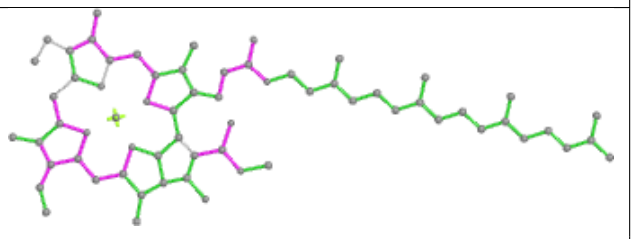
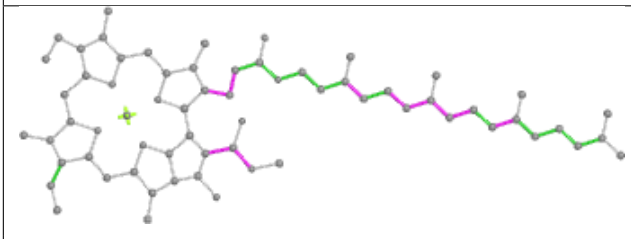


Bond angles



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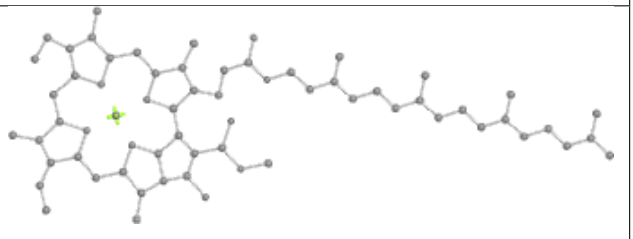
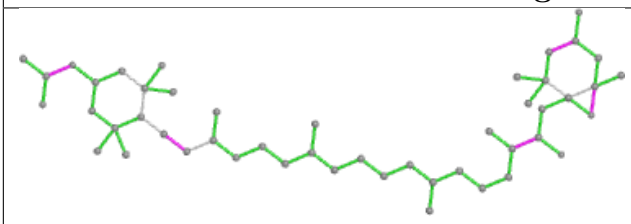


Rings

Ligand A86 5 303



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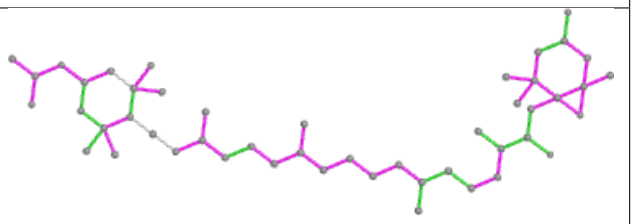

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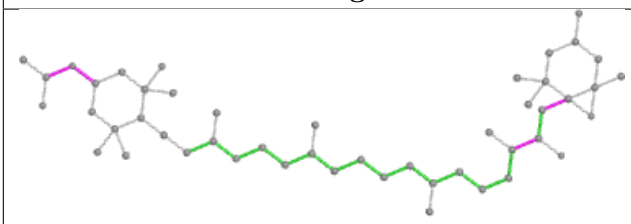

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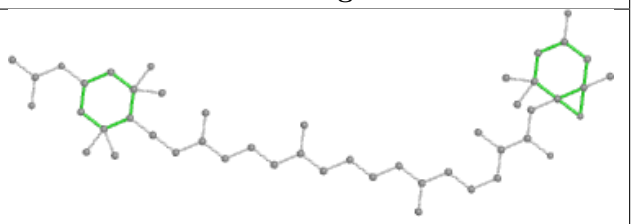
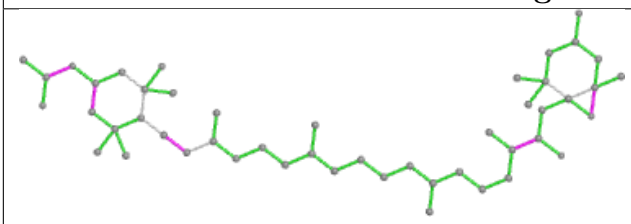


Rings

Ligand A86 3 302



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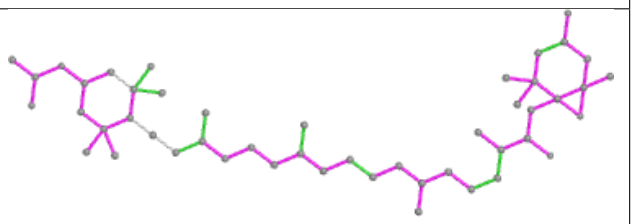

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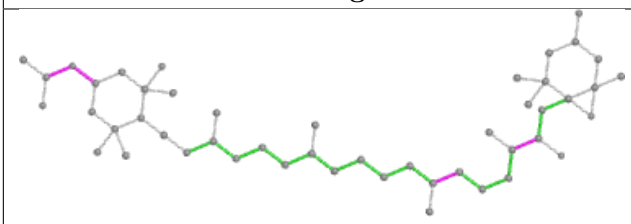

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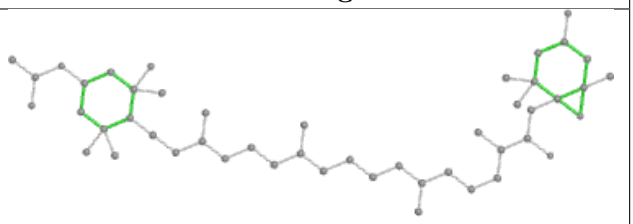
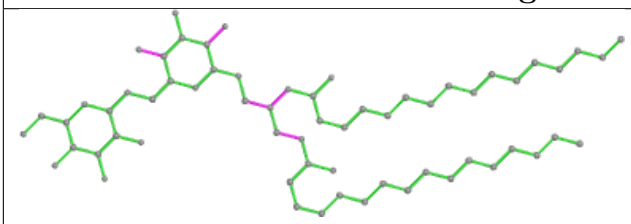


Rings

Ligand DGD H 102



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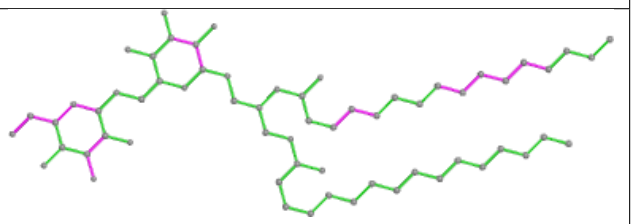

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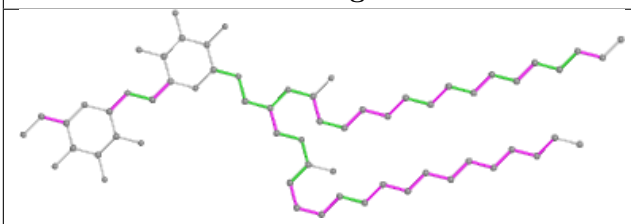

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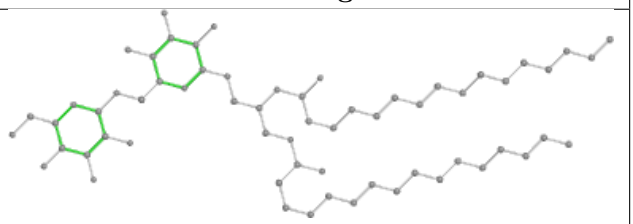
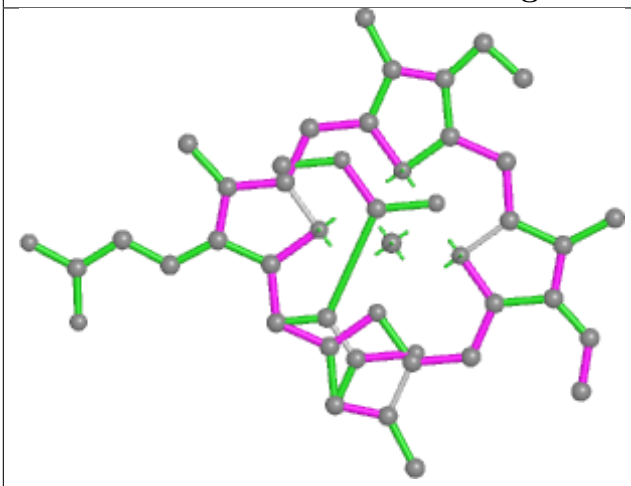


Rings

Ligand KC2 13 309



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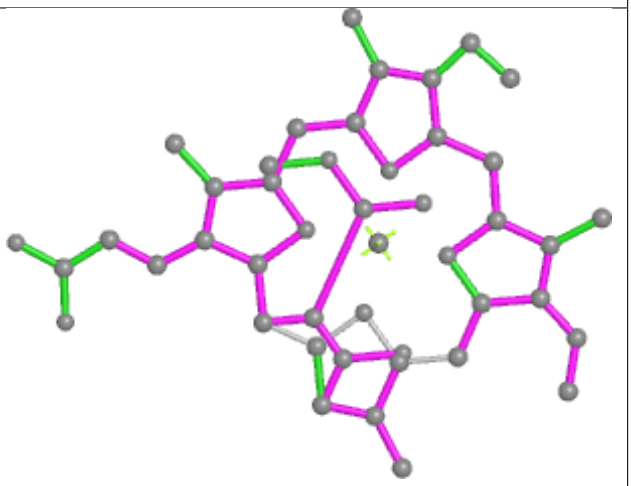
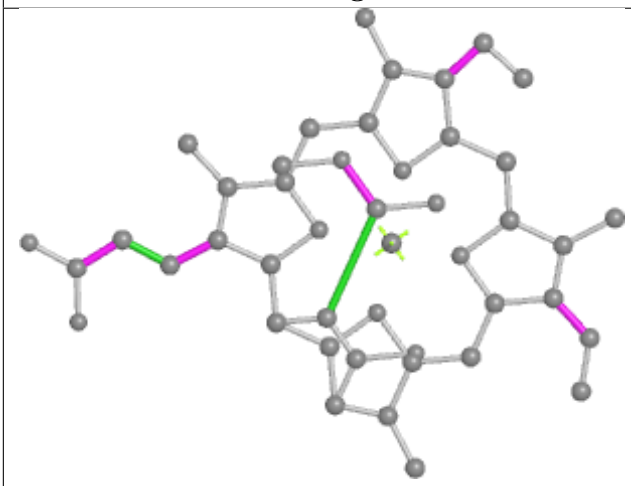


Bond angles



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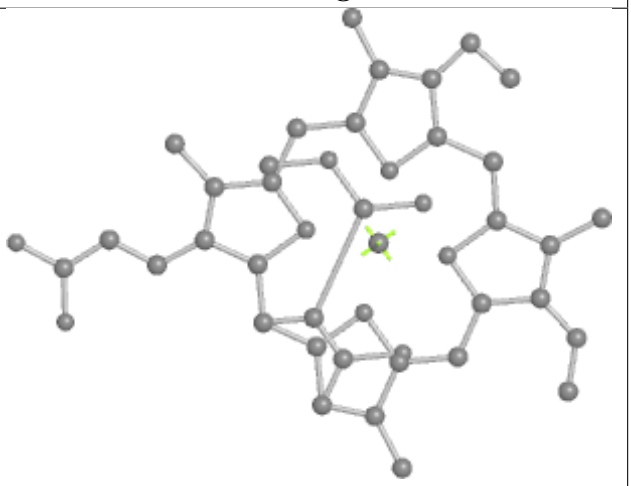
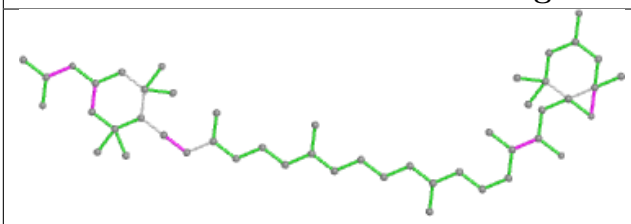


Rings

Ligand A86 6 302



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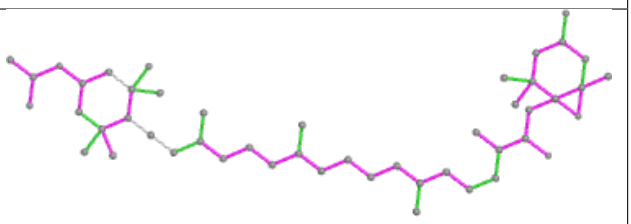
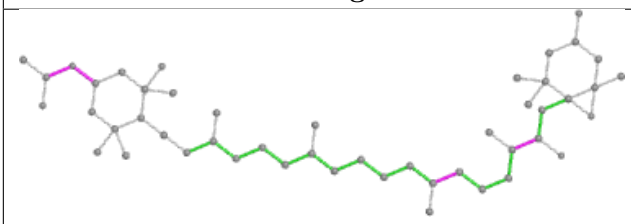


Bond angles



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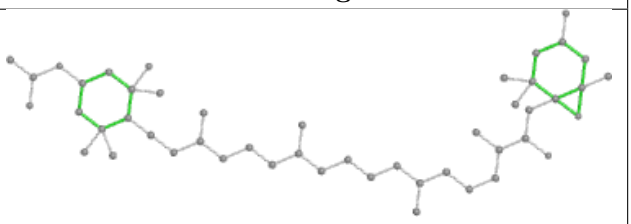
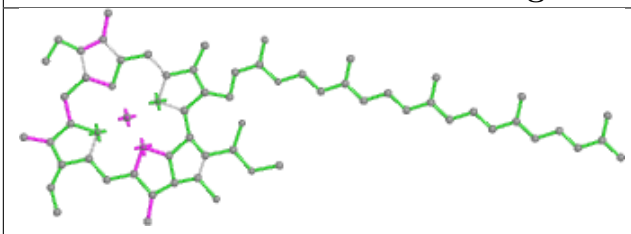
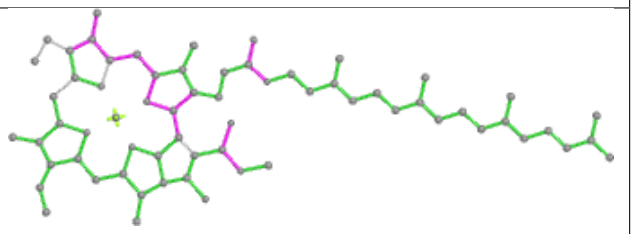


Rings

Ligand CLA b 610



Bond lengths



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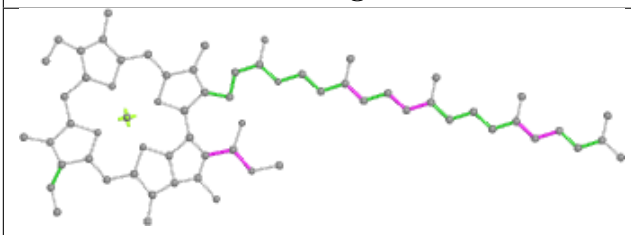
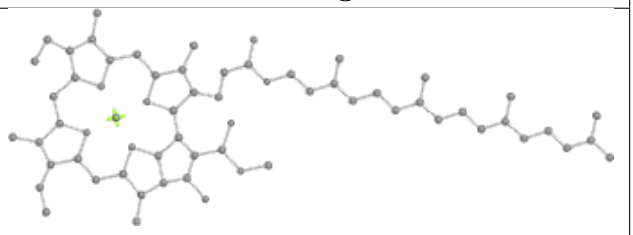
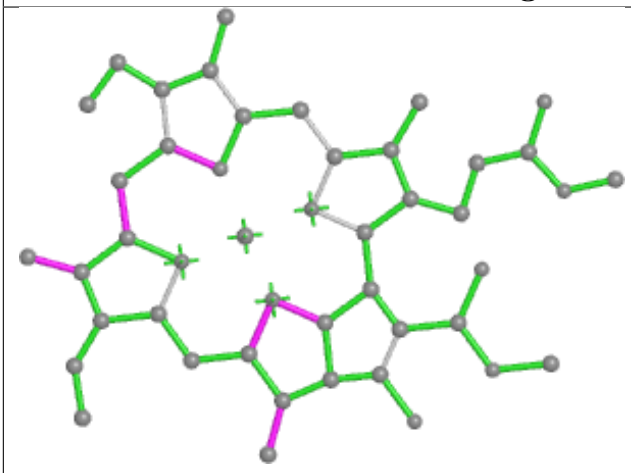


Torsions



Rings

Ligand CLA 19 311



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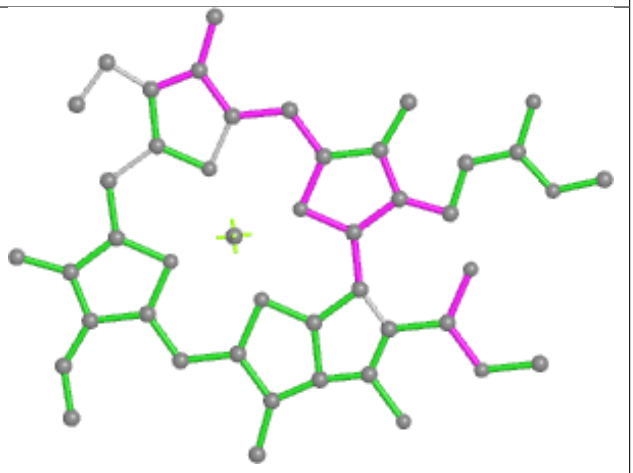

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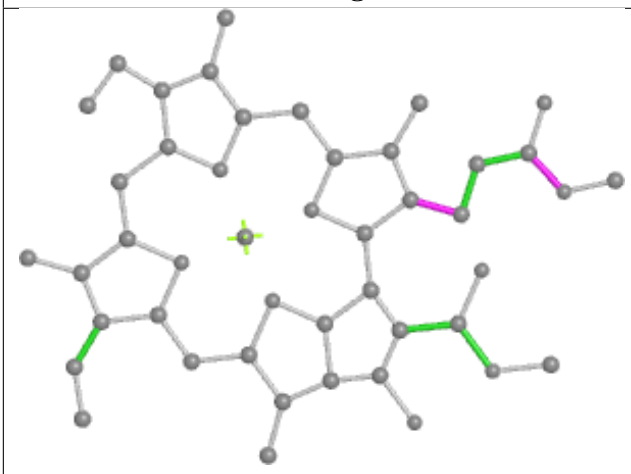

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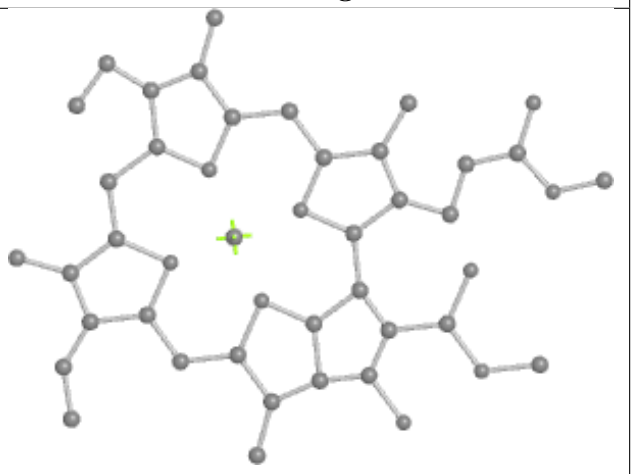
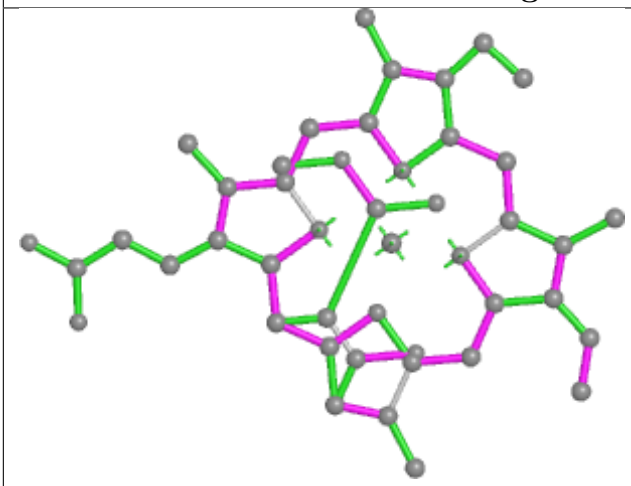


Rings

Ligand KC2 19 309



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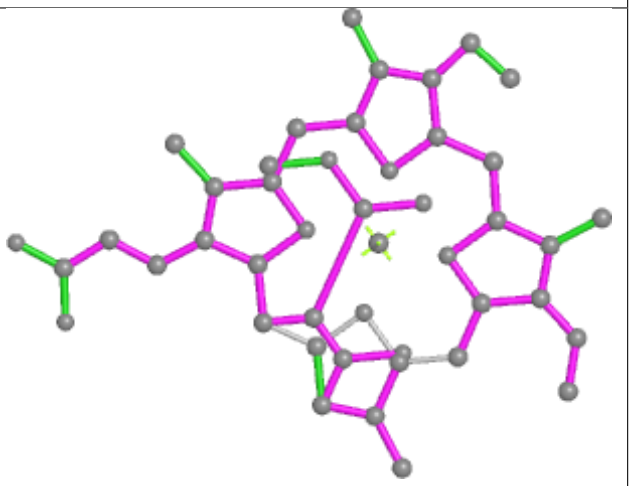

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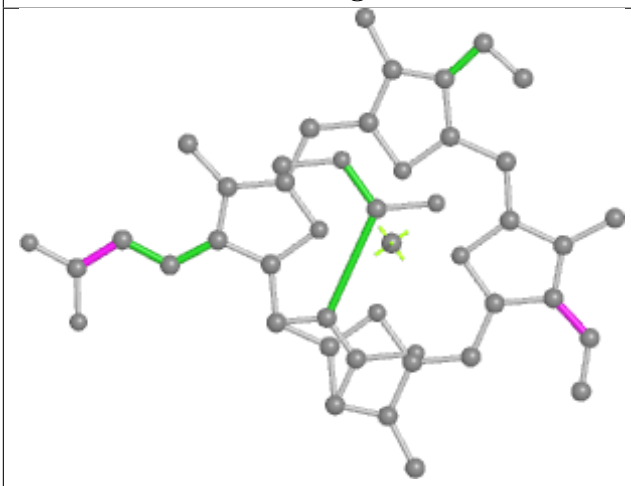

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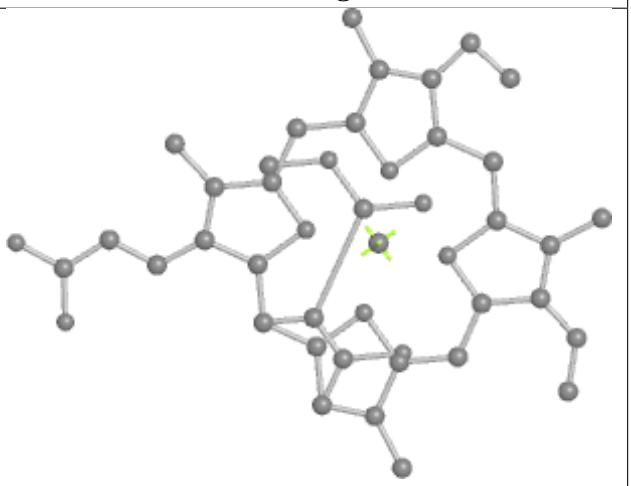
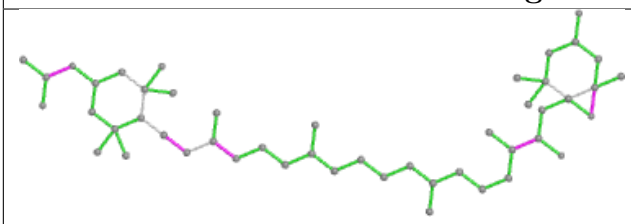


Rings

Ligand A86 10 302



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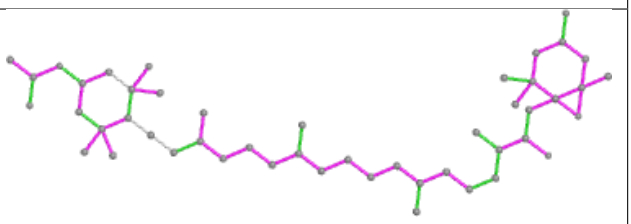

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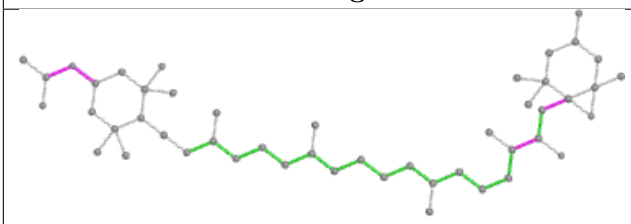

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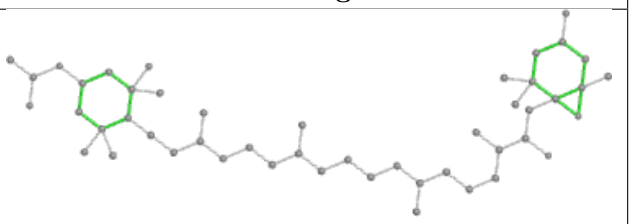
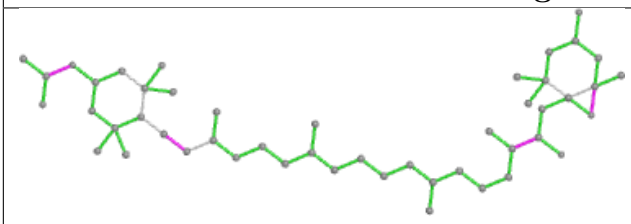


Rings

Ligand A86 1 319



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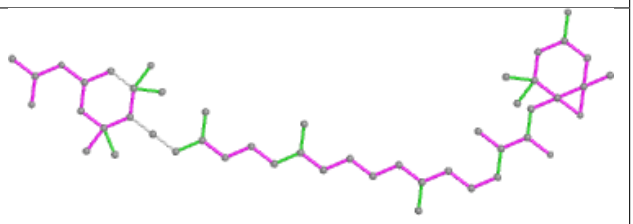

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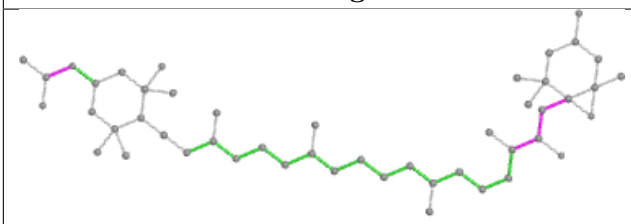

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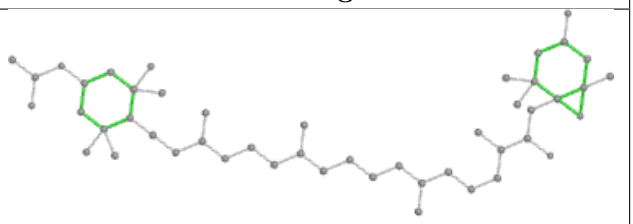
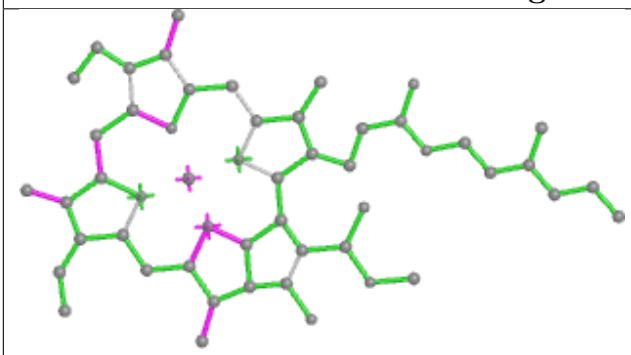


Rings

Ligand CLA 8 309



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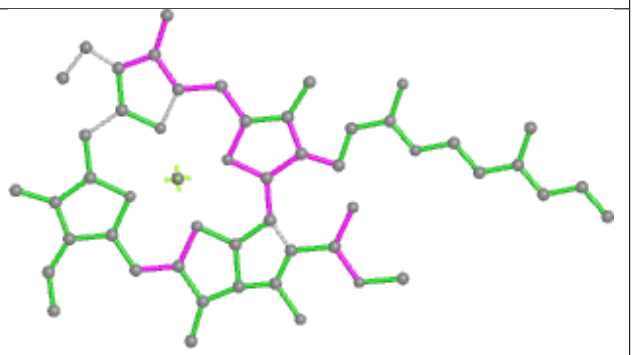

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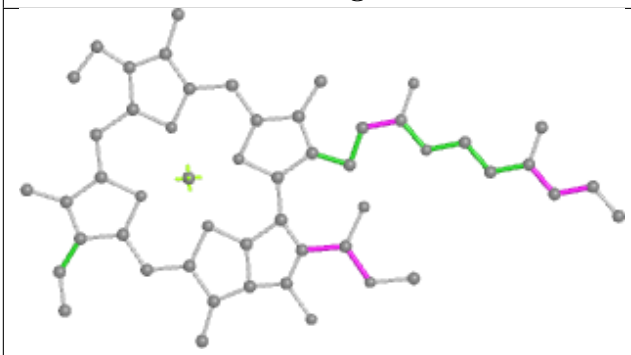

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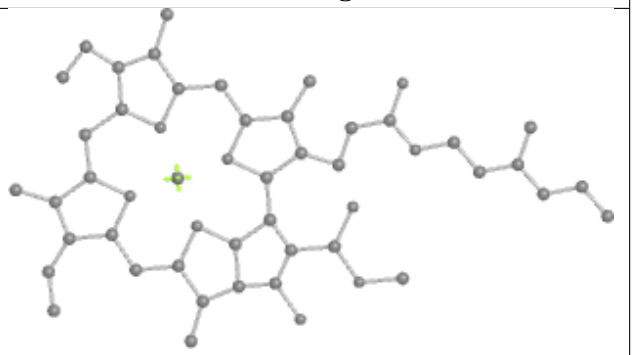
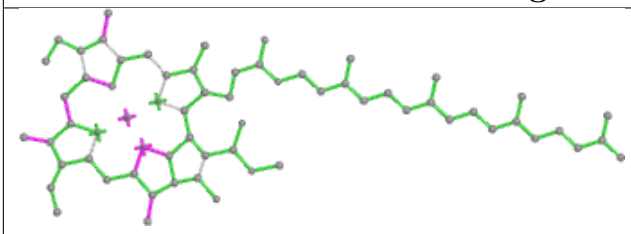


Rings

Ligand CLA c 513



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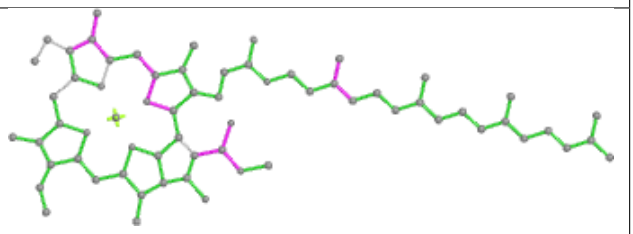

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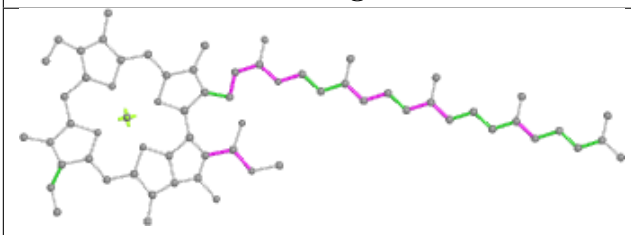

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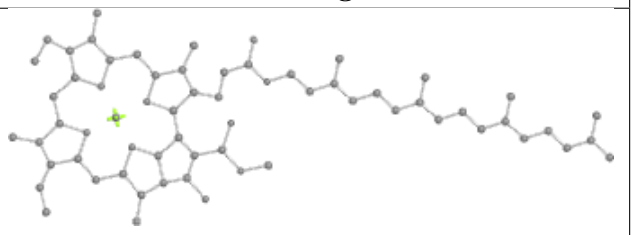
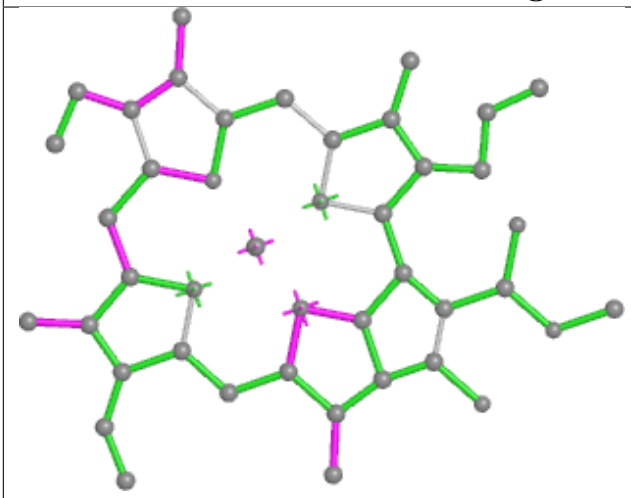


Rings

Ligand CLA p 607



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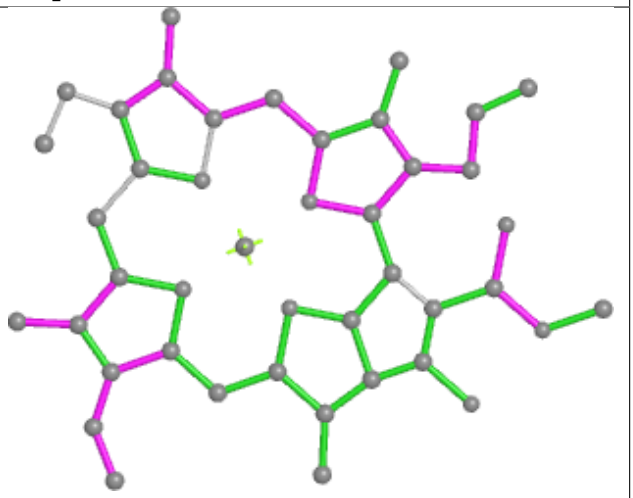

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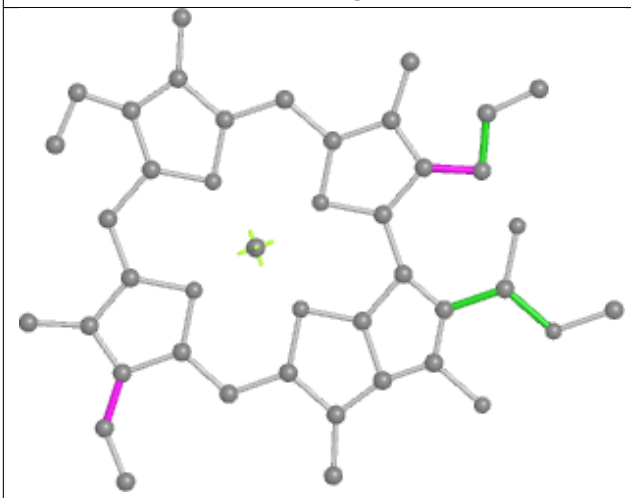

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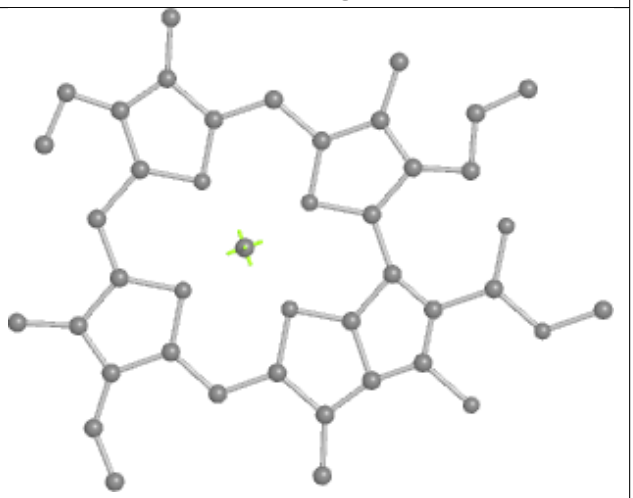
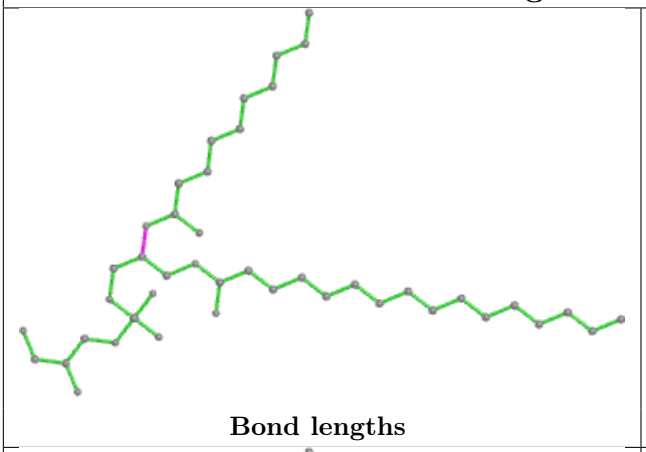


Rings

Ligand LHG b 623



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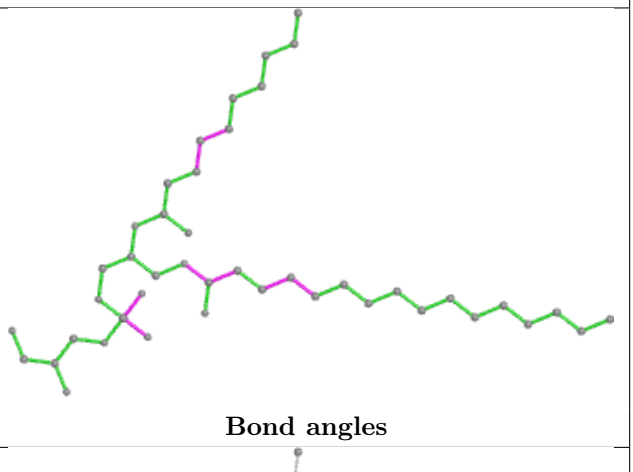

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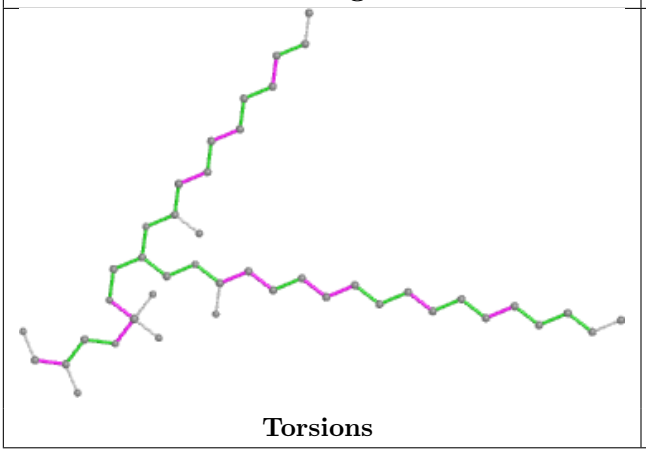

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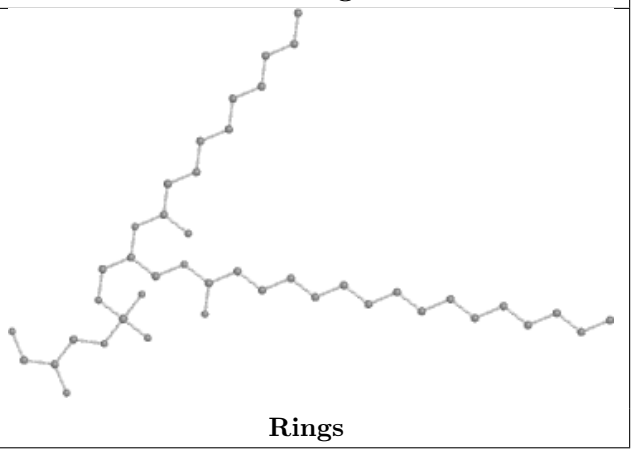
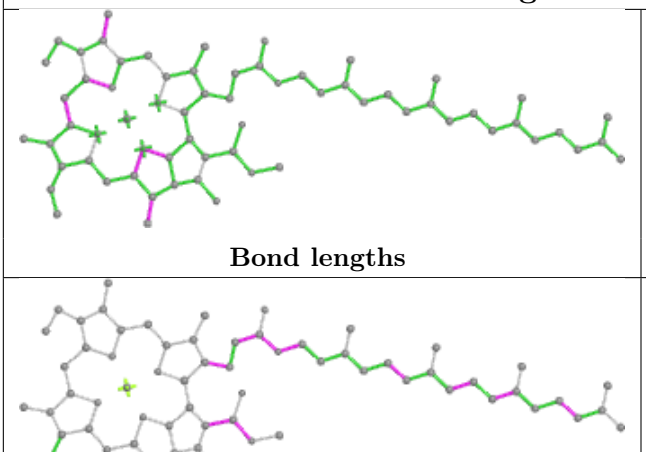


Rings

Ligand CLA 13 316



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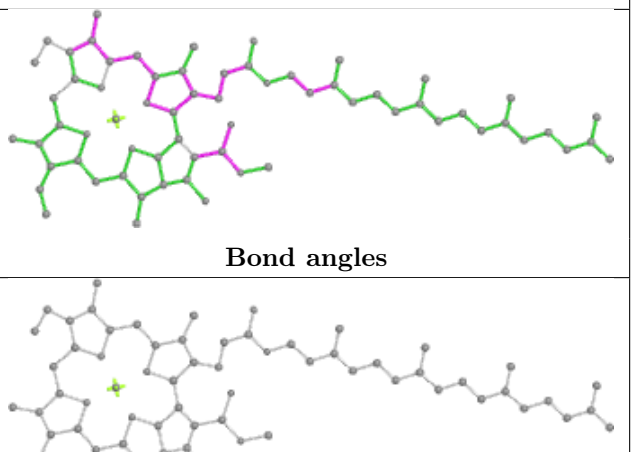

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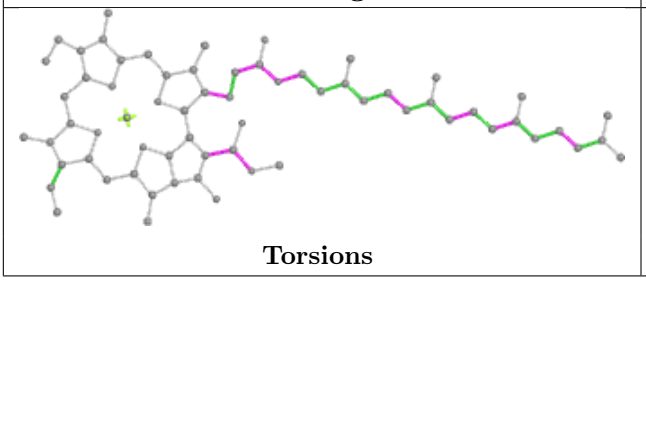

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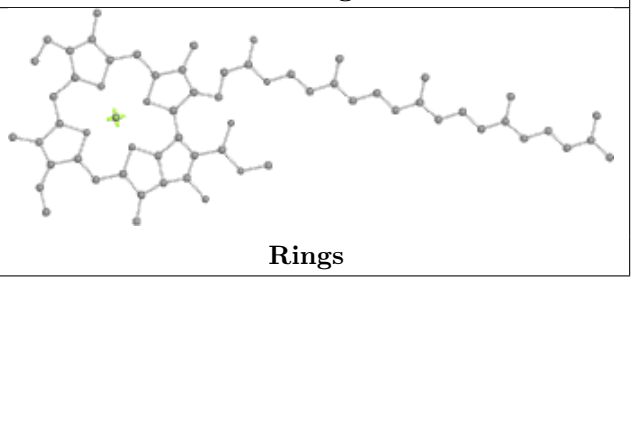
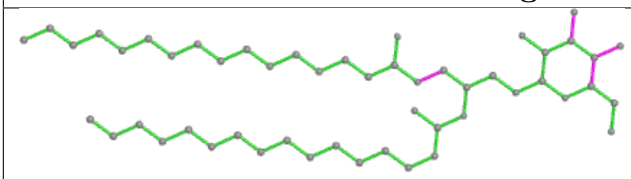


Rings

Ligand LMG B 620



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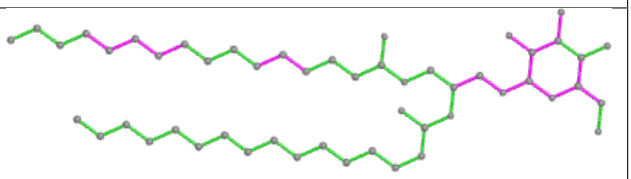

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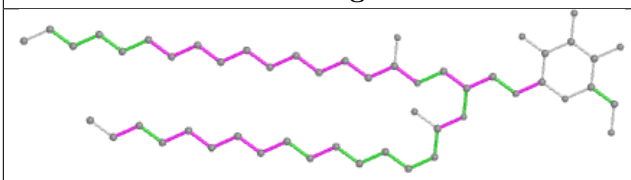

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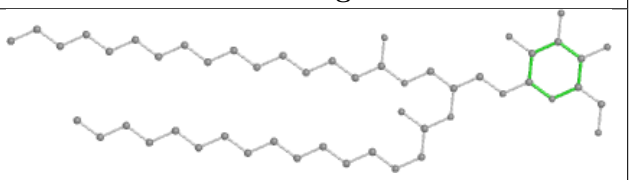

Rings

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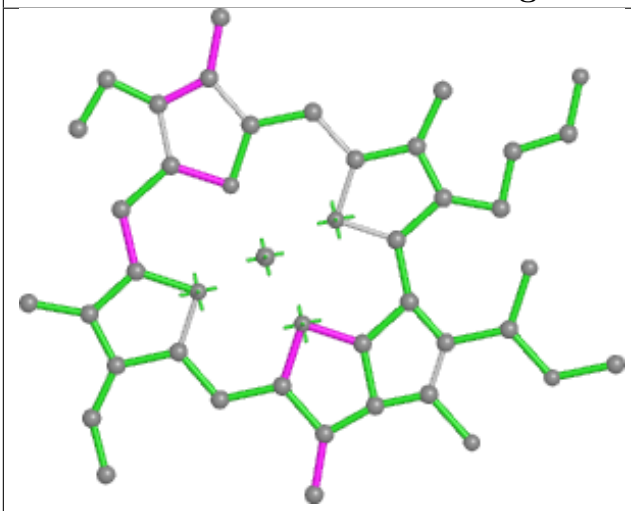

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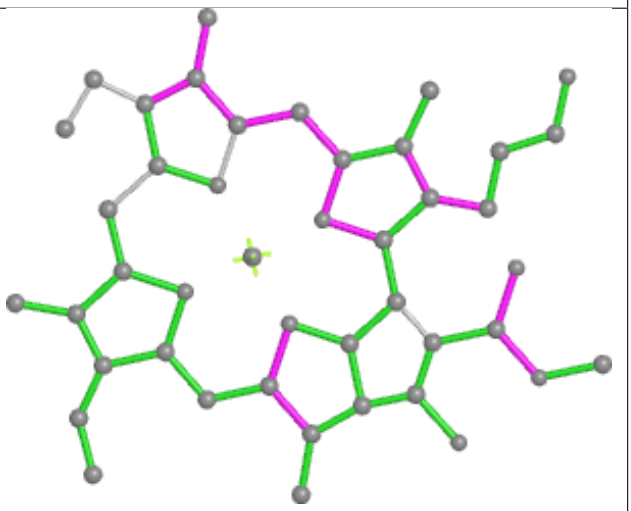

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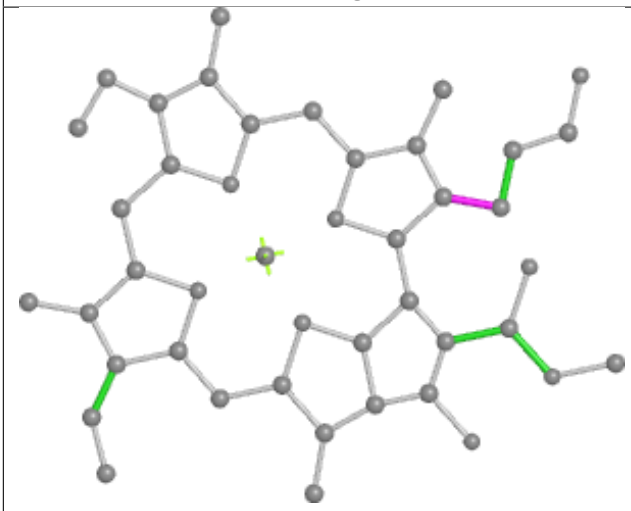

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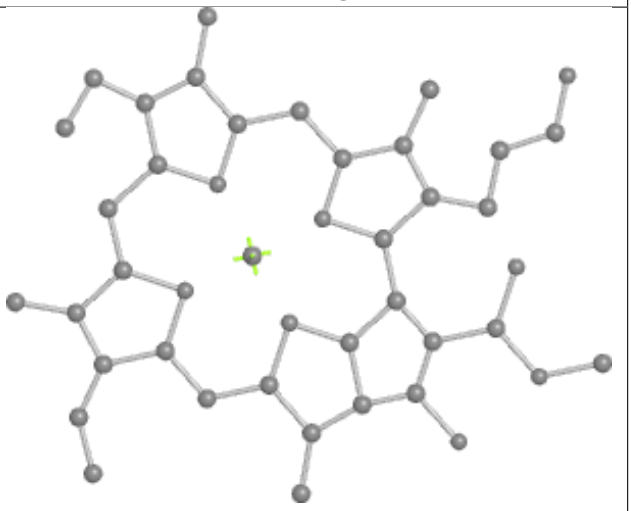
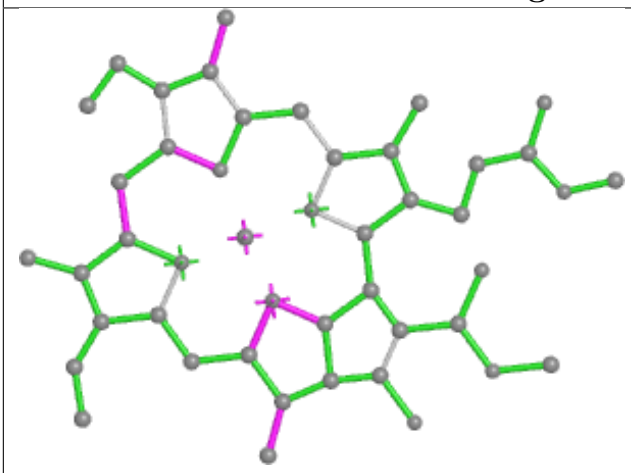


Rings

Ligand CLA 4 311



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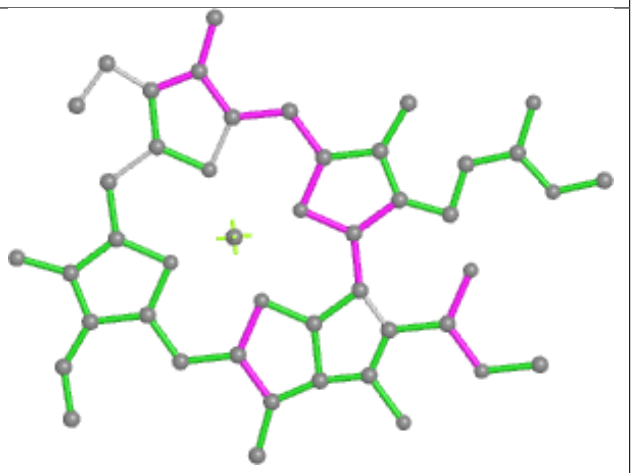

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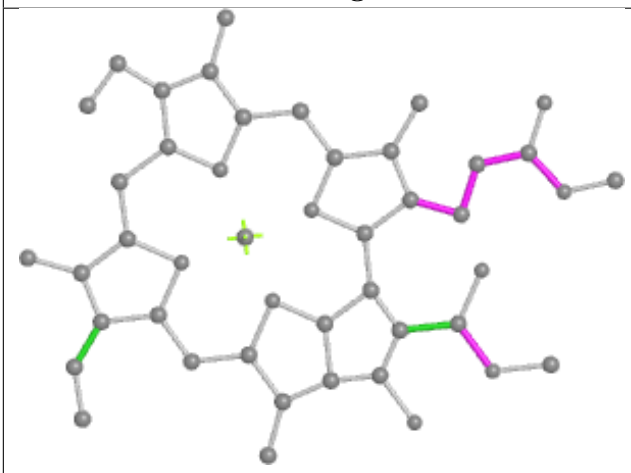

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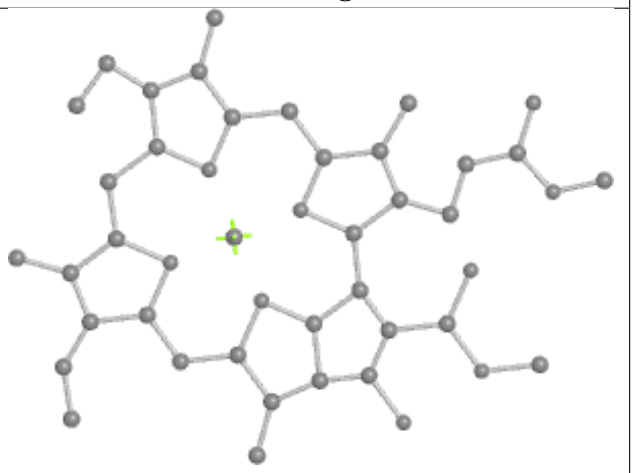
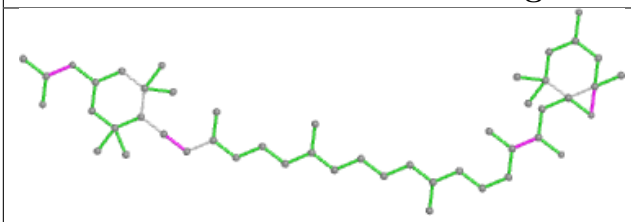


Rings

Ligand A86 11 303



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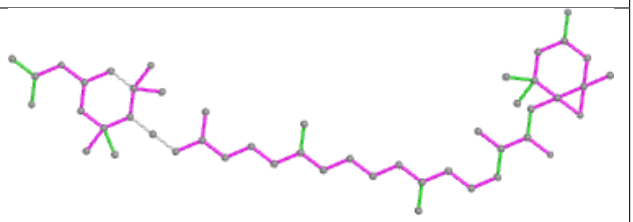
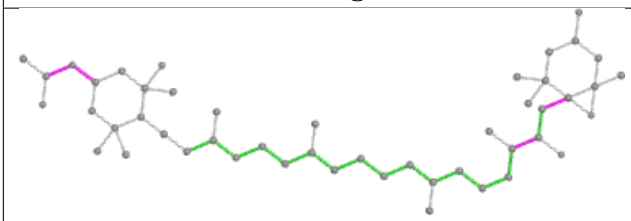


Bond angles



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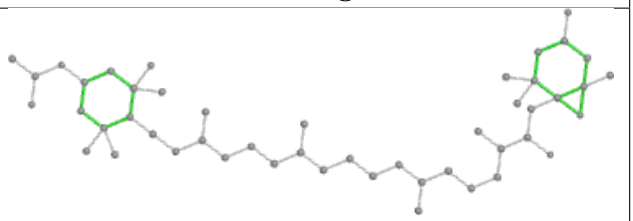
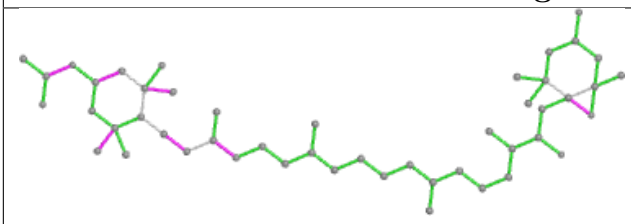


Rings

Ligand A86 2 304



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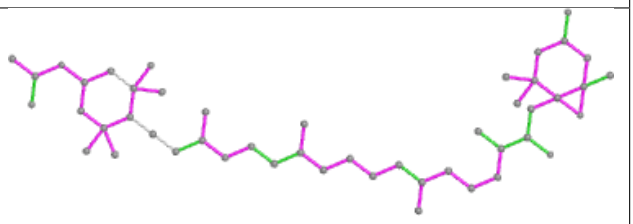

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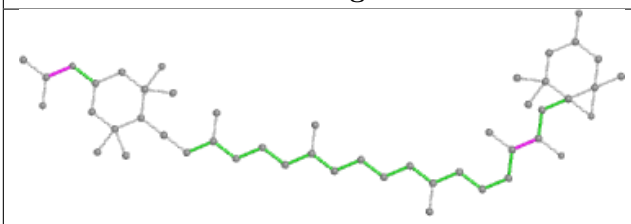
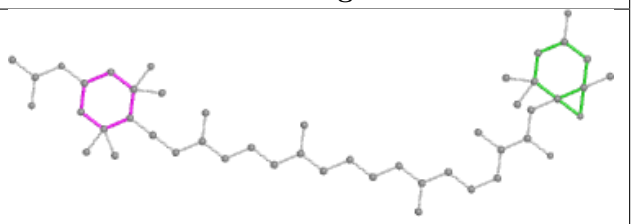
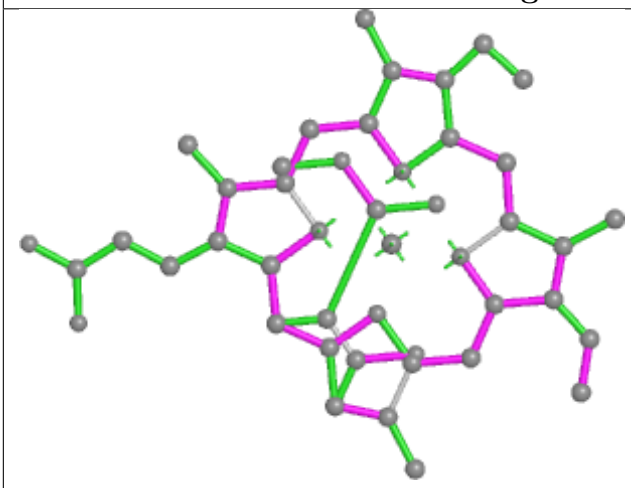


Torsions



Rings

Ligand KC2 16 312



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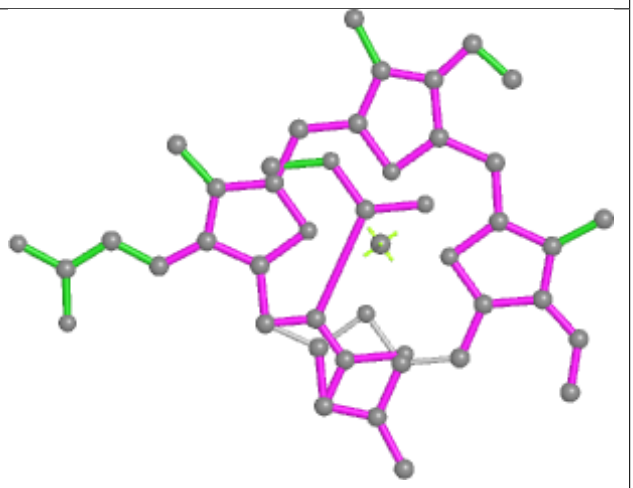

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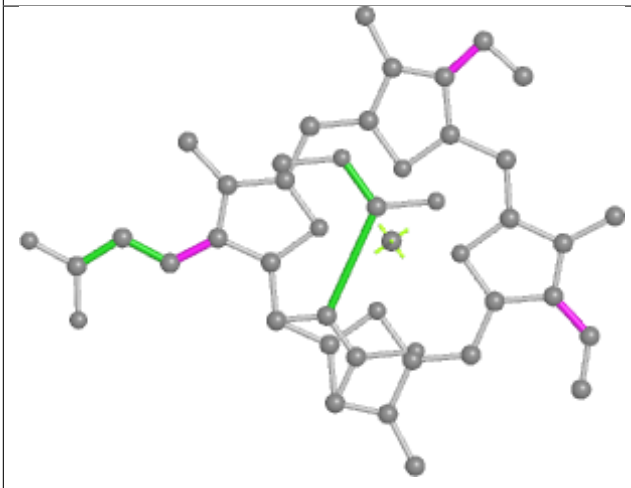

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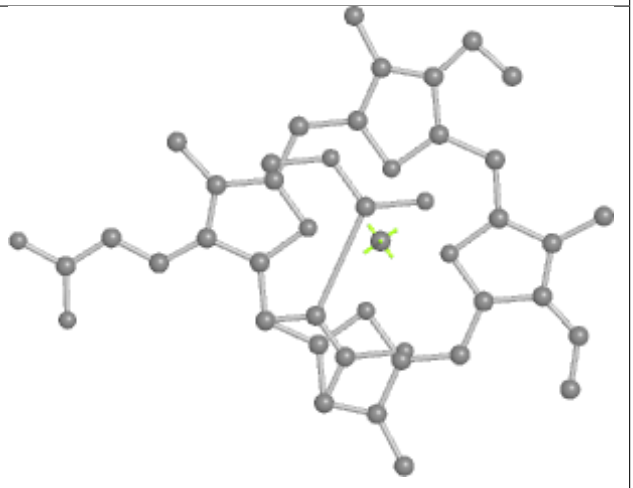
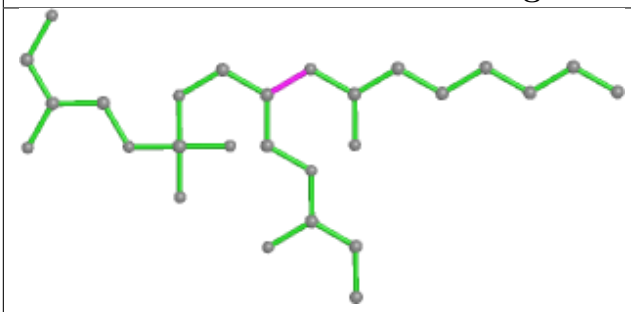


Rings

Ligand LHG P 615



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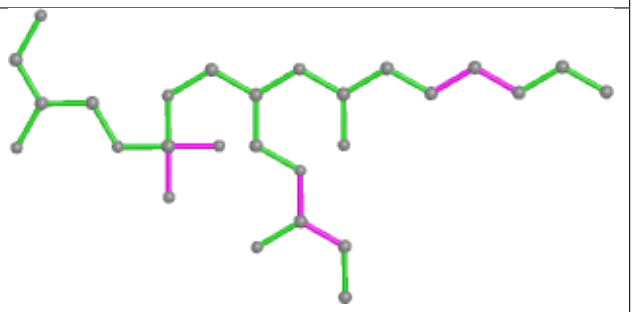

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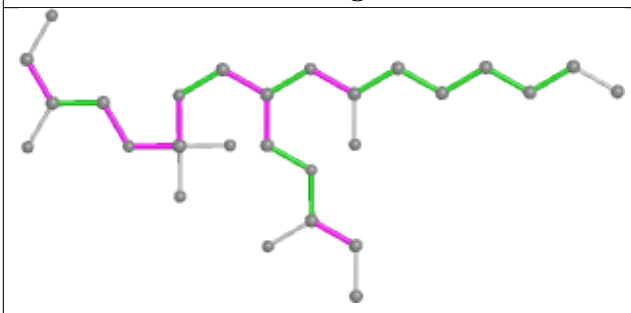

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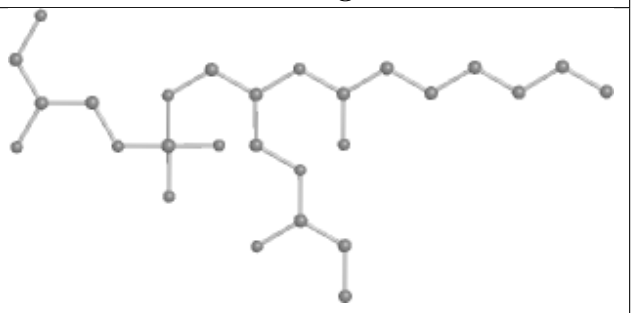
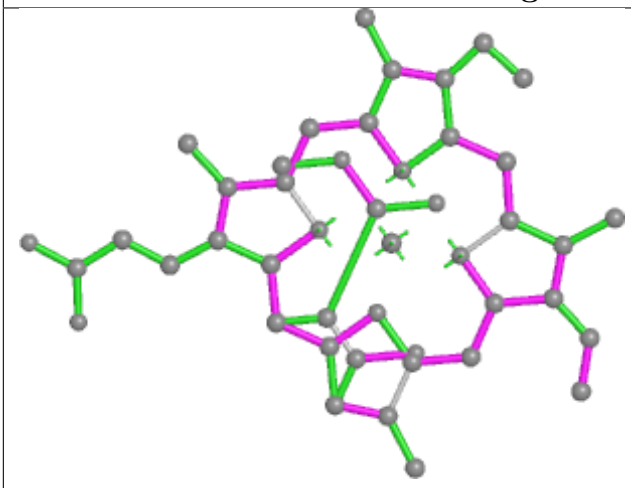


Rings

Ligand KC2 17 309



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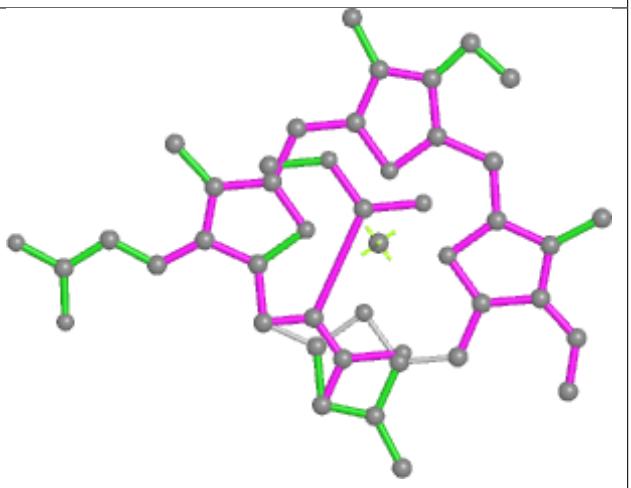

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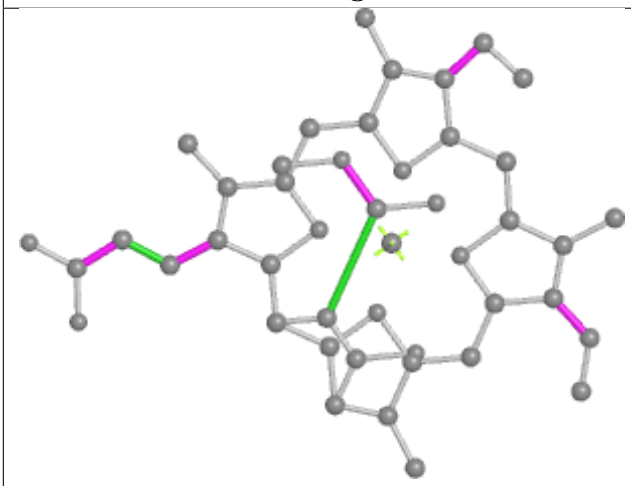

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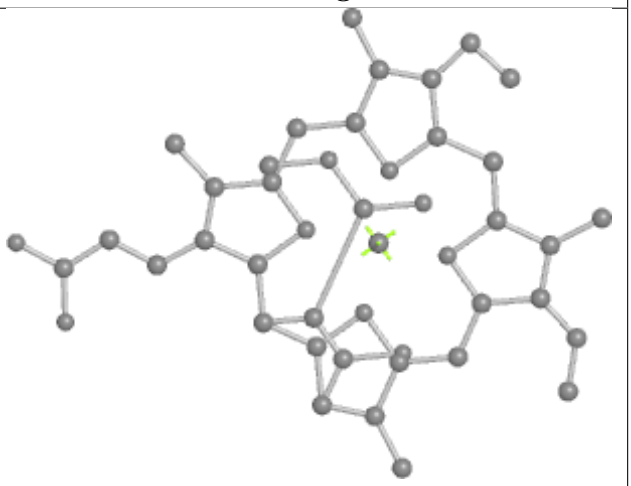
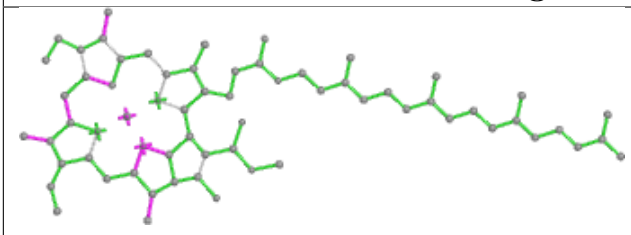


Rings

Ligand CLA 4 307



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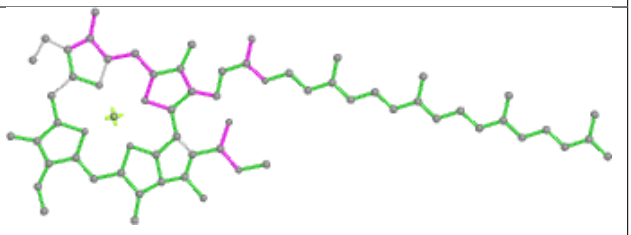

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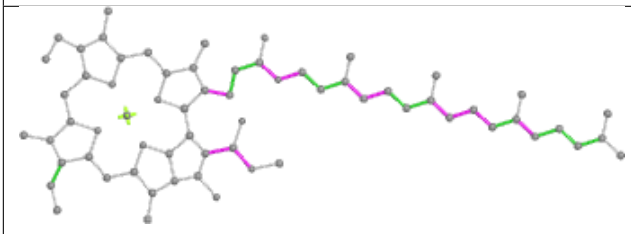

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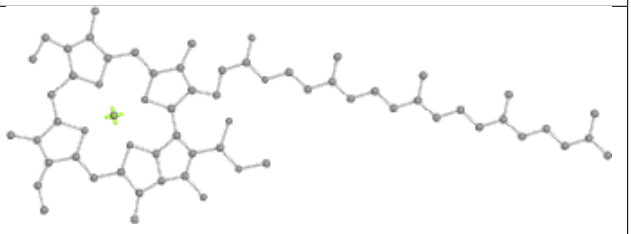
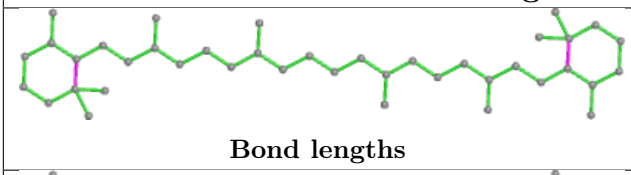


Rings

Ligand BCR C 517



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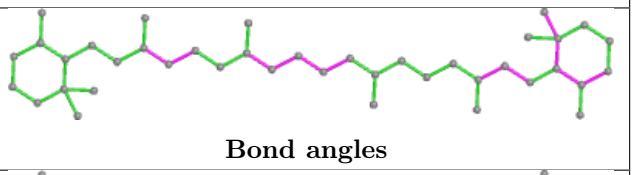

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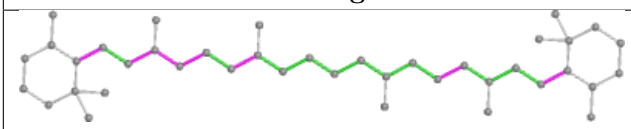

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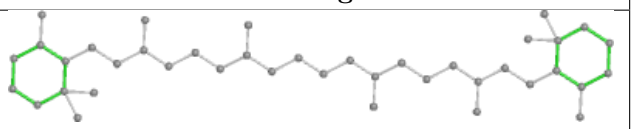
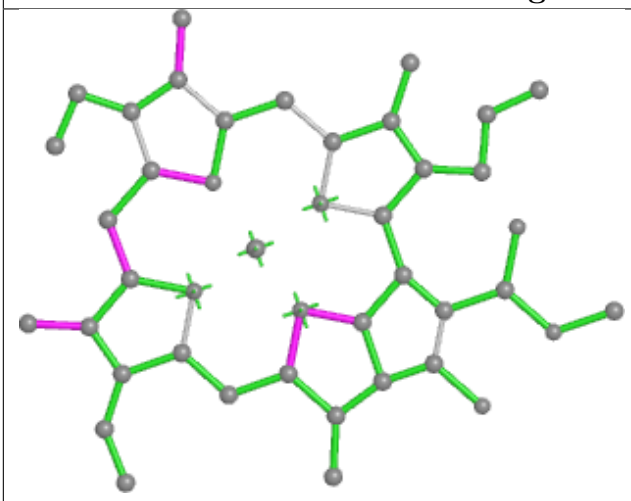


Rings

Ligand CLA 2 309



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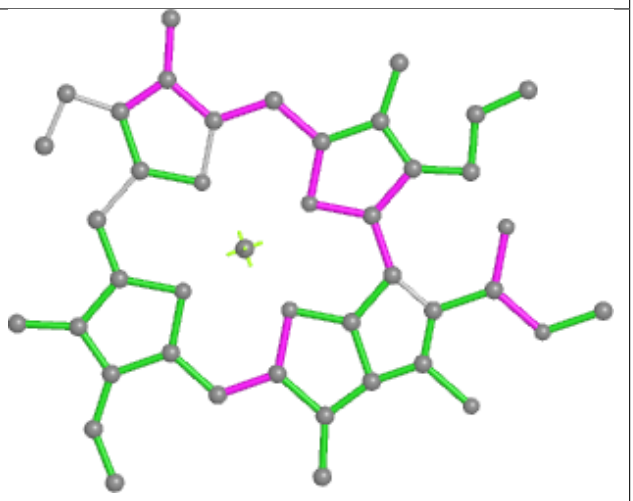

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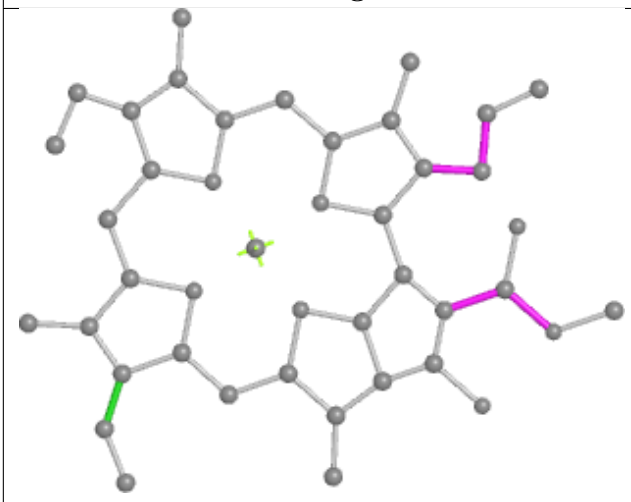

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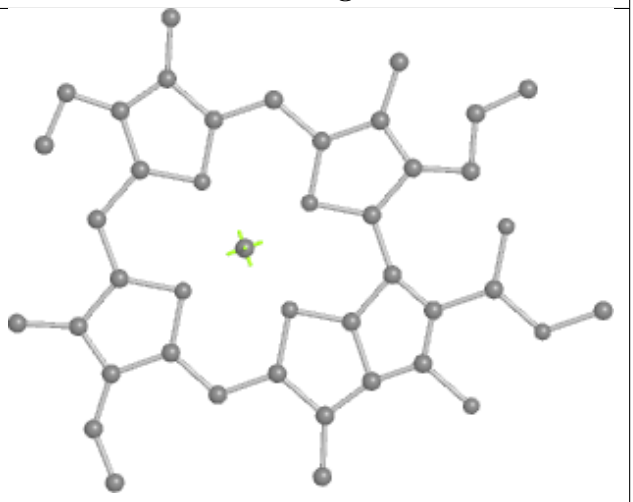
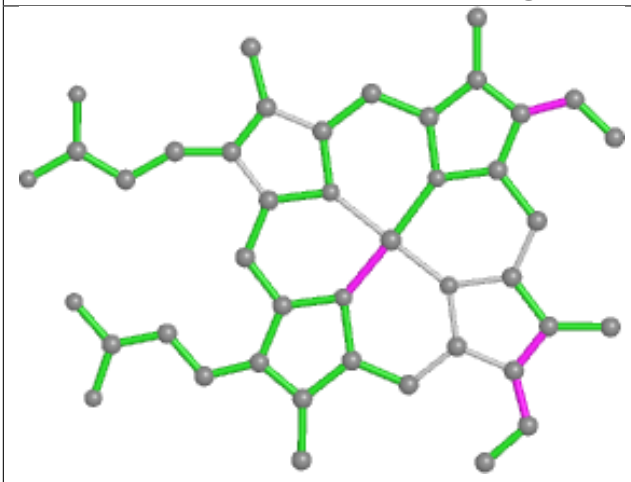


Rings

Ligand HEM E 101



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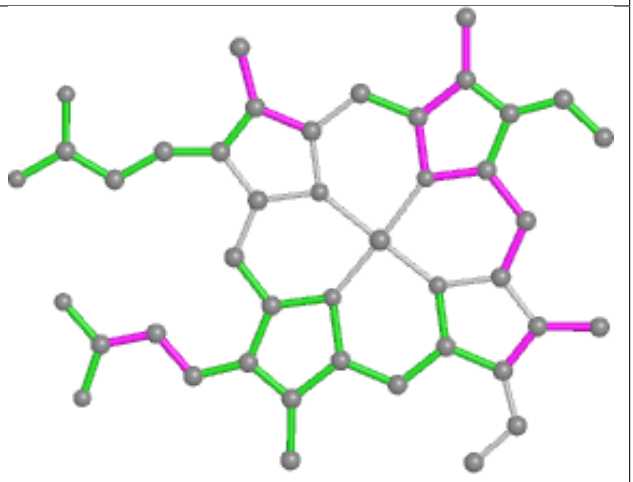

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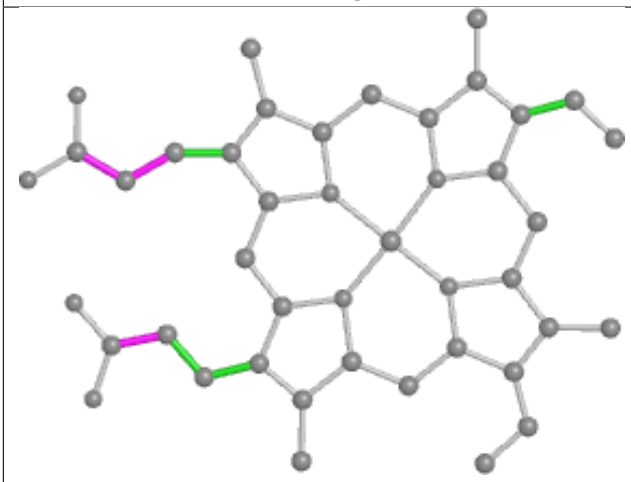

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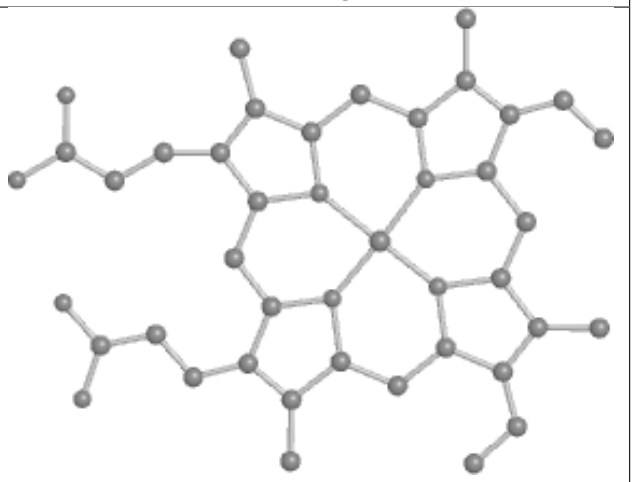
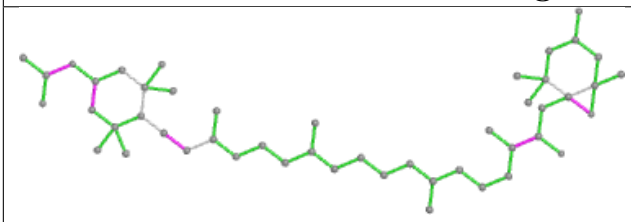


Rings

Ligand A86 2 302



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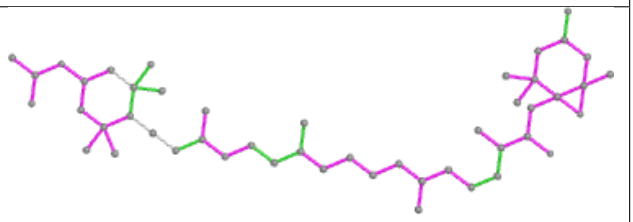

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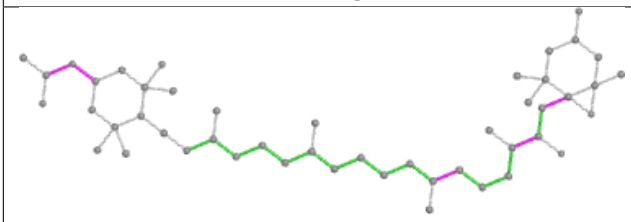

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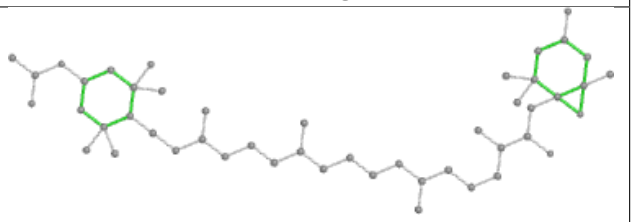
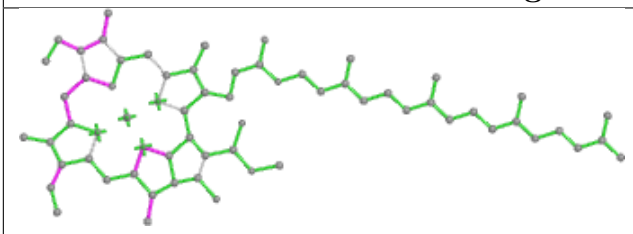


Rings

Ligand CLA B 603



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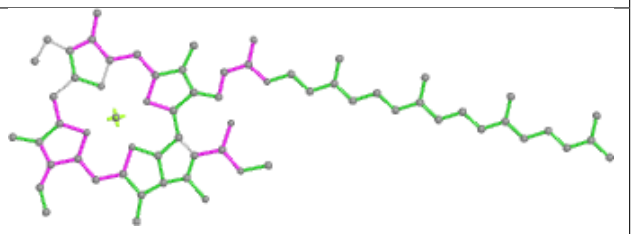

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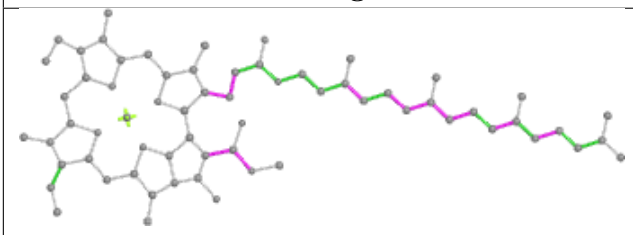

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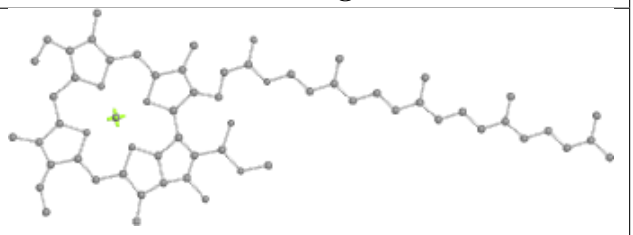
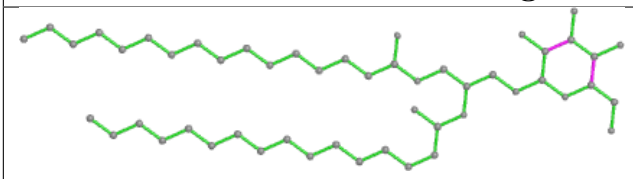


Rings

Ligand LMG C 522



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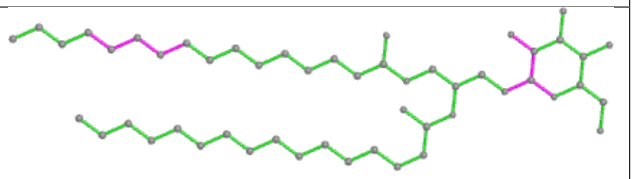

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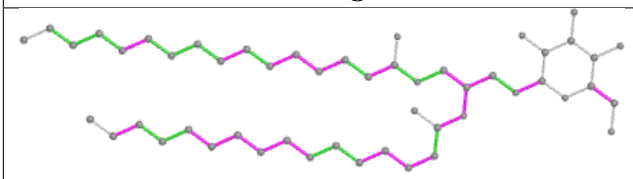

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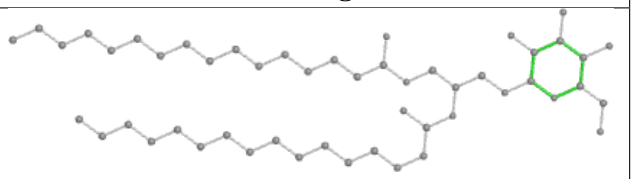
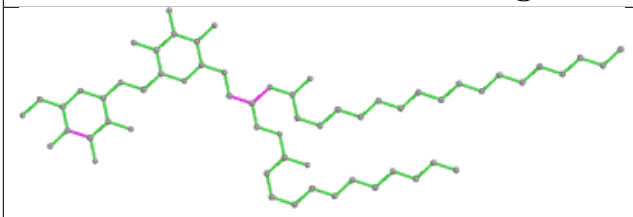


Rings

Ligand DGD 11 318



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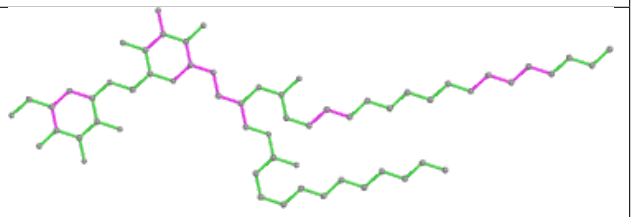
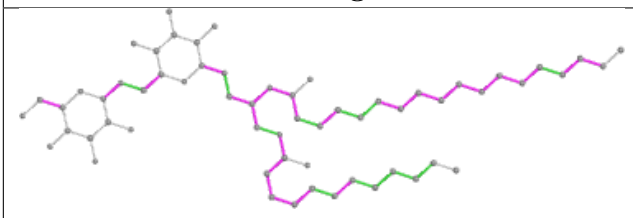


Bond angles



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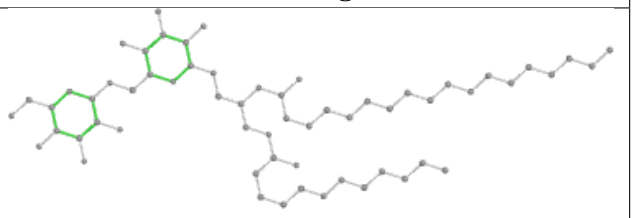
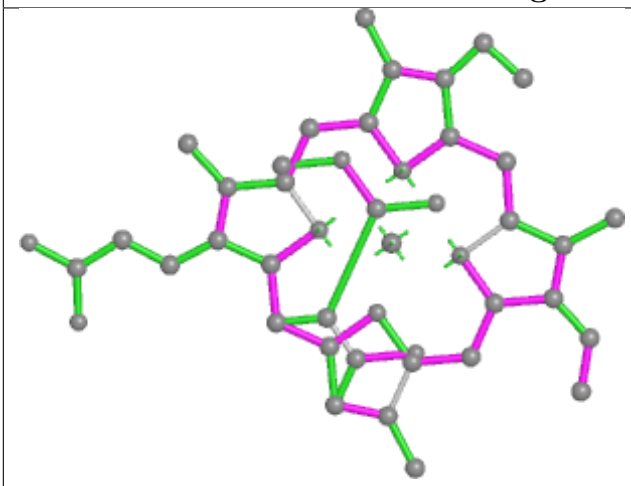


Rings

Ligand KC2 1 309



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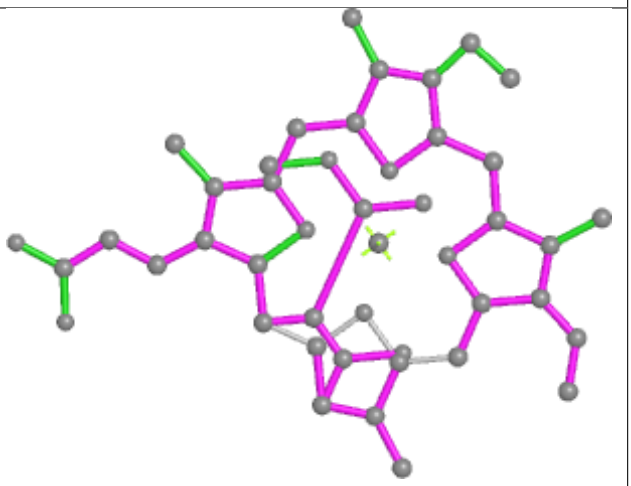

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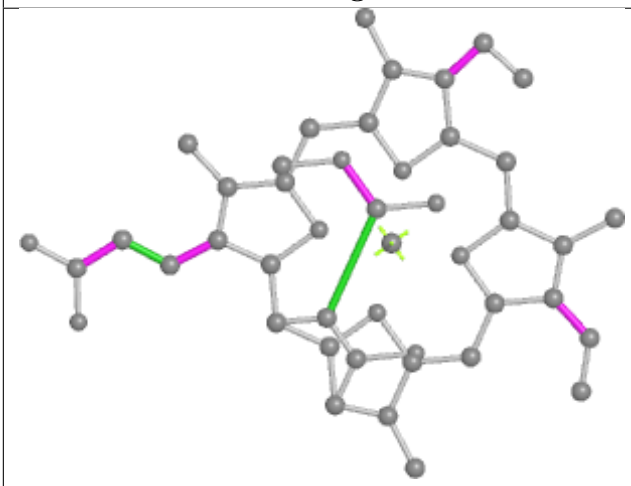

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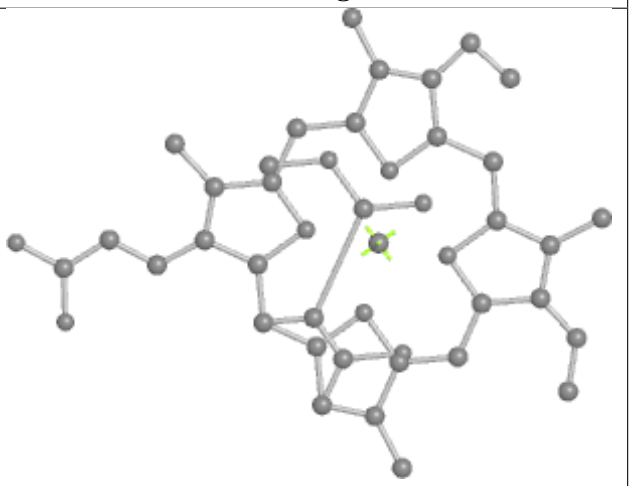
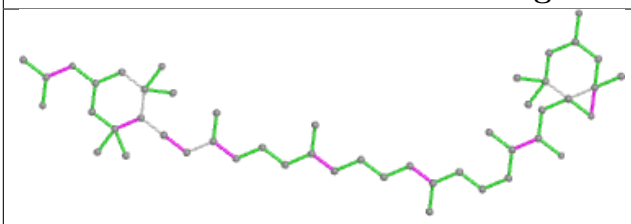


Rings

Ligand A86 8 303



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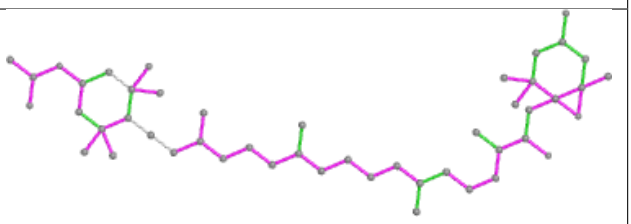

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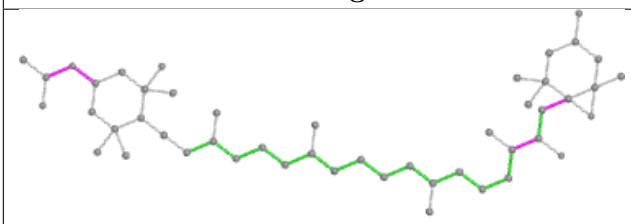

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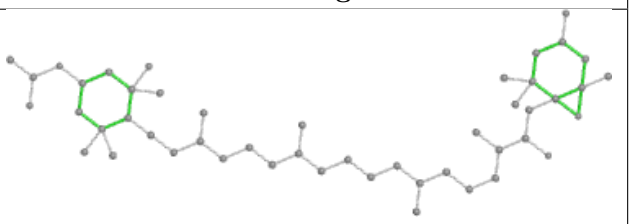
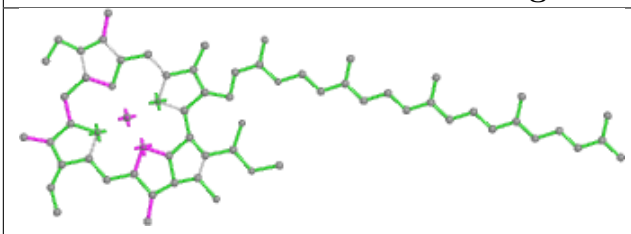


Rings

Ligand CLA c 506



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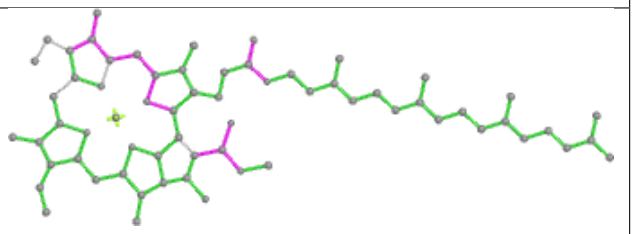

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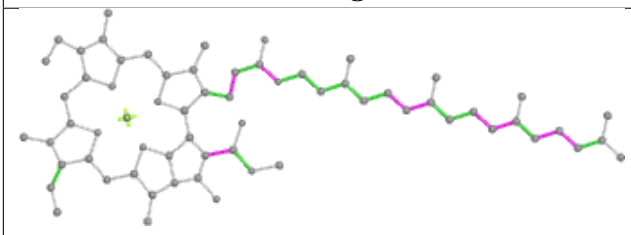
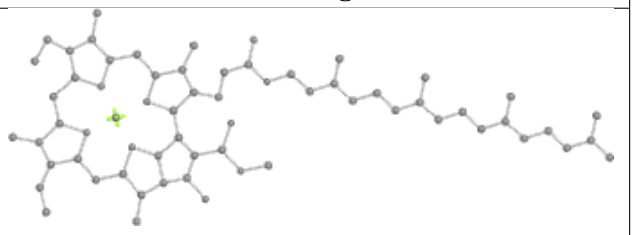
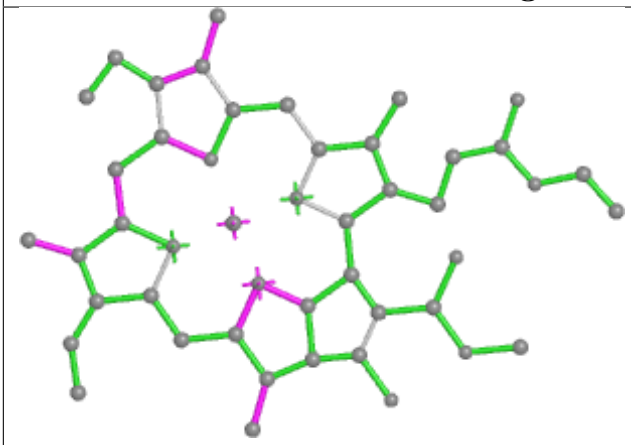


Torsions



Rings

Ligand CLA 17 312



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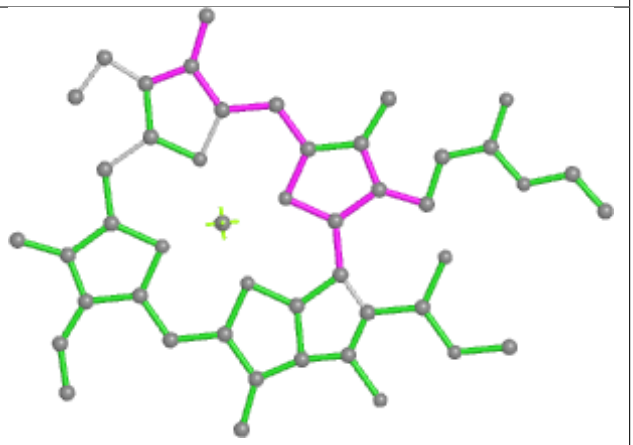

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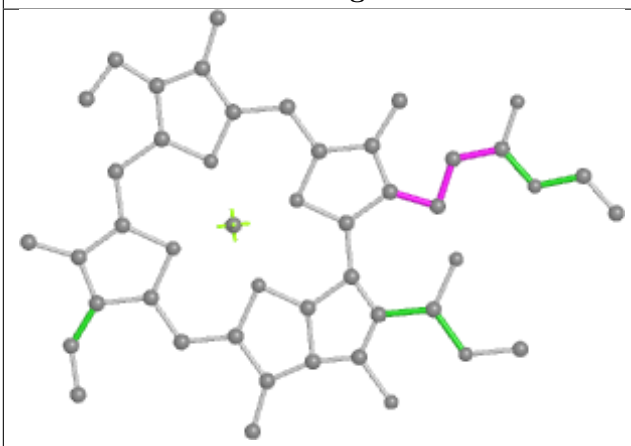

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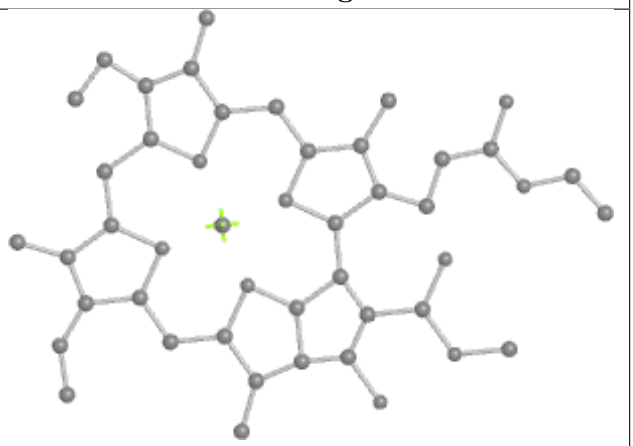
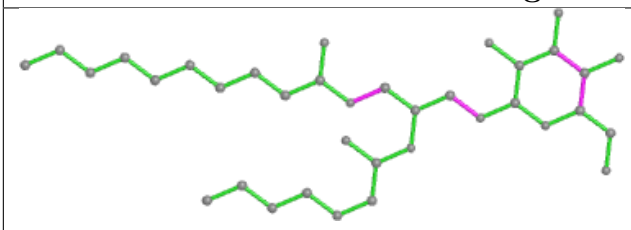


Rings

Ligand LMG 5 316



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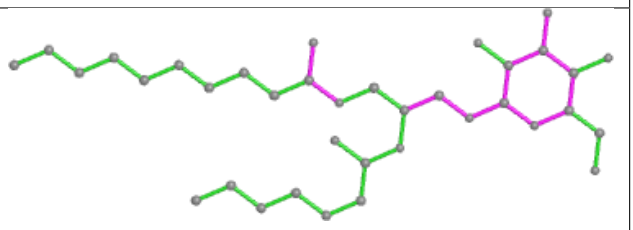

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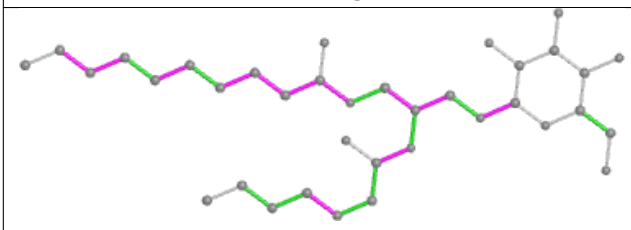

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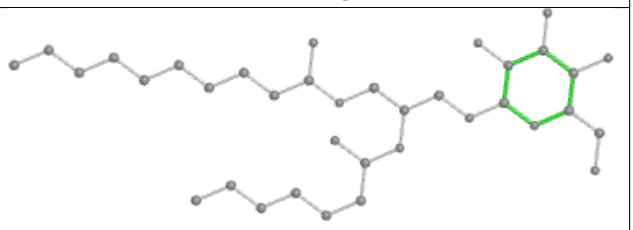
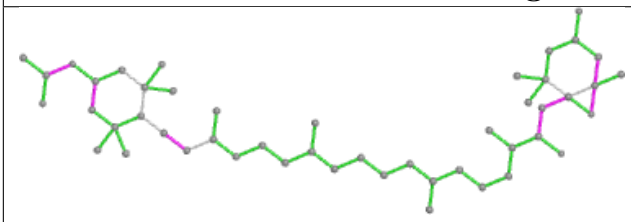


Rings

Ligand A86 16 306



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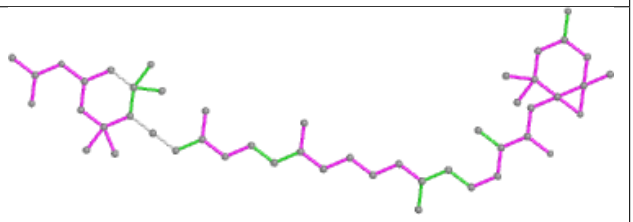

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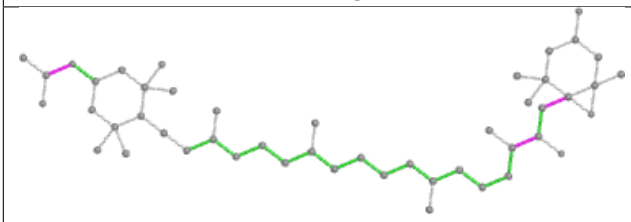

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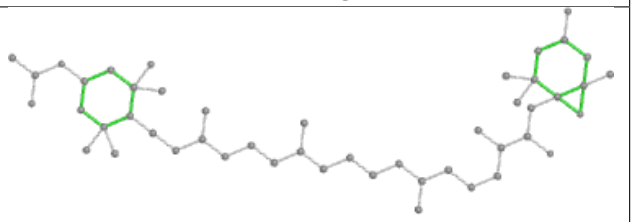
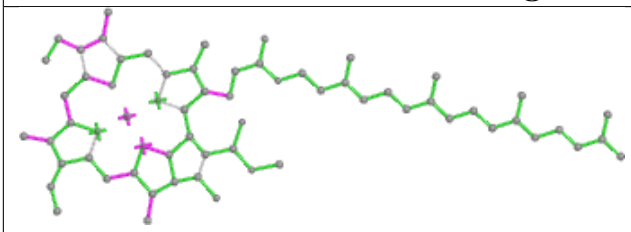


Rings

Ligand CLA D 404



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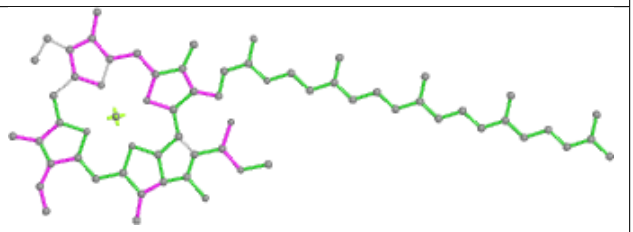

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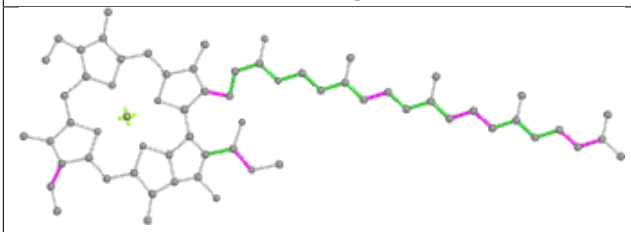

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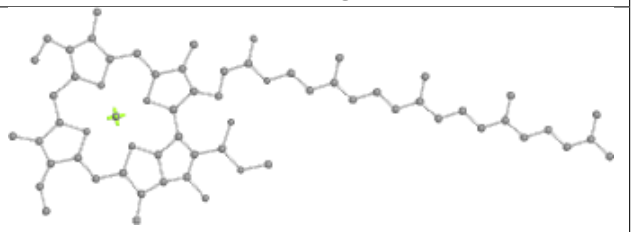
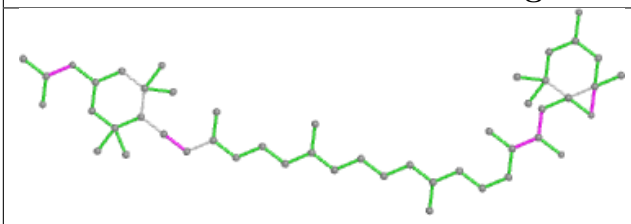


Rings

Ligand A86 18 303



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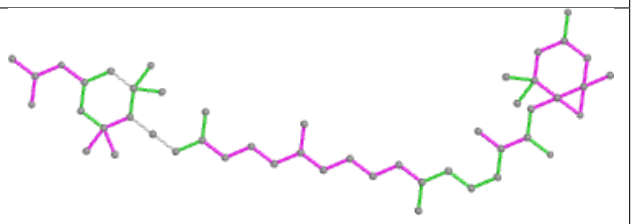

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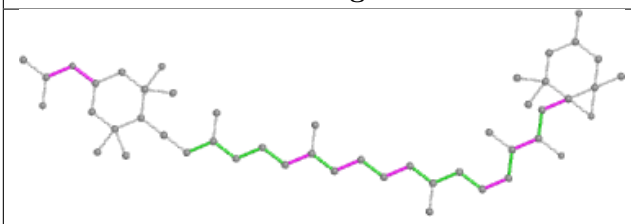

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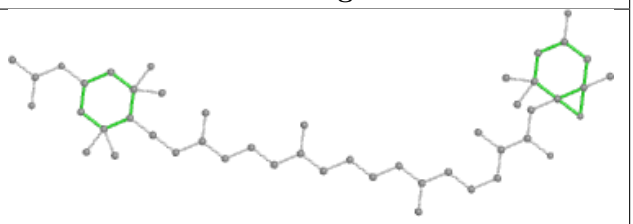
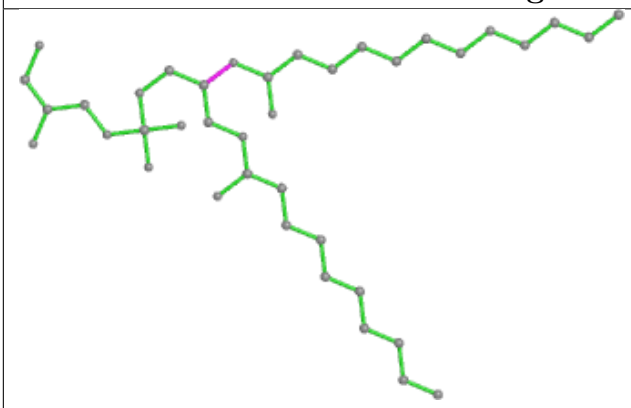


Rings

Ligand LHG 8 315



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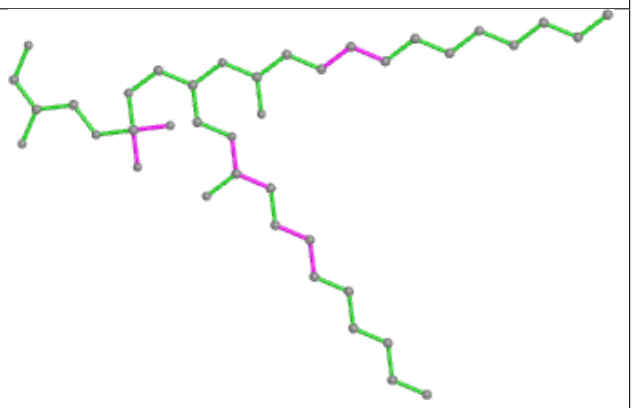

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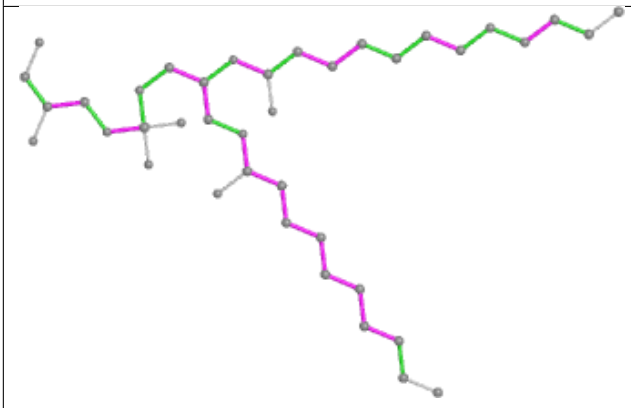

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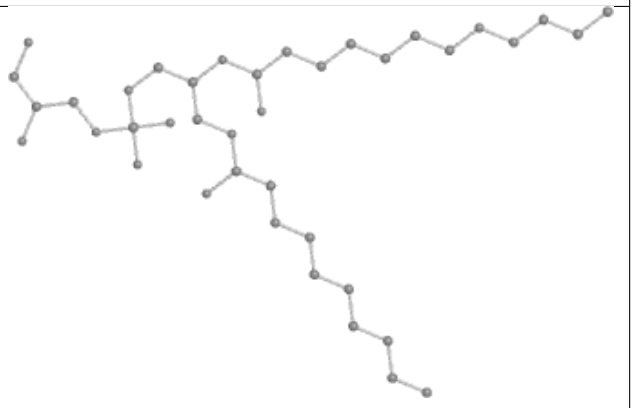
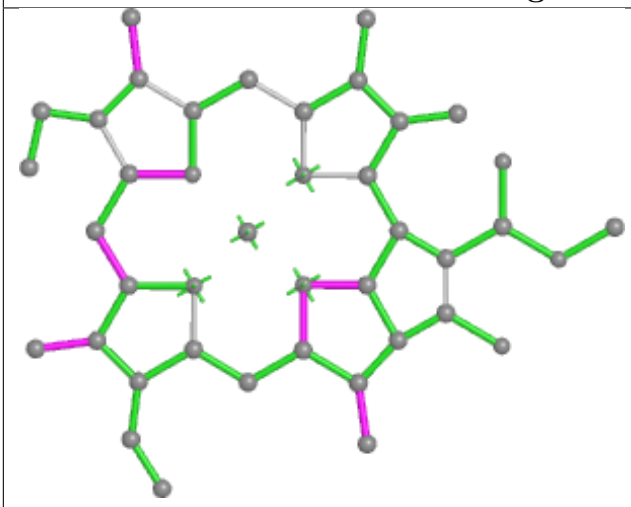


Rings

Ligand CLA p 605



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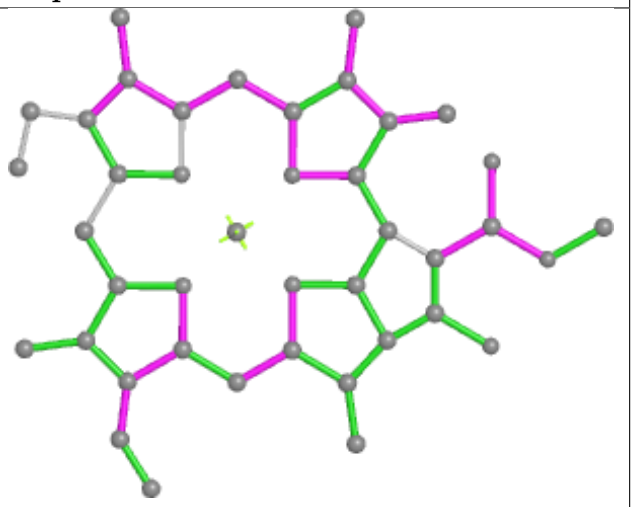

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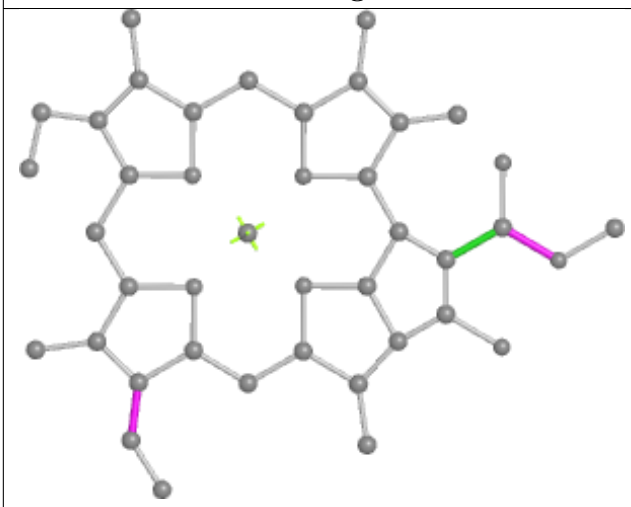

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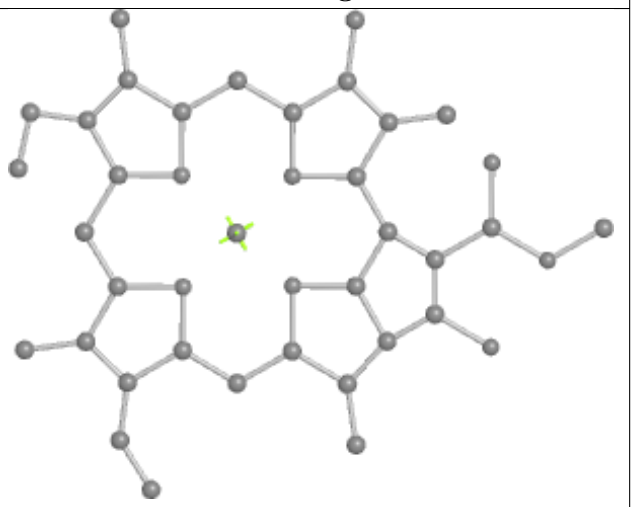
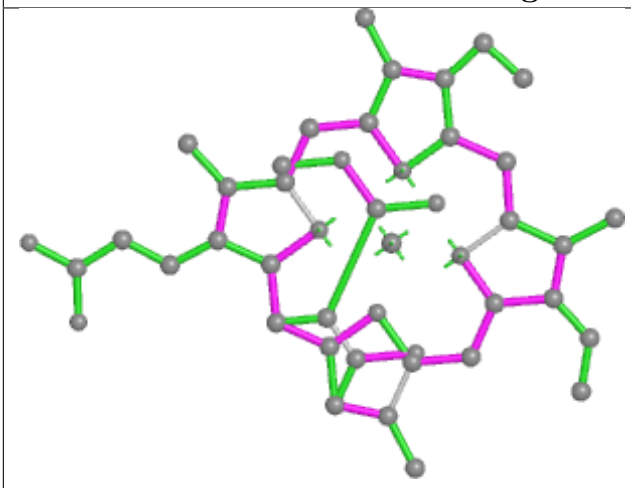


Rings

Ligand KC1 16 301



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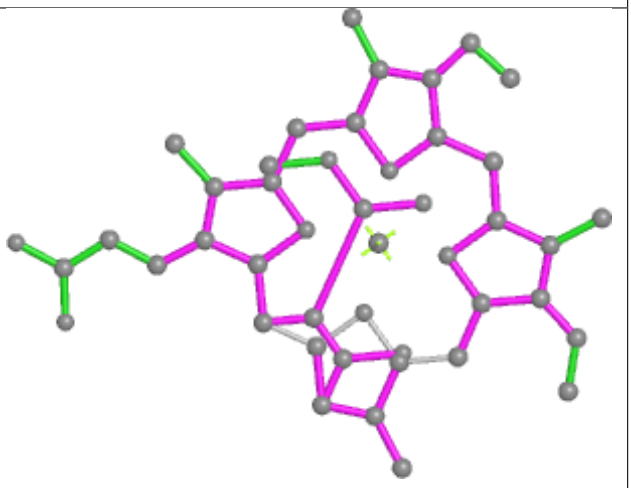

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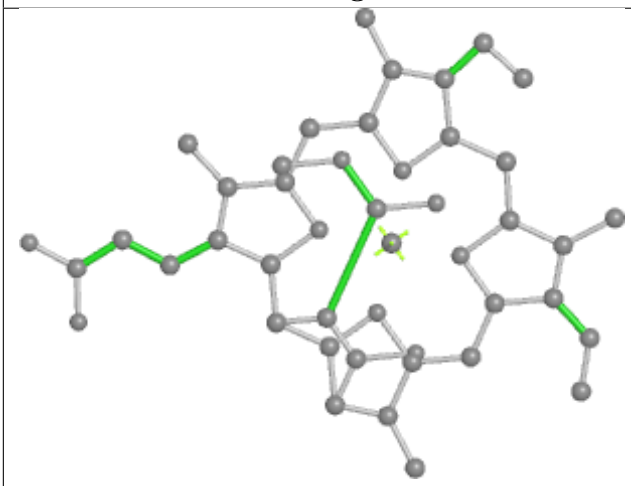

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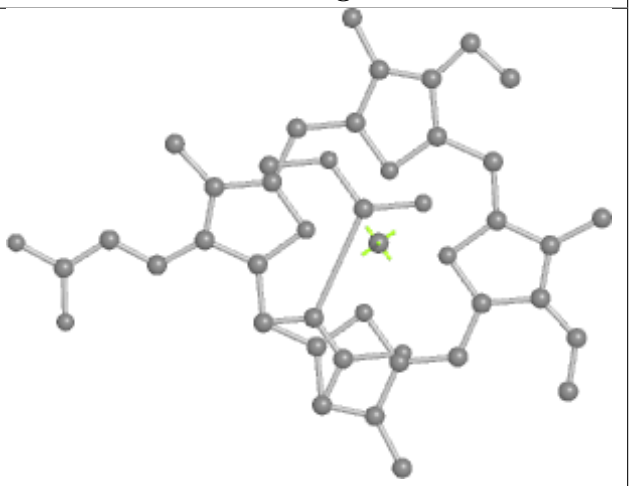
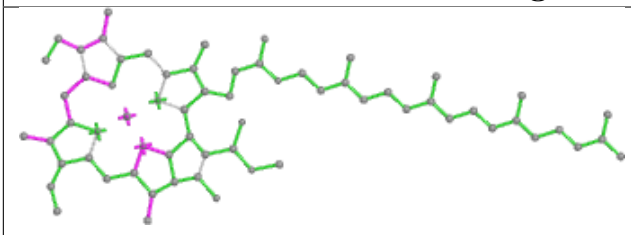


Rings

Ligand CLA c 507



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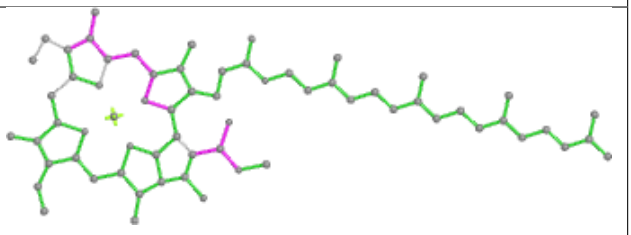

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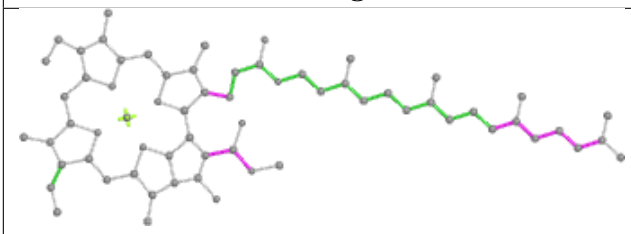

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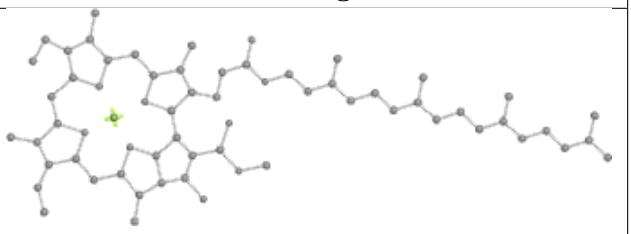
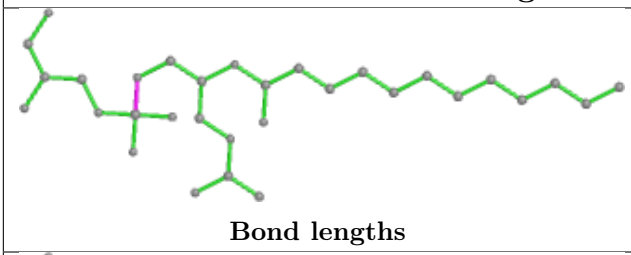


Rings

Ligand LHG 18 316



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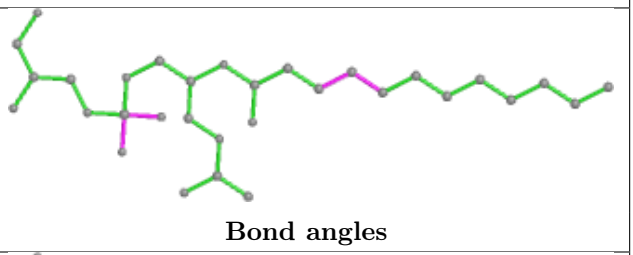

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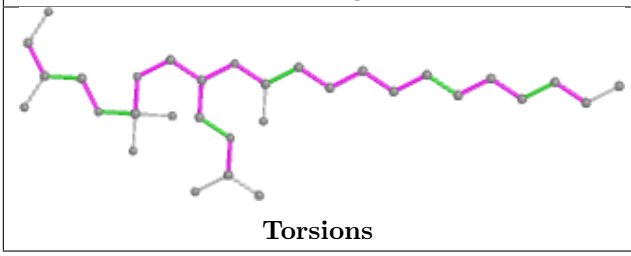

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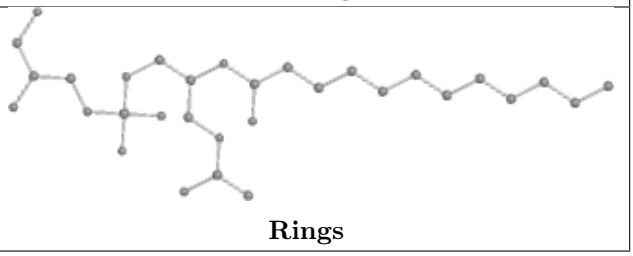
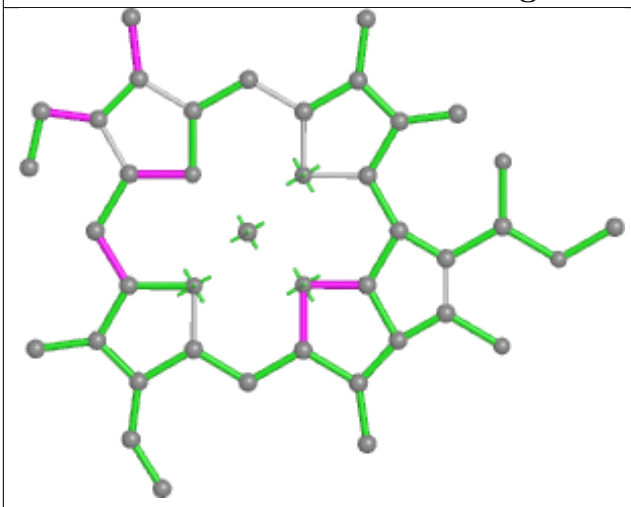


Rings

Ligand CLA 13 310



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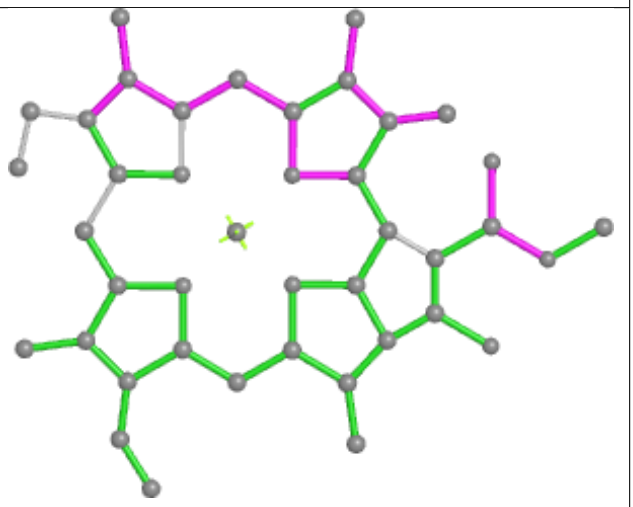
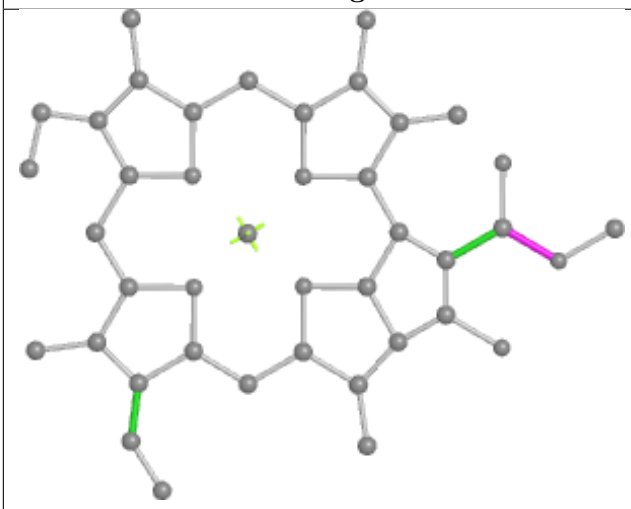


Bond angles



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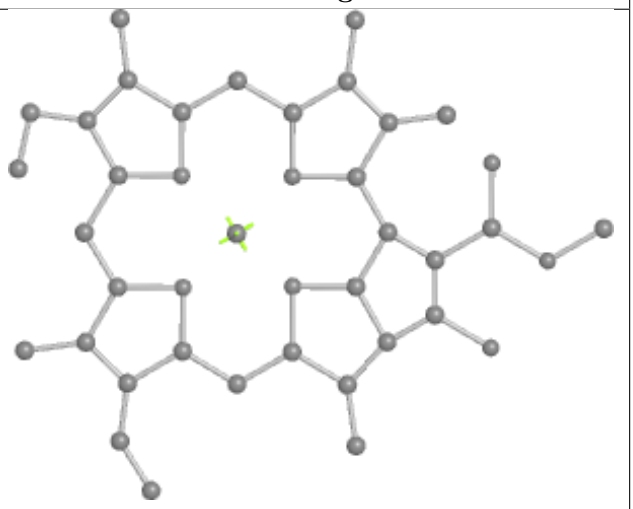
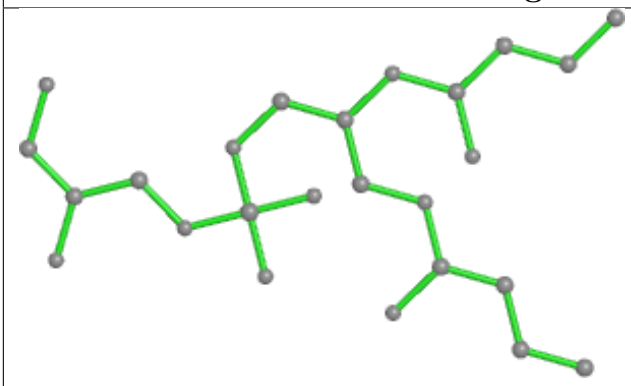


Rings

Ligand LHG Z 103



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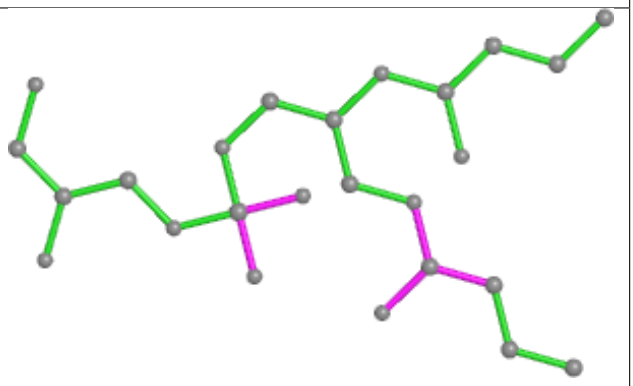
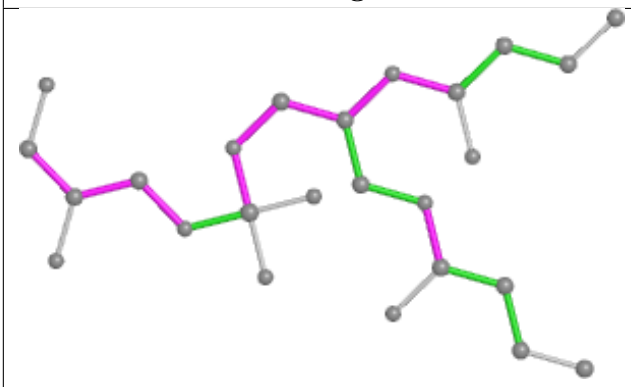


Bond angles



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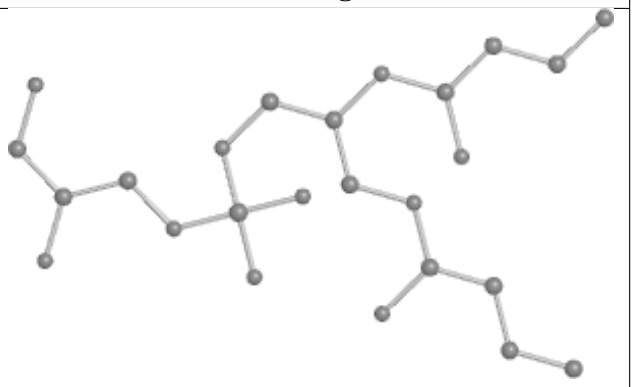
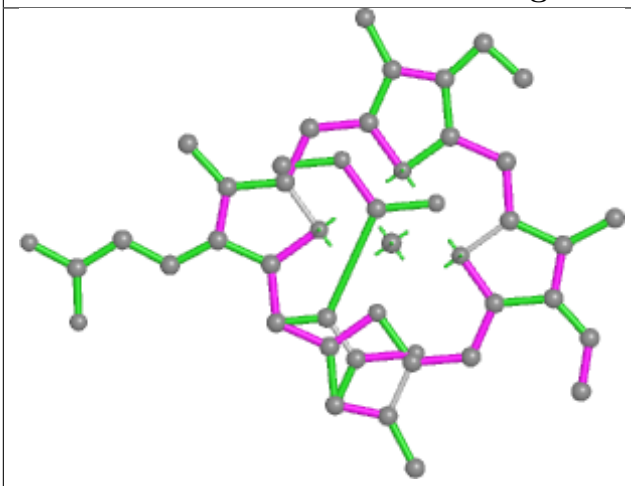


Rings

Ligand KC2 1 311



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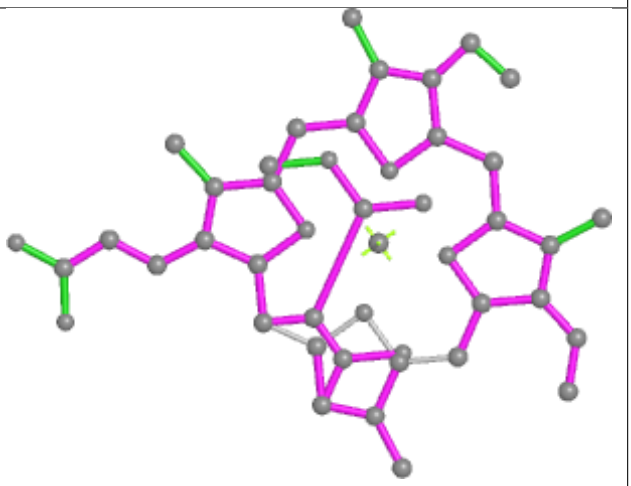
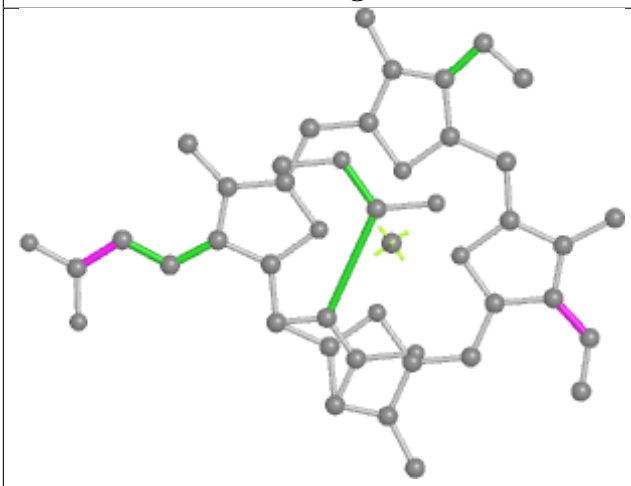


Bond angles



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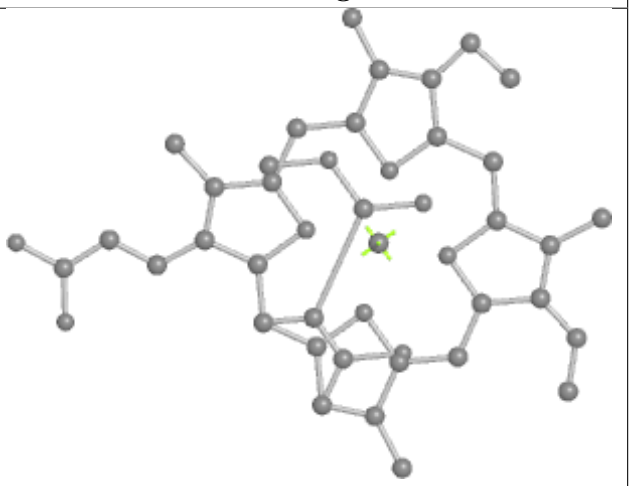
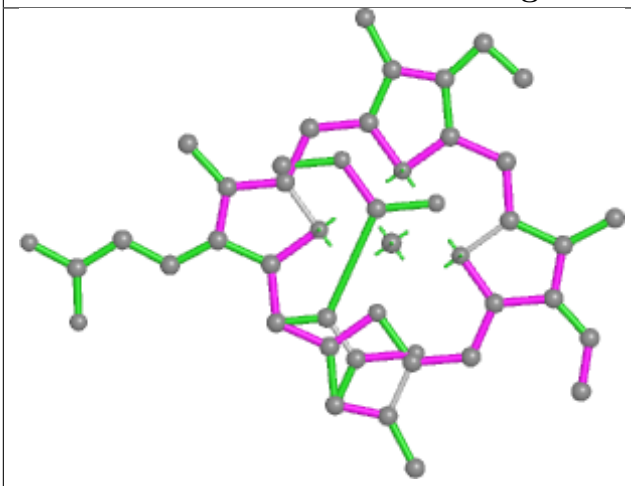


Rings

Ligand KC2 15 308



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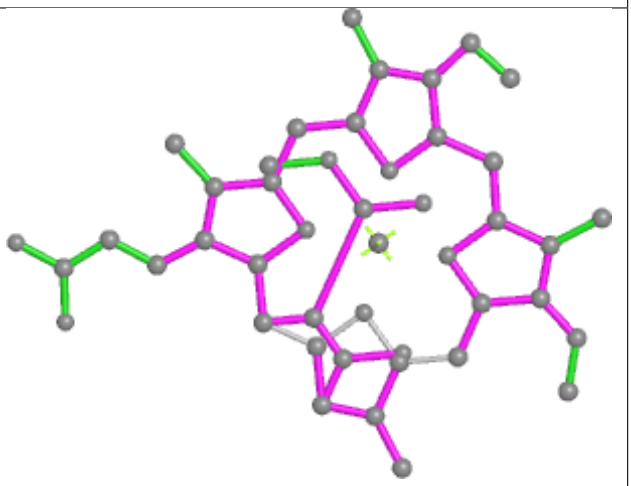

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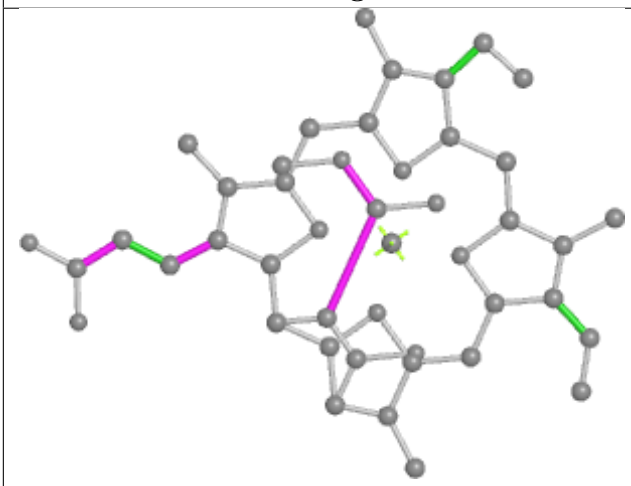
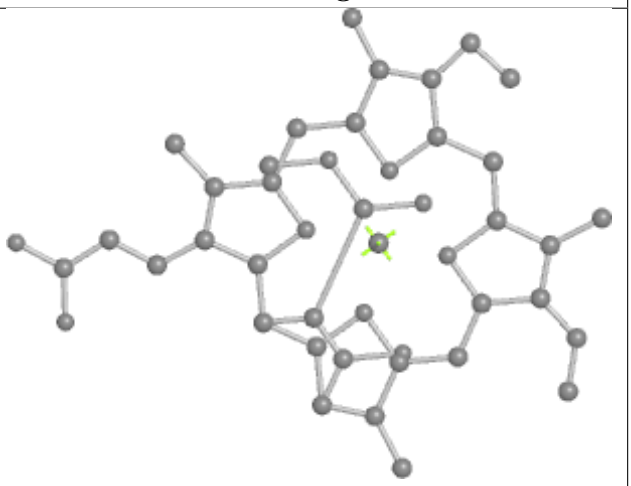
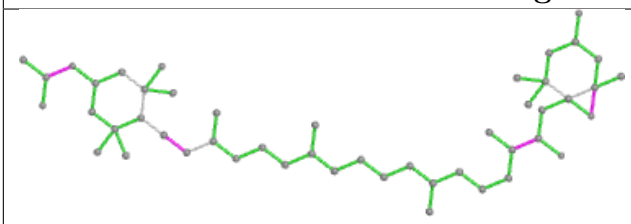


Torsions



Rings

Ligand A86 7 303



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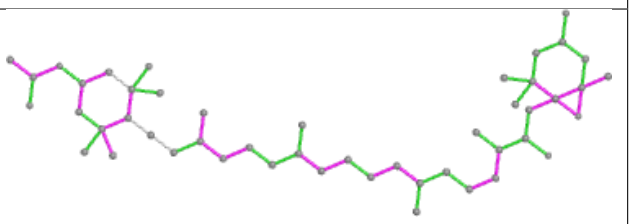

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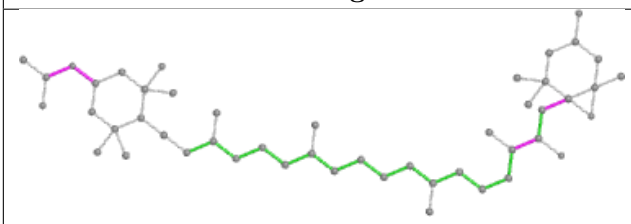

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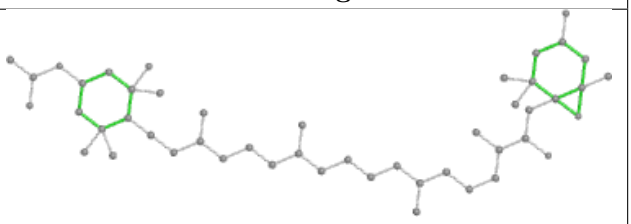
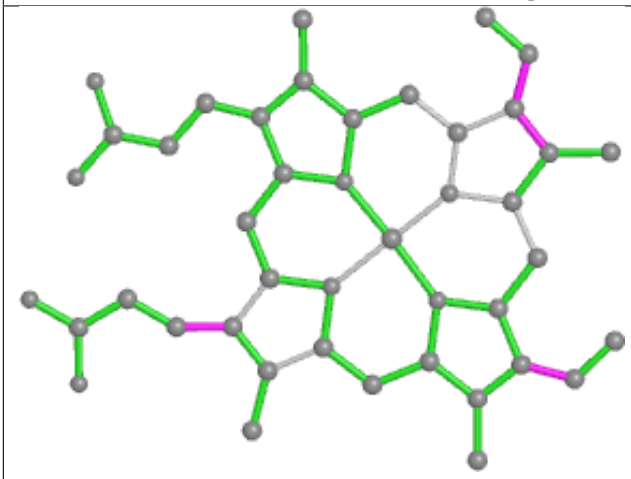


Rings

Ligand HEM v 201



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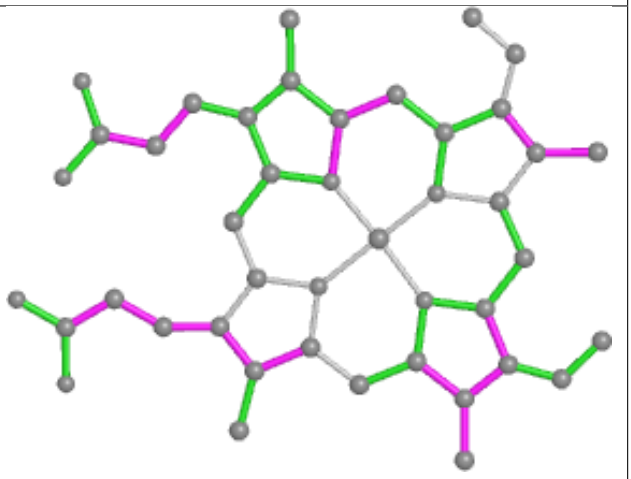

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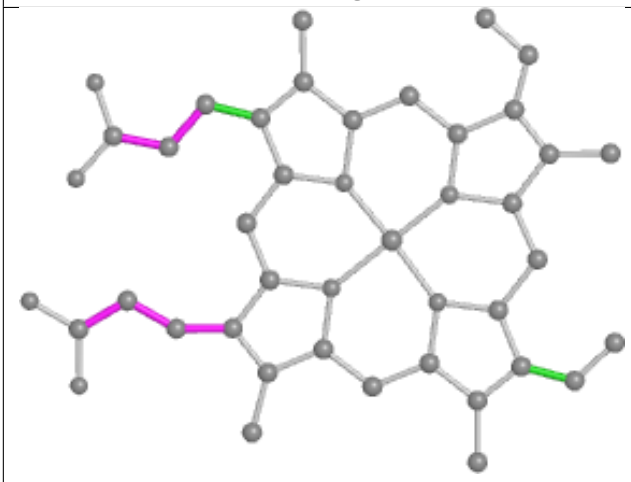

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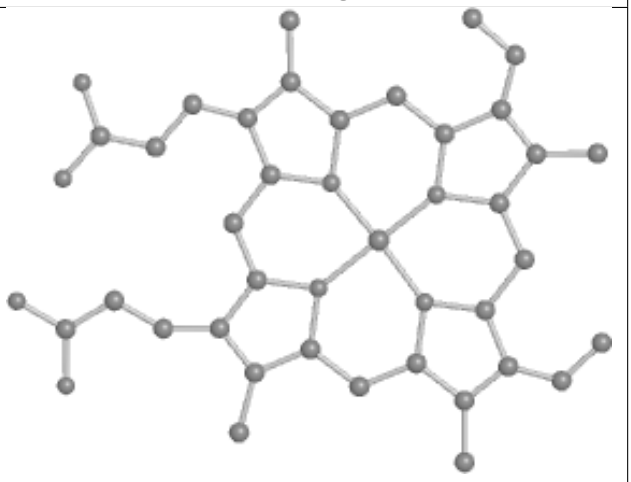

Rings

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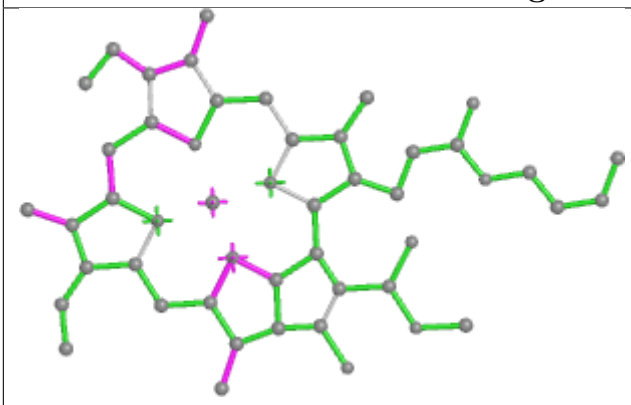

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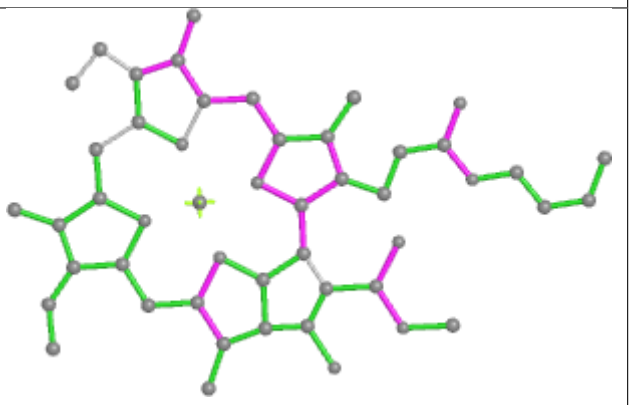

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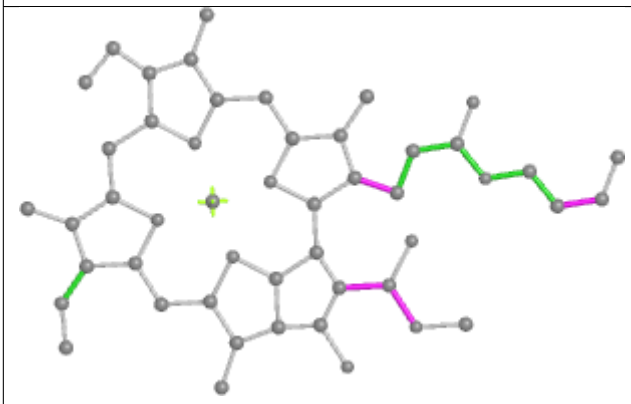

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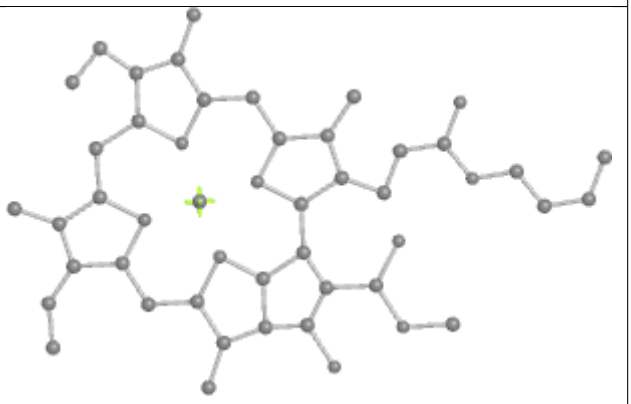
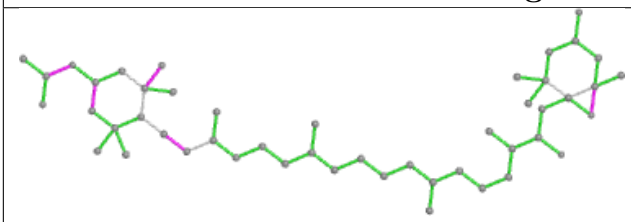


Rings

Ligand A86 16 307



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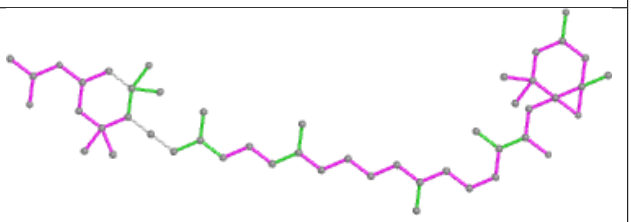

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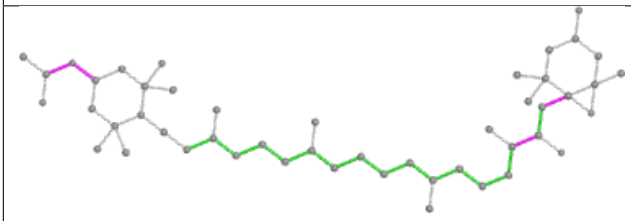

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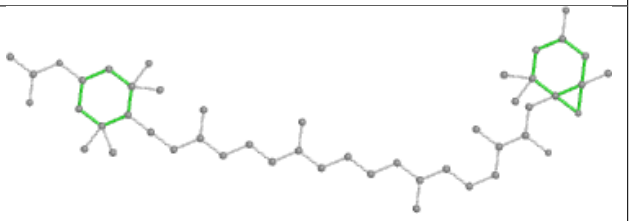

Rings

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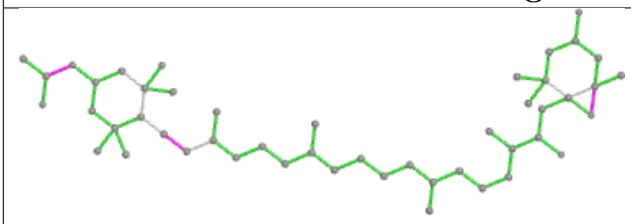

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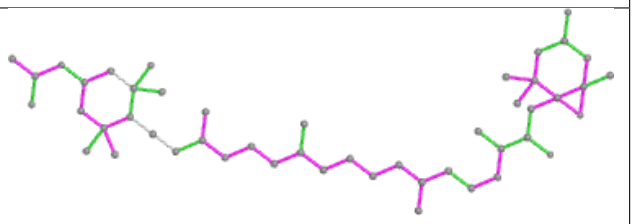

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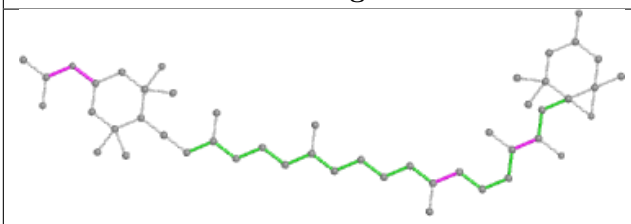

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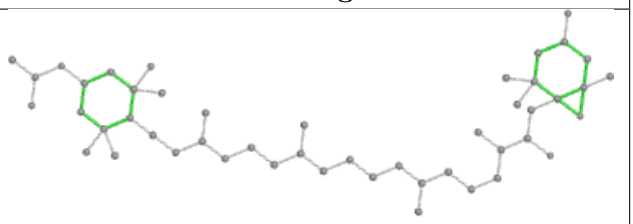

Rings

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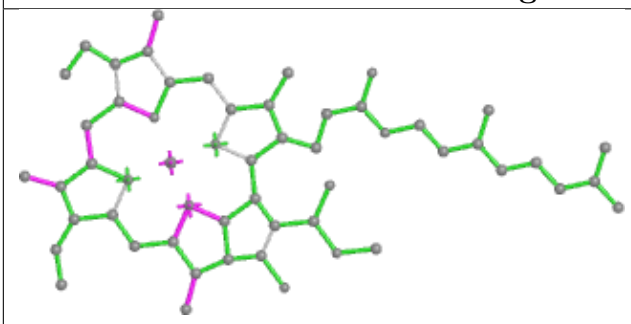

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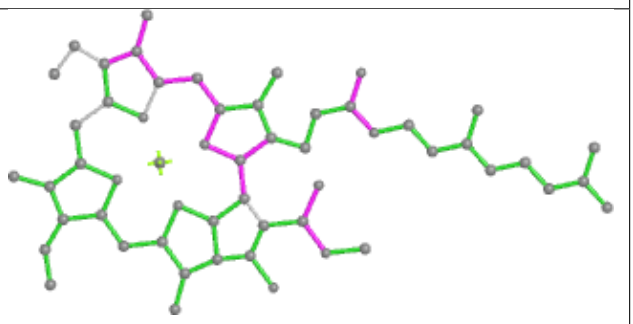

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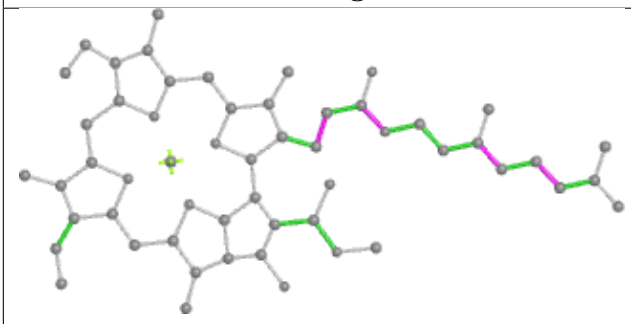

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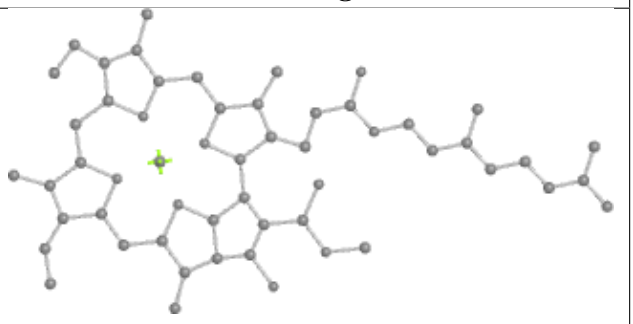

Rings

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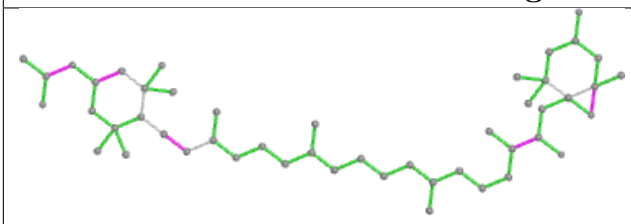

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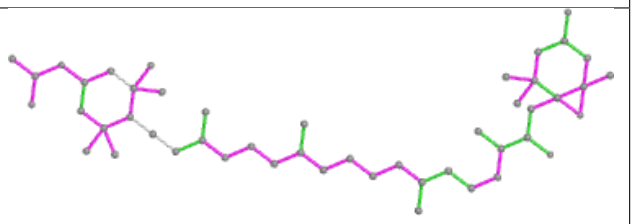

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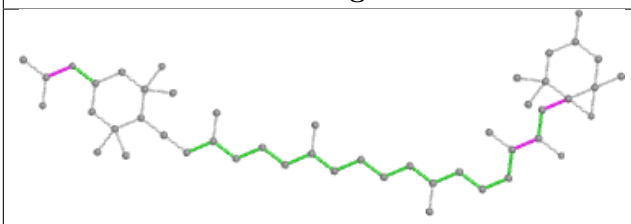

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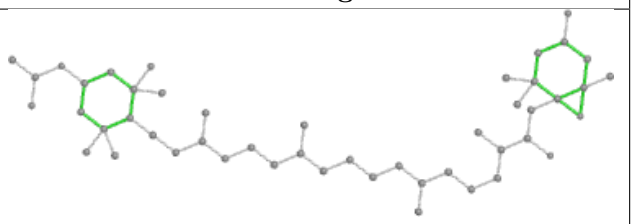

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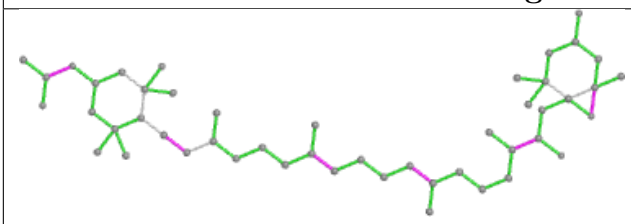

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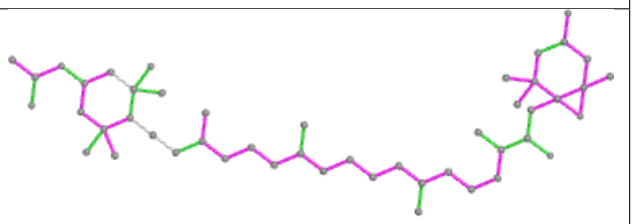

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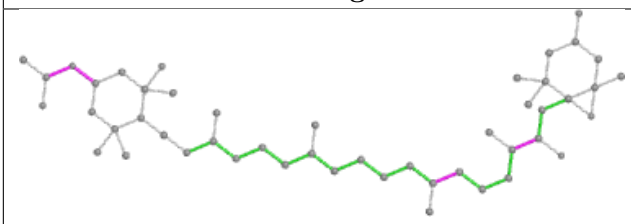

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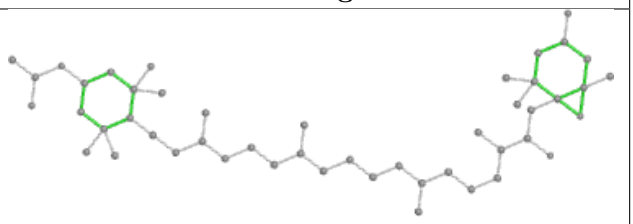

Rings

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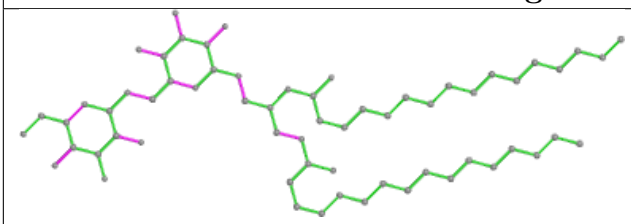

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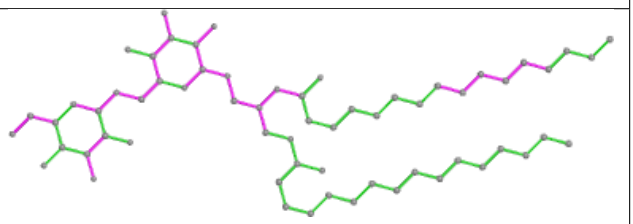

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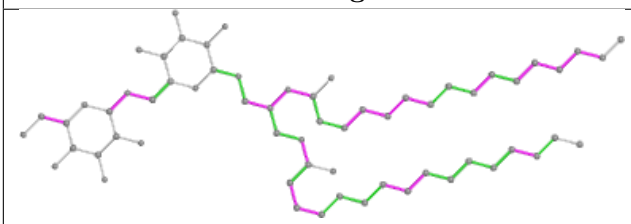

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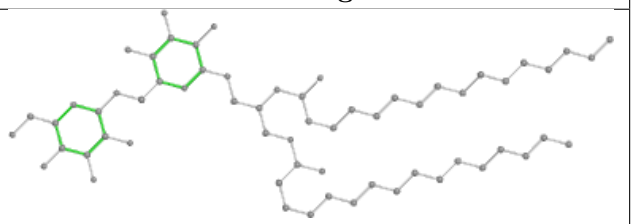
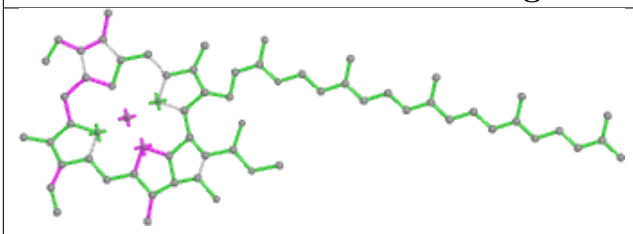


Rings

Ligand CLA D 401



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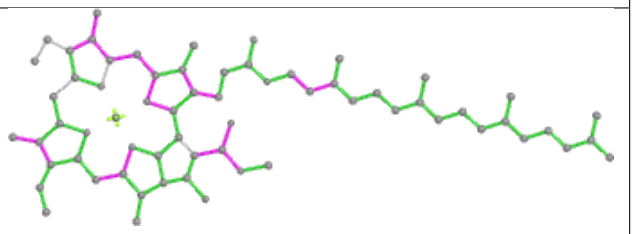

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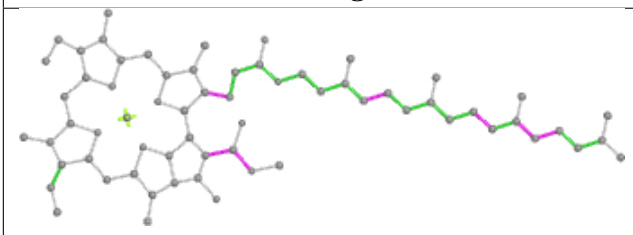

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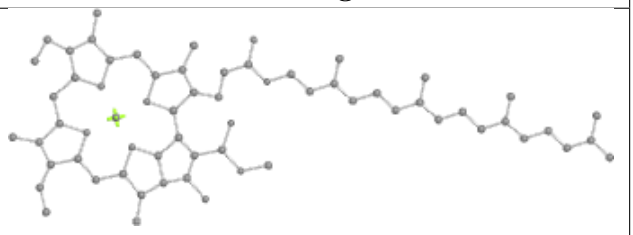
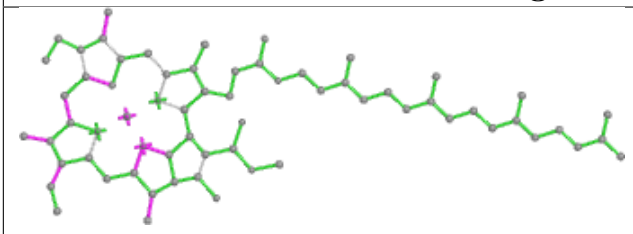


Rings

Ligand CLA c 511



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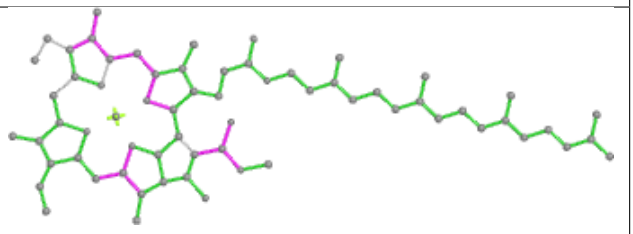

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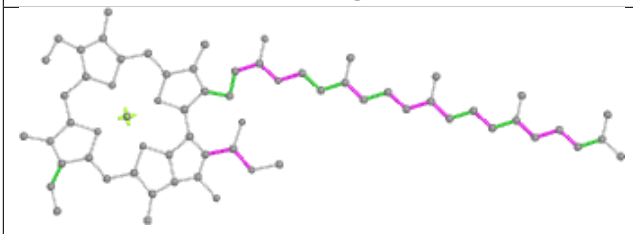

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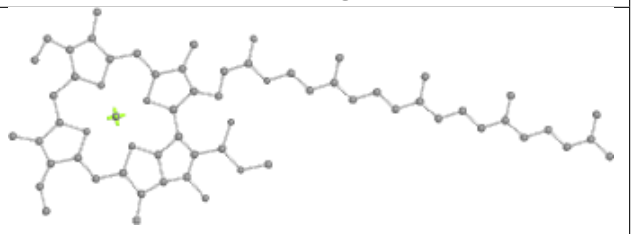
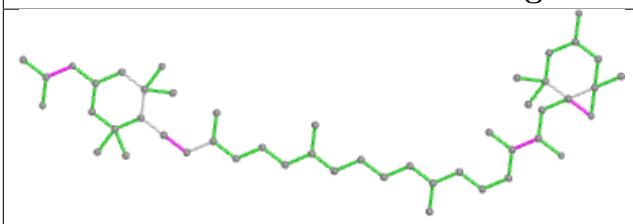


Rings

Ligand A86 19 304



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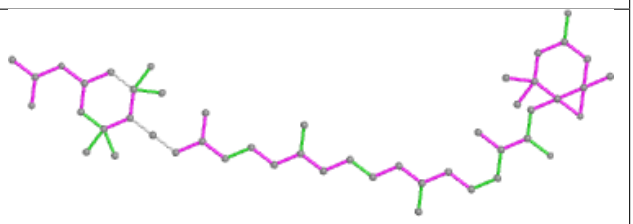
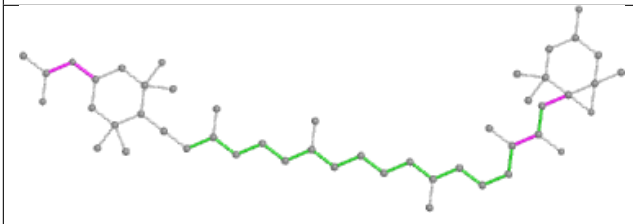


Bond angles



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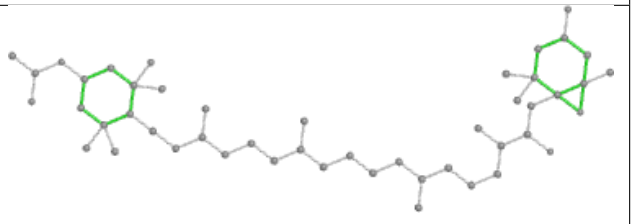
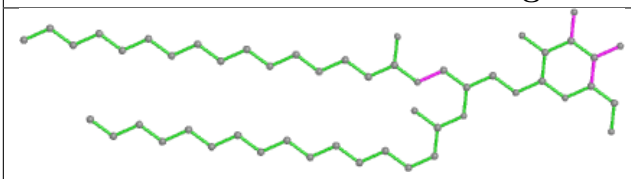


Rings

Ligand LMG b 621



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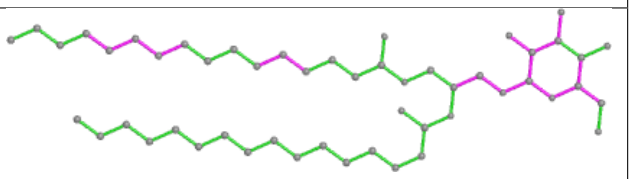

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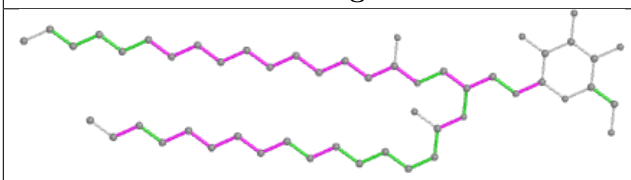

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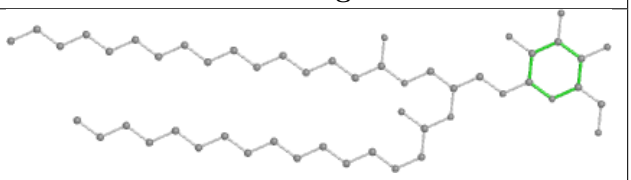
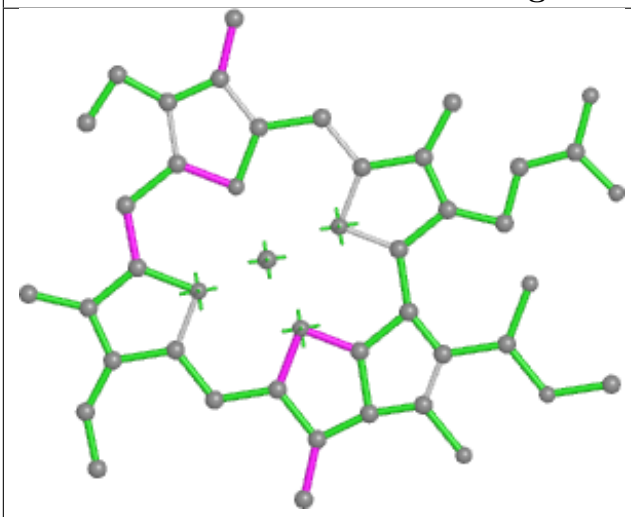
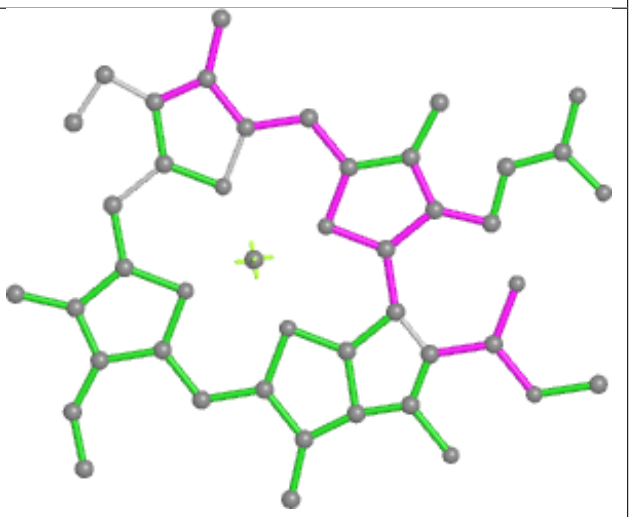


Rings

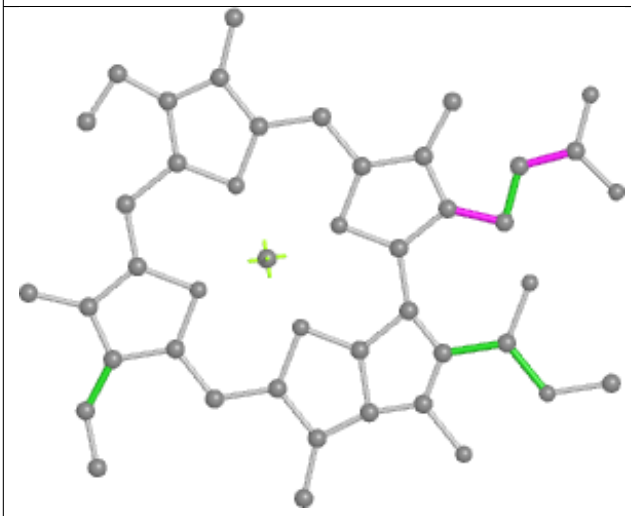
Ligand CLA 3 312



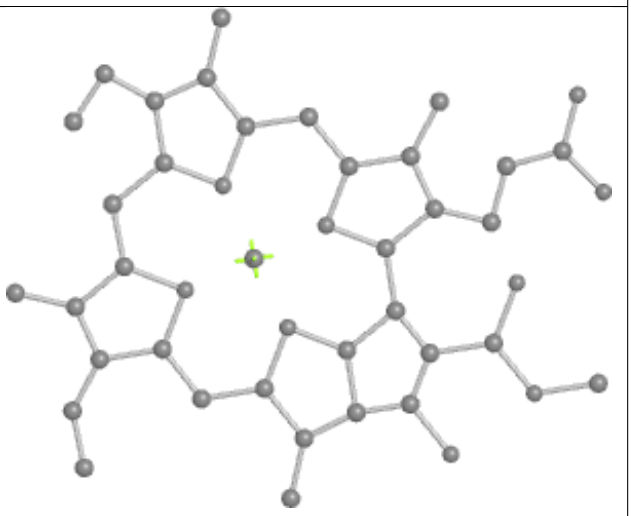
Bond lengths



Bond angles

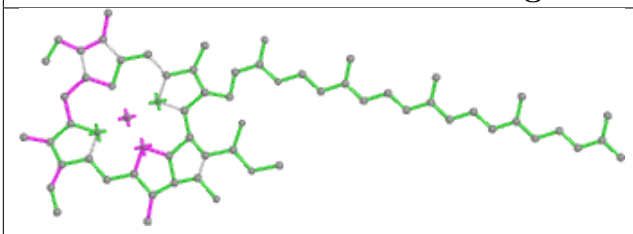


Torsions



Rings

Ligand CLA C 505



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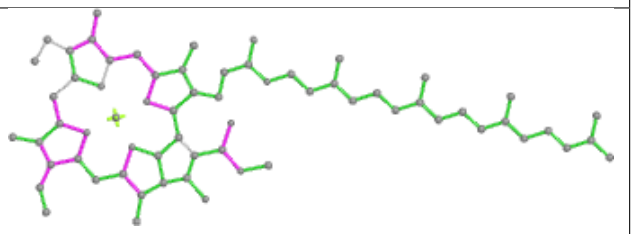

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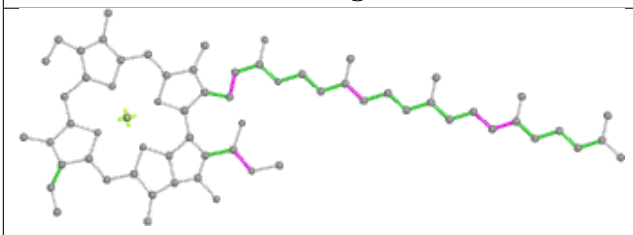

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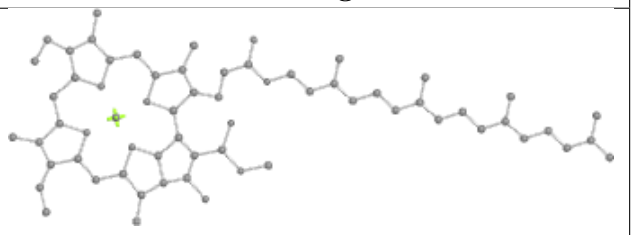
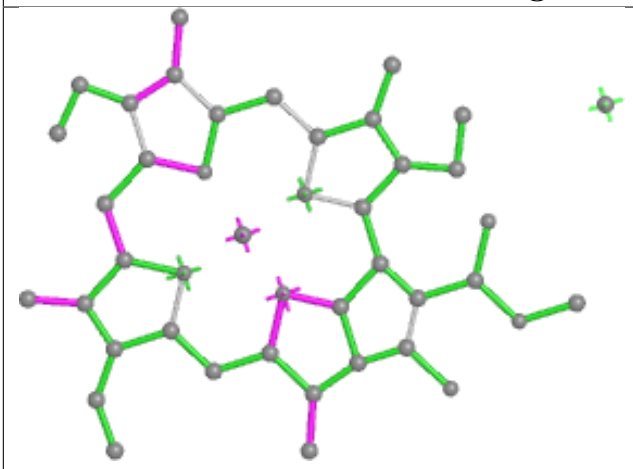


Rings

Ligand CLA 0 313



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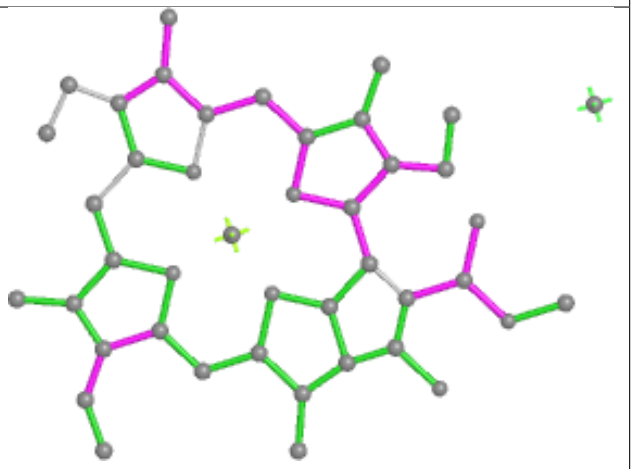

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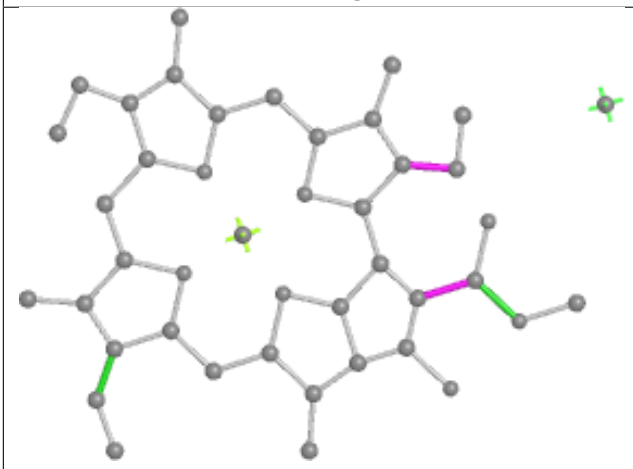

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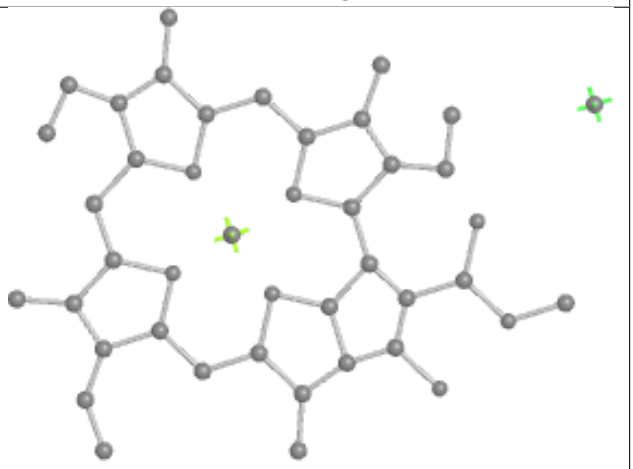
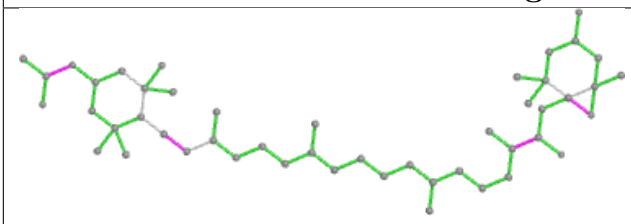


Rings

Ligand A86 10 304



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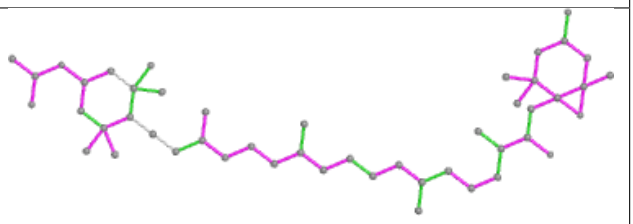

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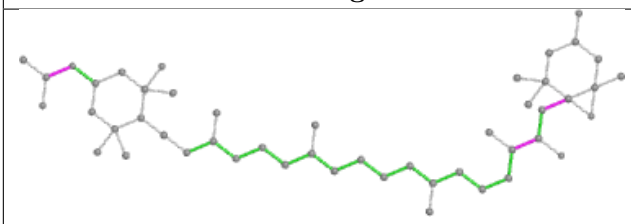

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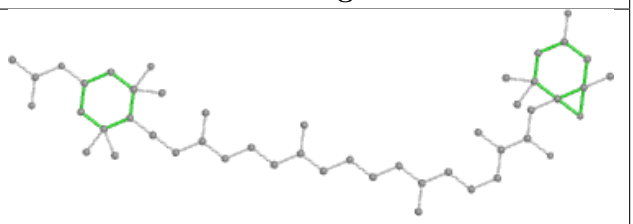
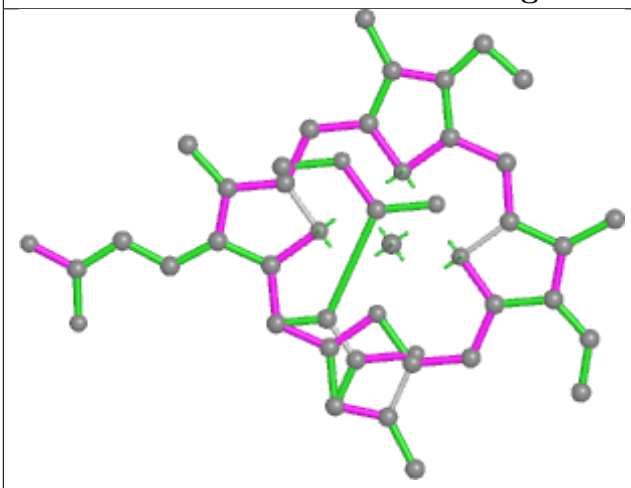


Rings

Ligand KC1 18 313



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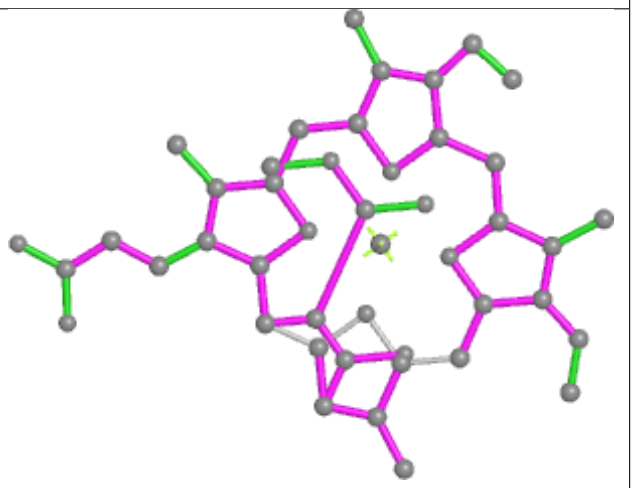

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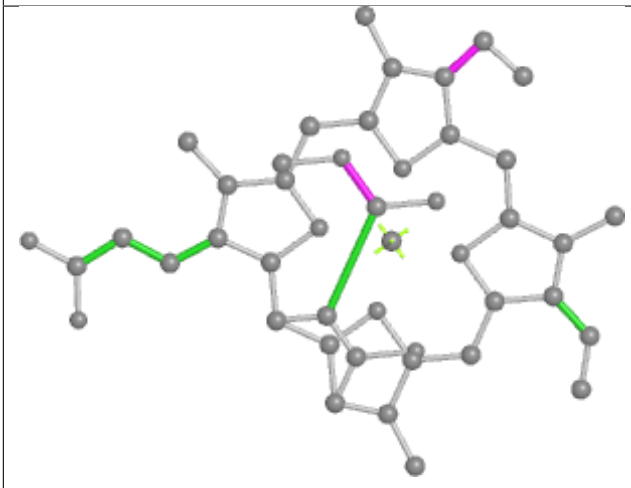

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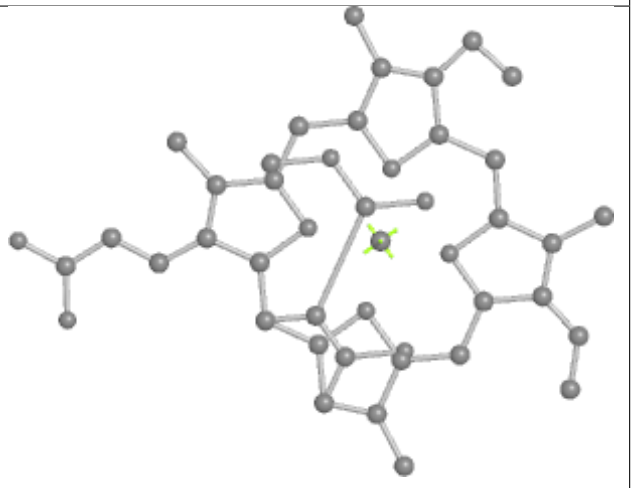
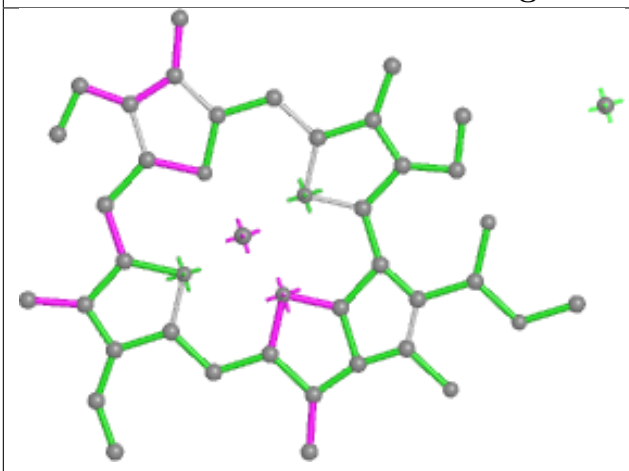


Rings

Ligand CLA 10 313



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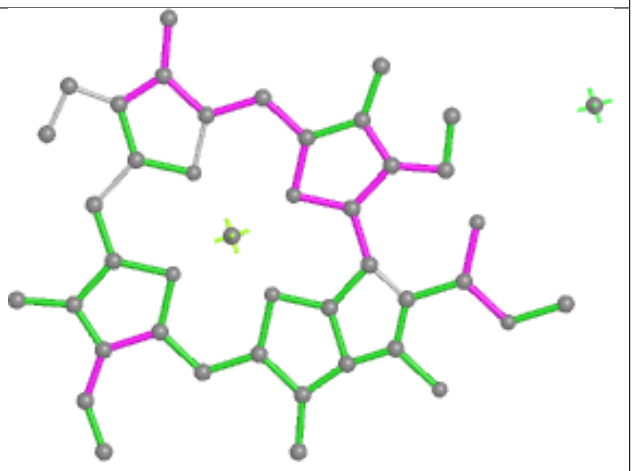

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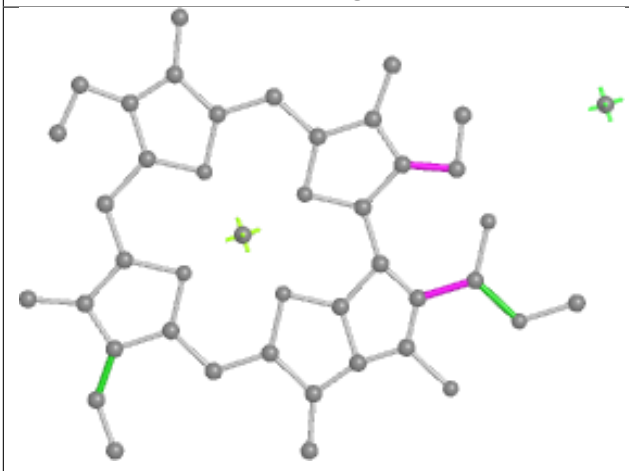

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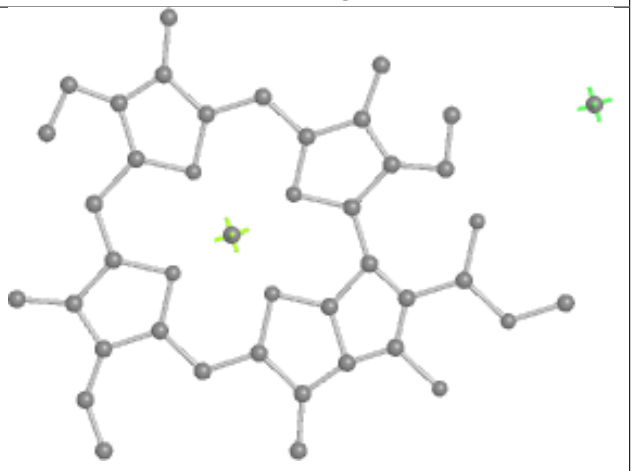
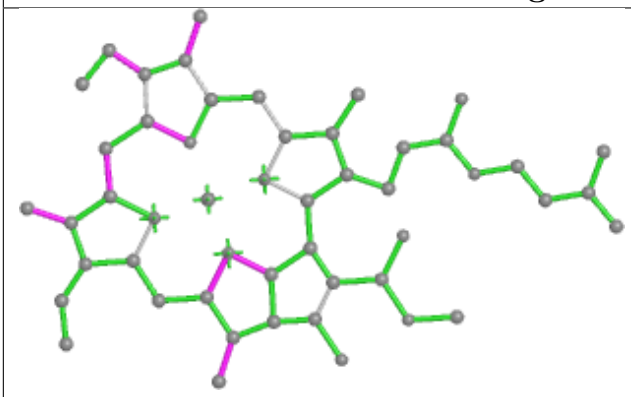


Rings

Ligand CLA 1 310



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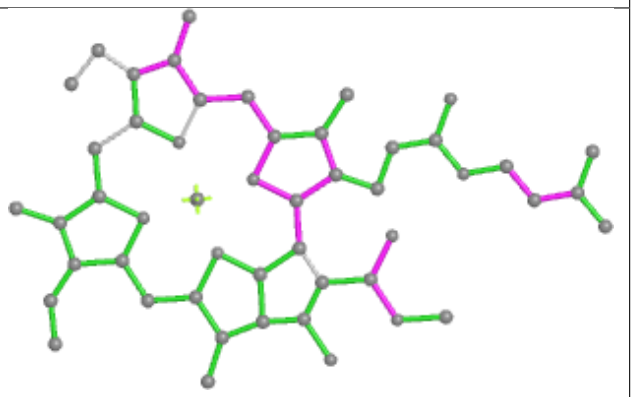

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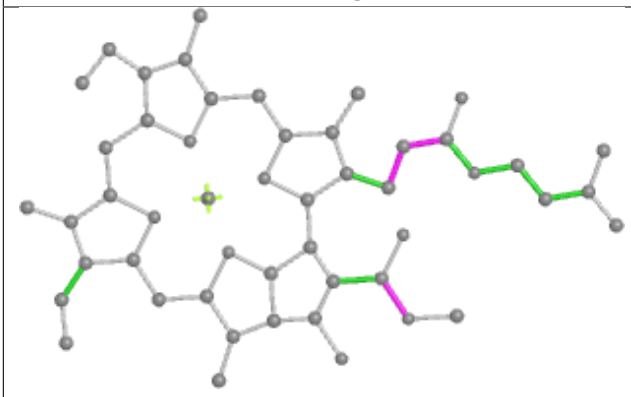

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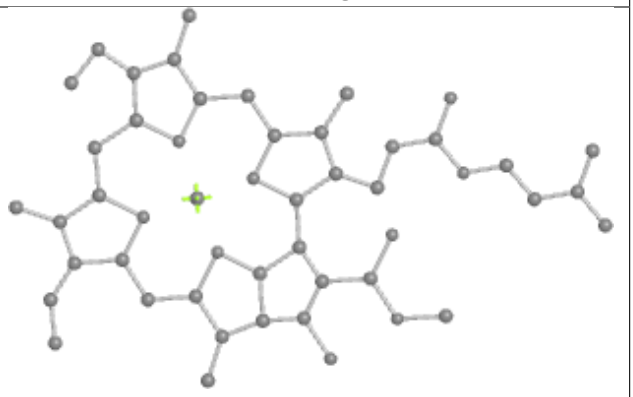
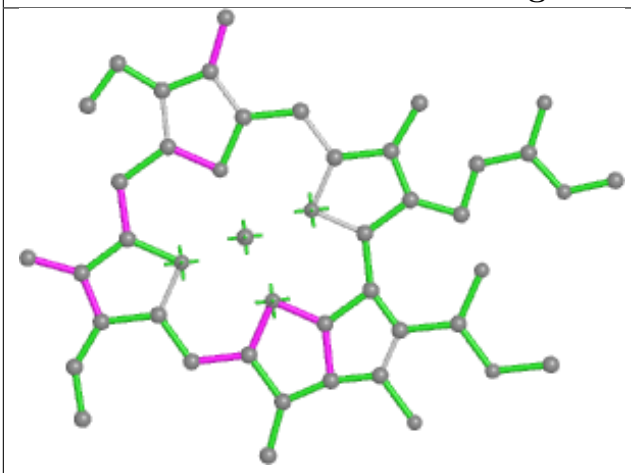


Rings

Ligand CLA 2 315



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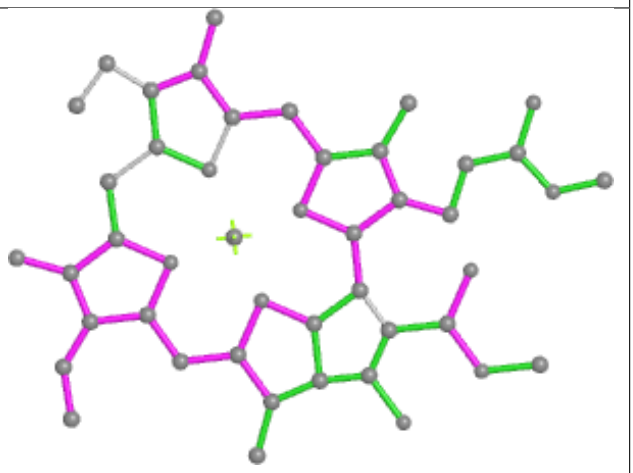

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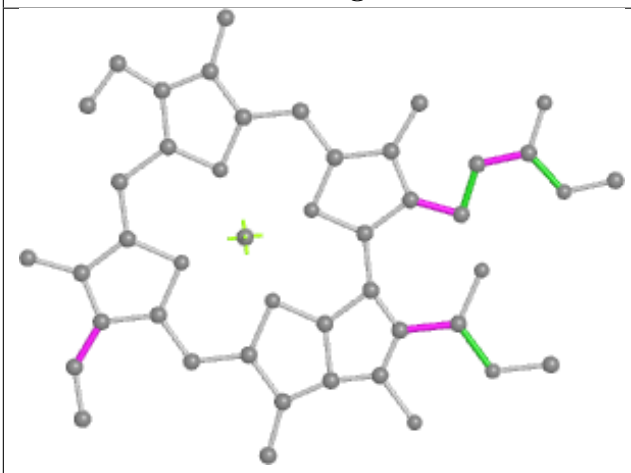

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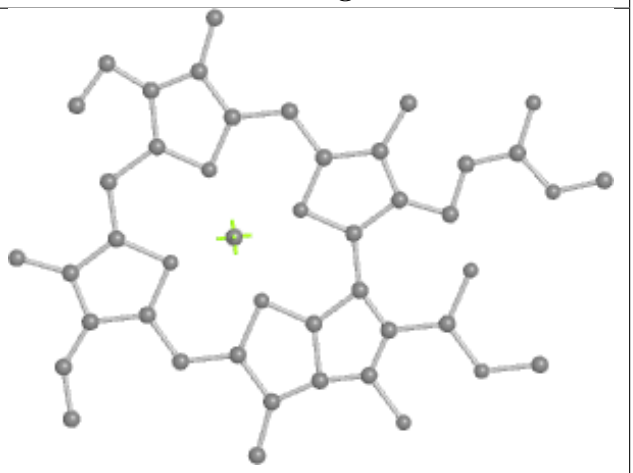
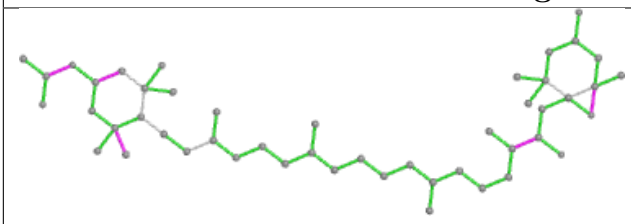


Rings

Ligand A86 1 320



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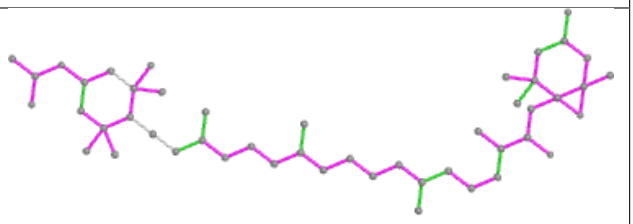

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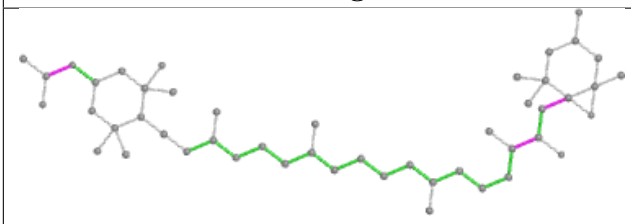

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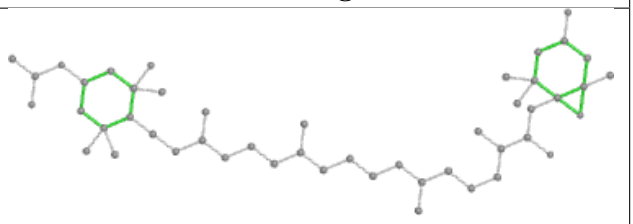
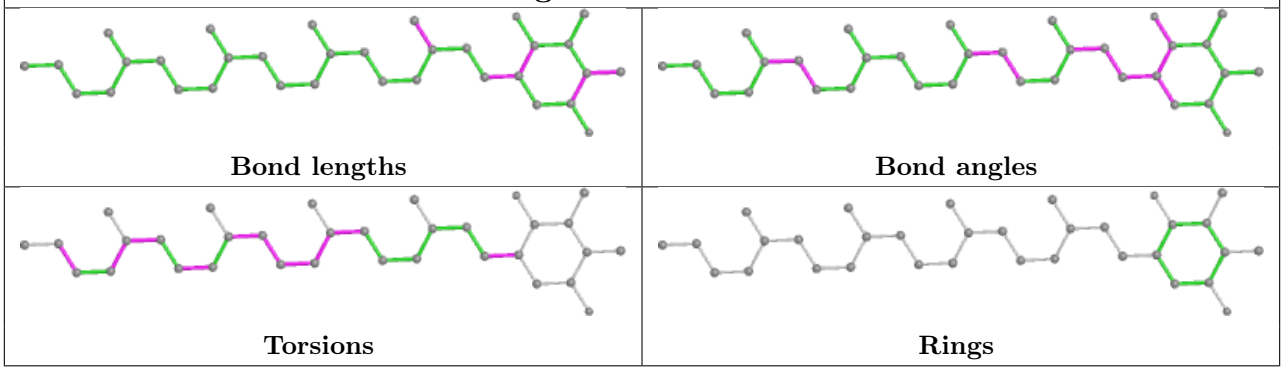


Rings

Ligand PL9 a 409



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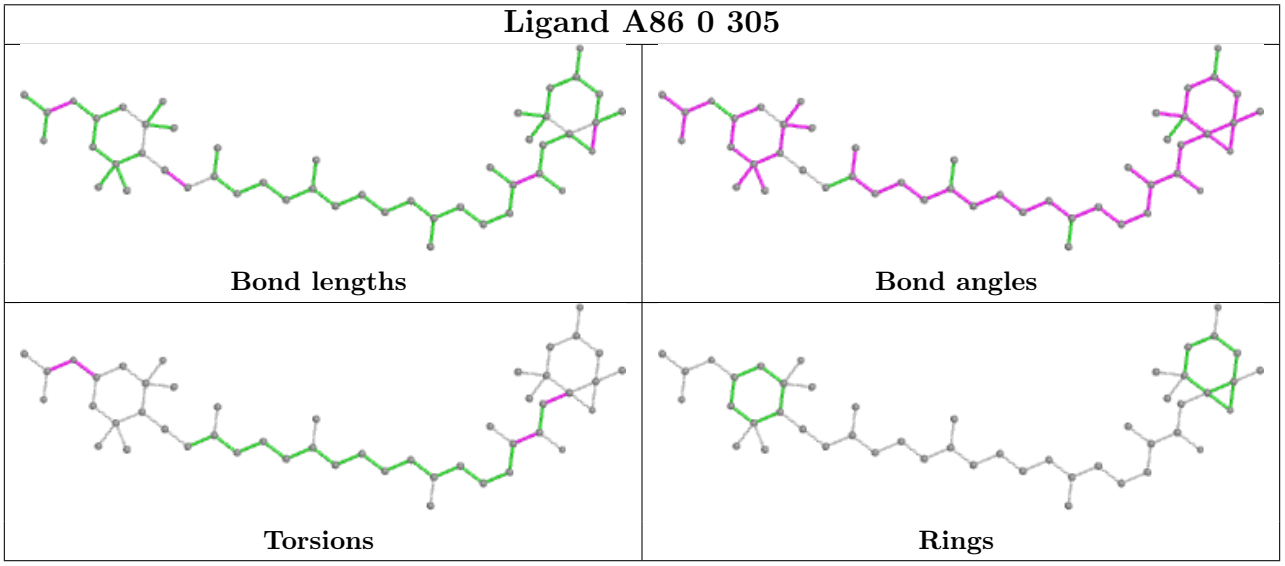

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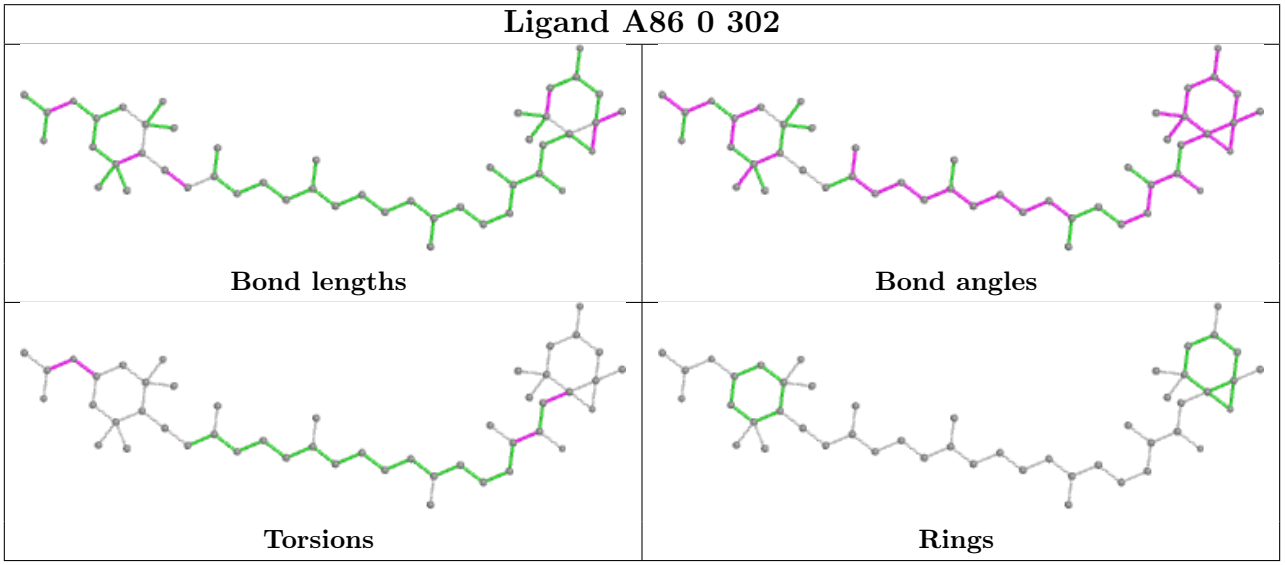
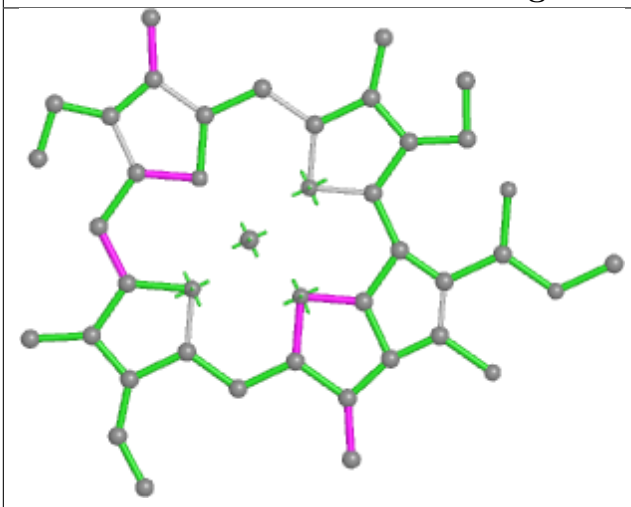
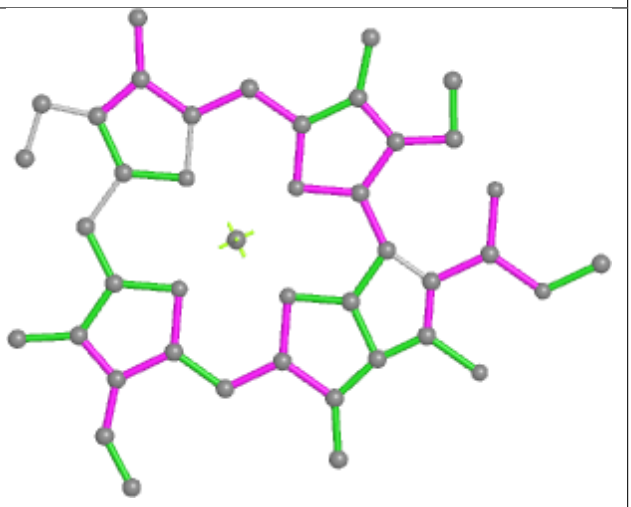


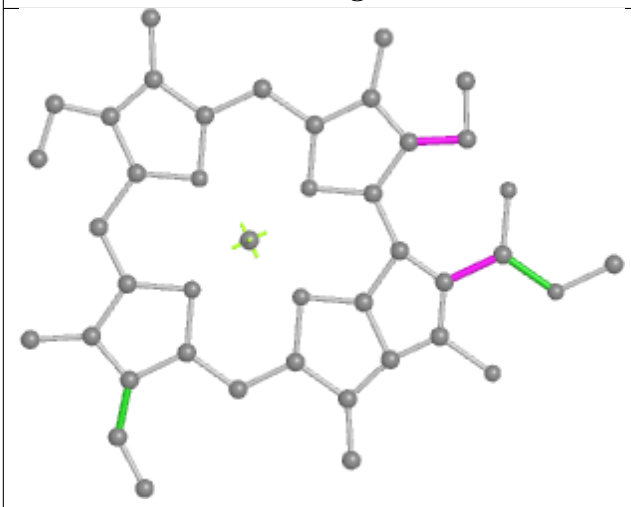
Ligand CLA 5 306



Bond lengths



Bond angles



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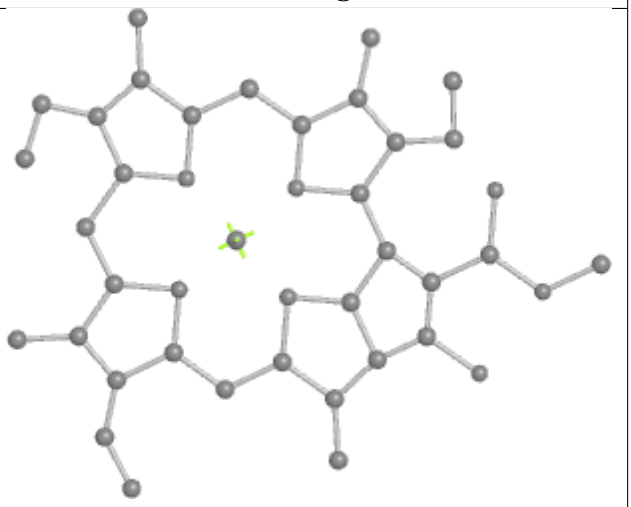
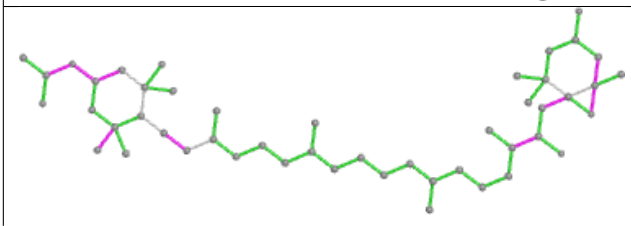


Rings

Ligand A86 3 305



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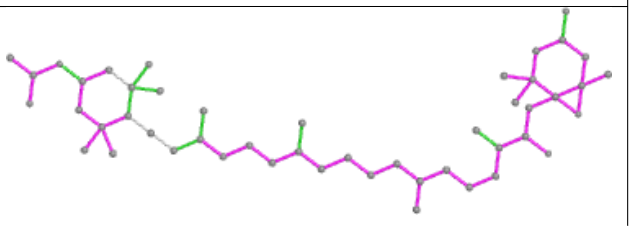
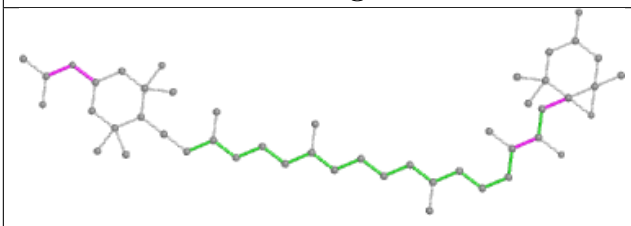


Bond angles



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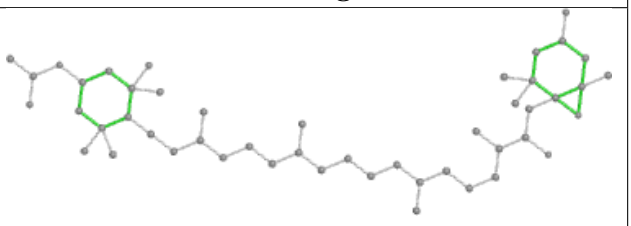
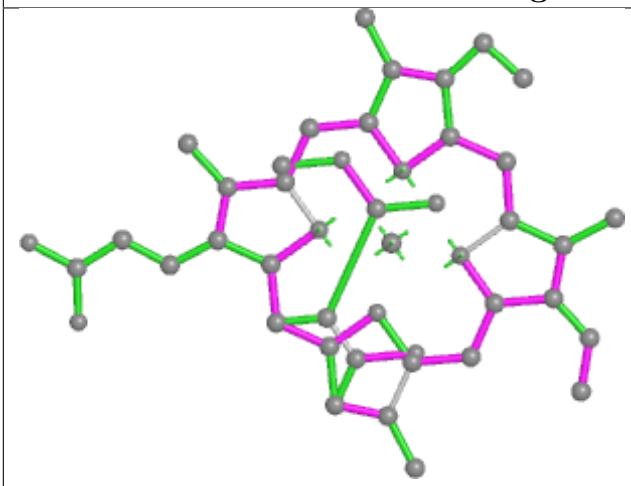


Rings

Ligand KC2 2 310



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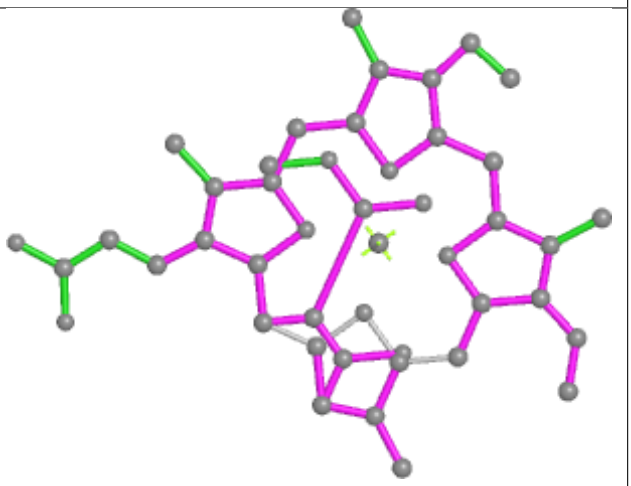

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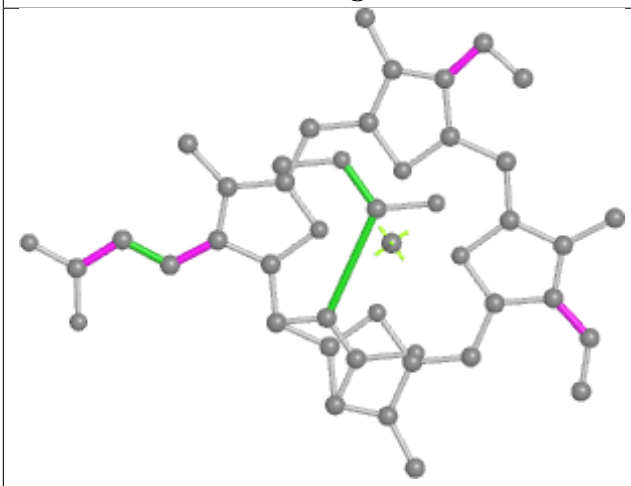

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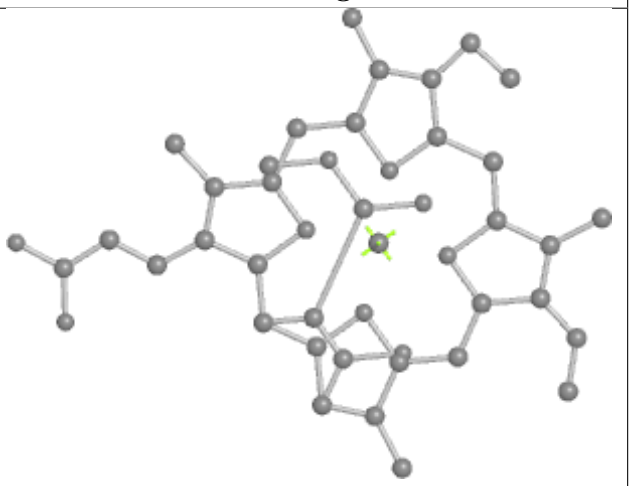
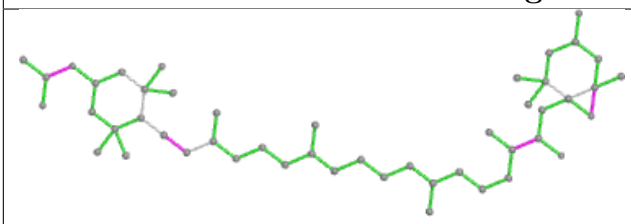


Rings

Ligand A86 19 306



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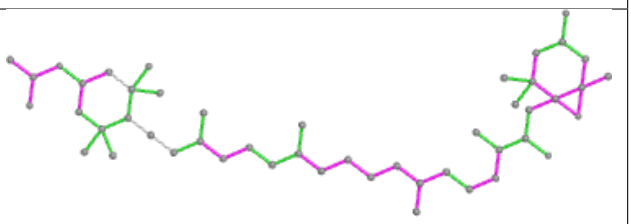
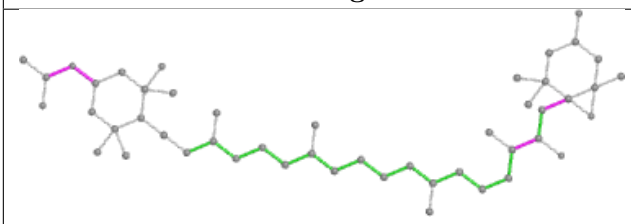


Bond angles



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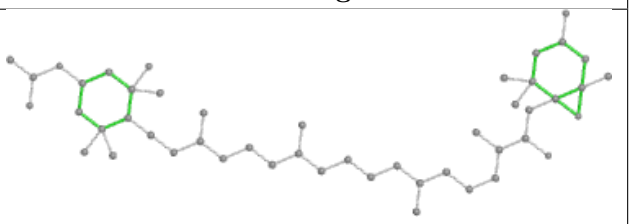
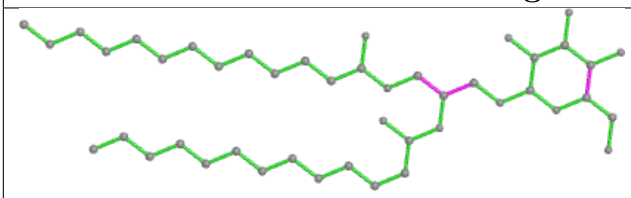


Rings

Ligand LMG 1 317



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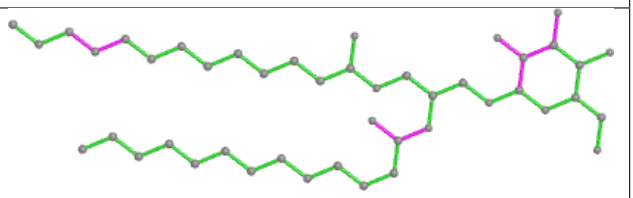

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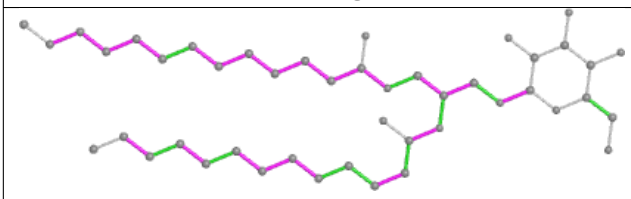

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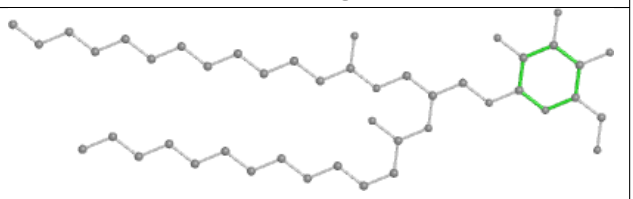
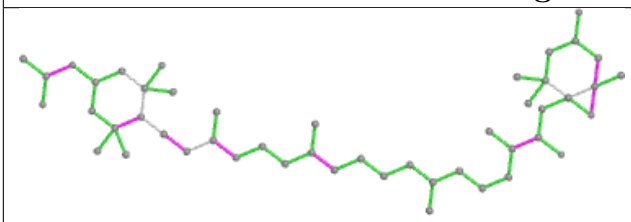


Rings

Ligand A86 7 302



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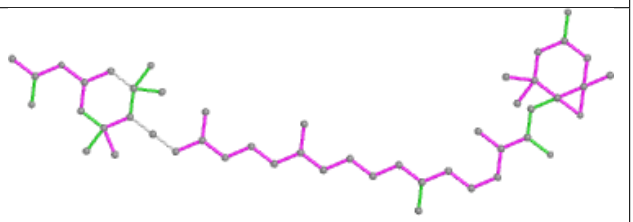

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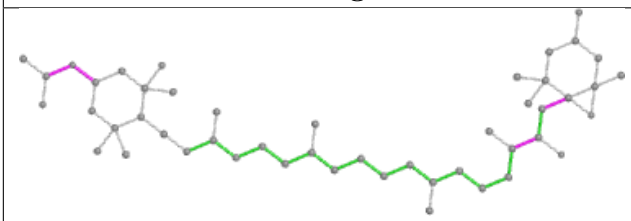

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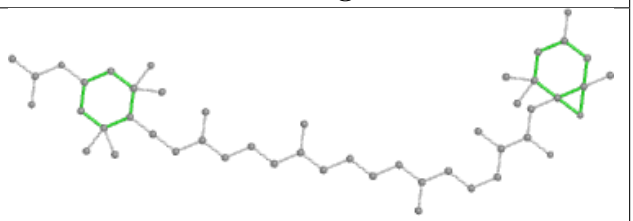

Rings

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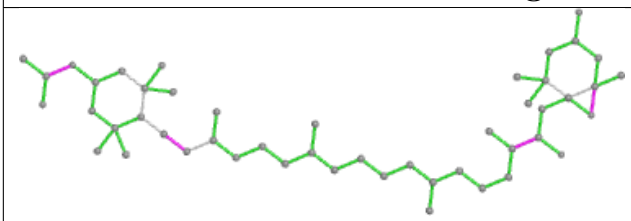

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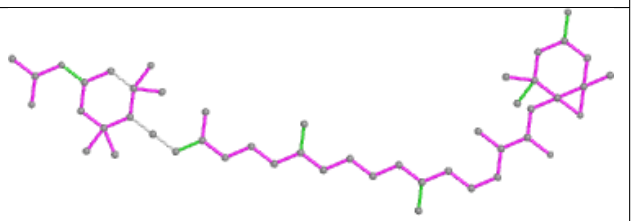

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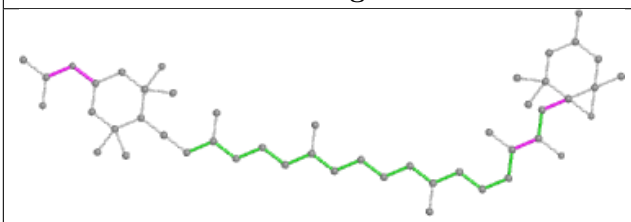

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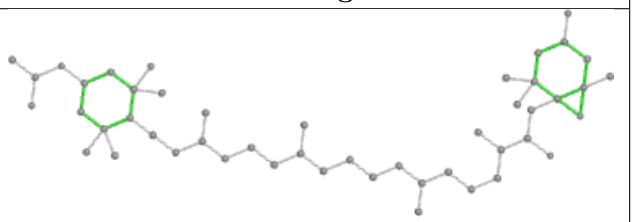

Rings

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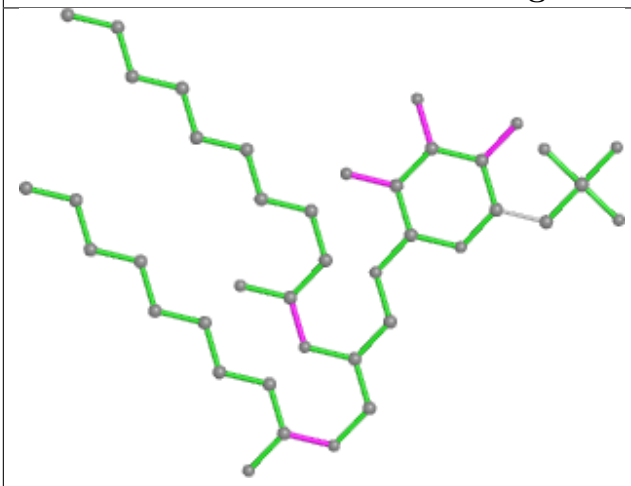

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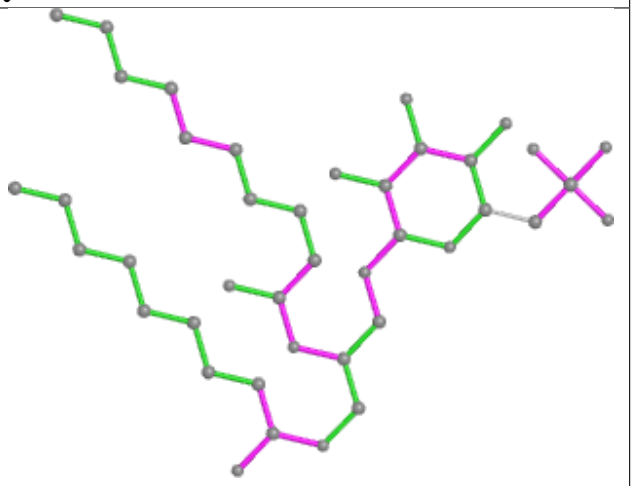

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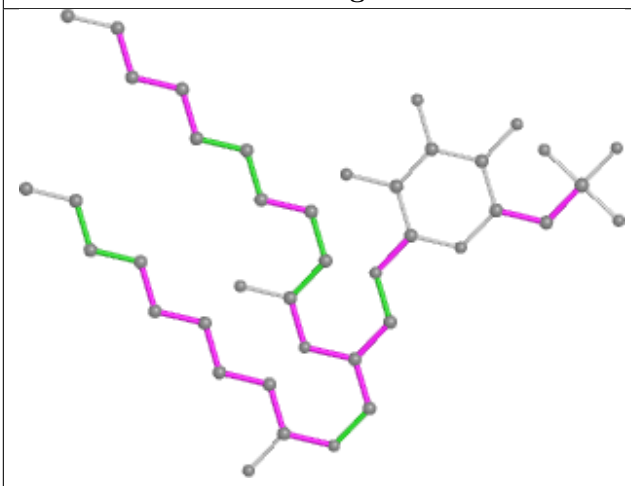

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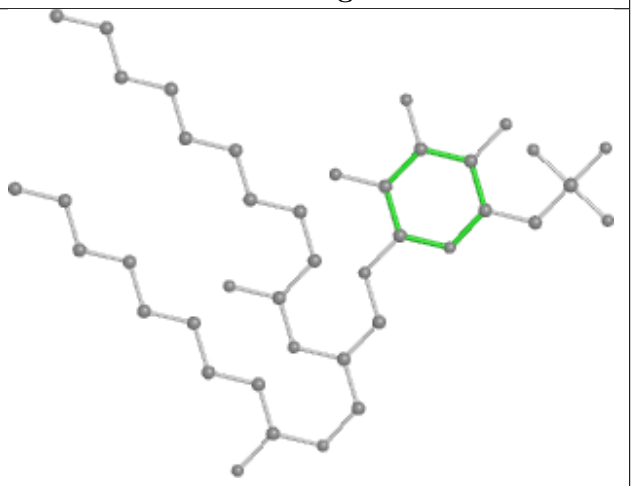
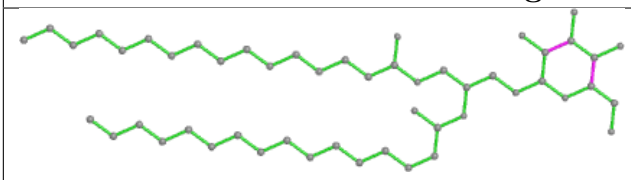


Rings

Ligand LMG c 521



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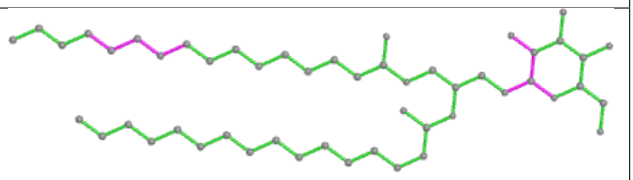

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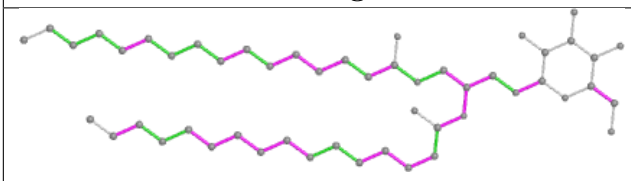

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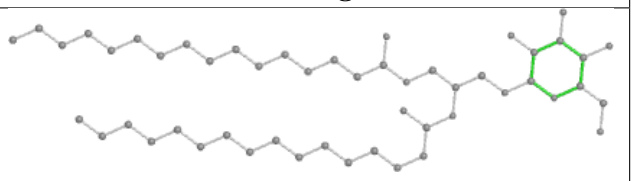

Rings

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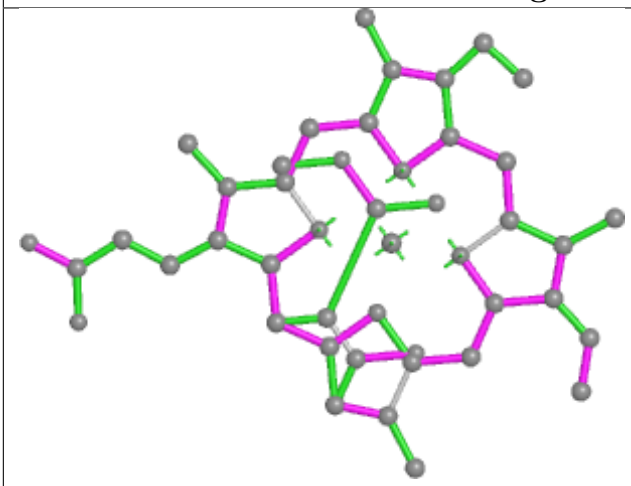

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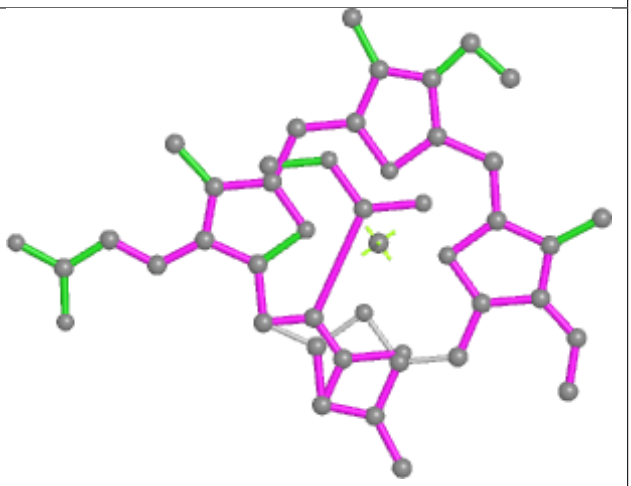

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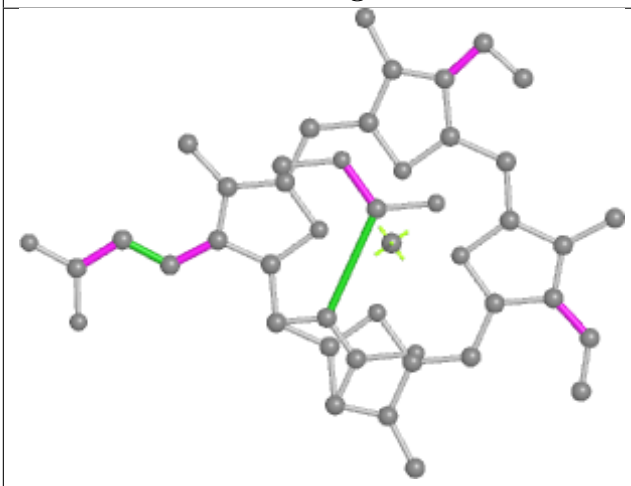

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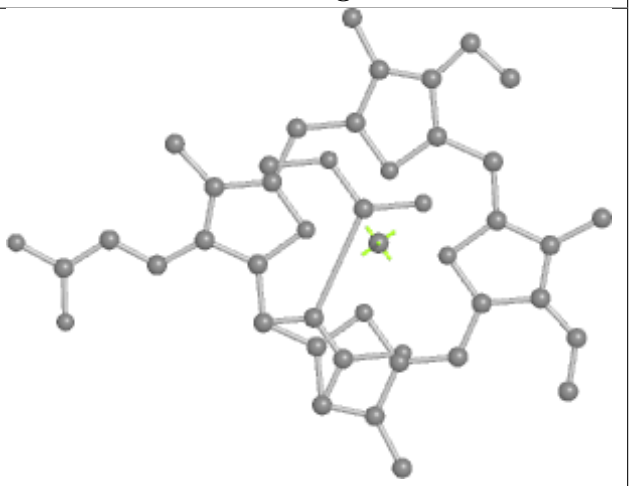

Rings

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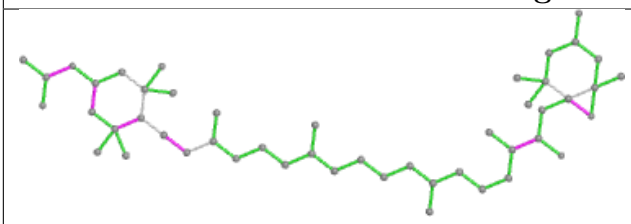

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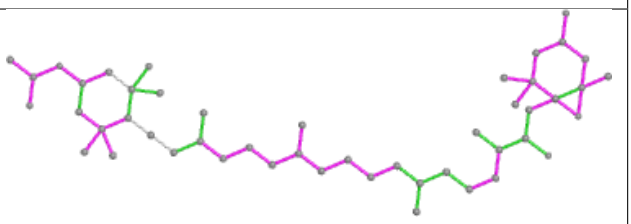

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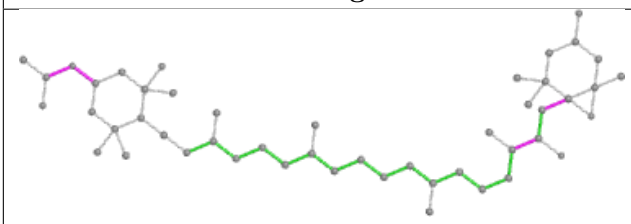

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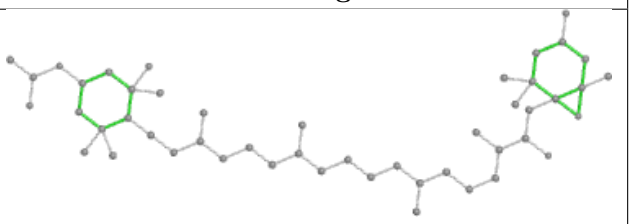

Rings

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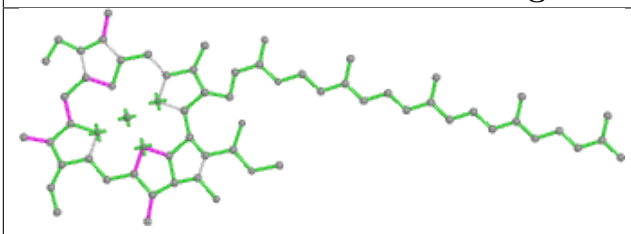

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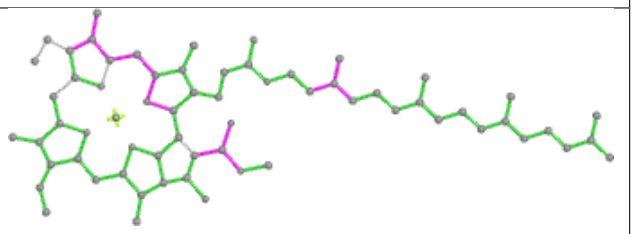

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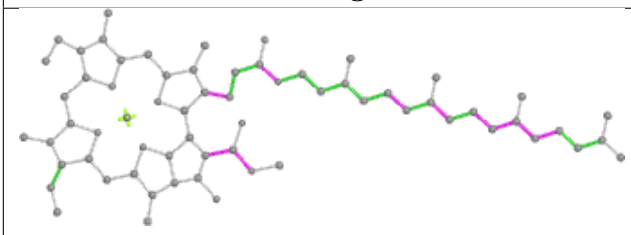

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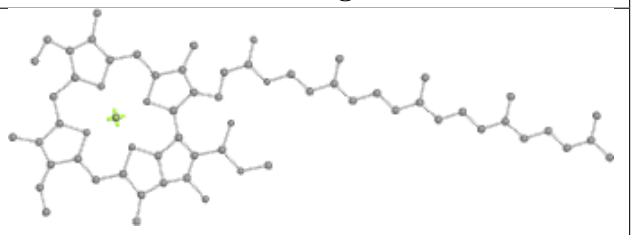
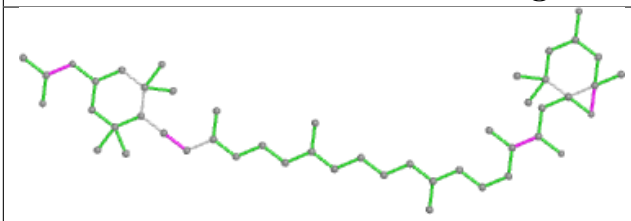


Rings

Ligand A86 P 613



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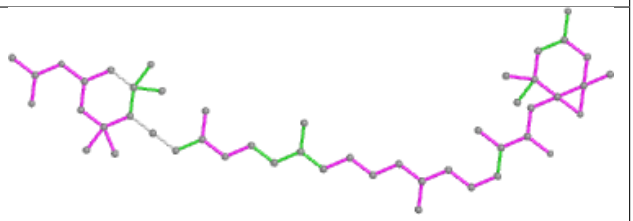

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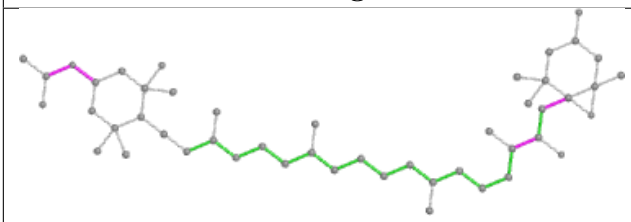

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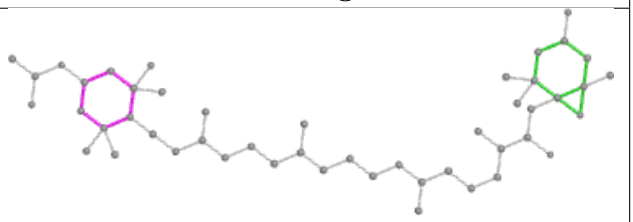

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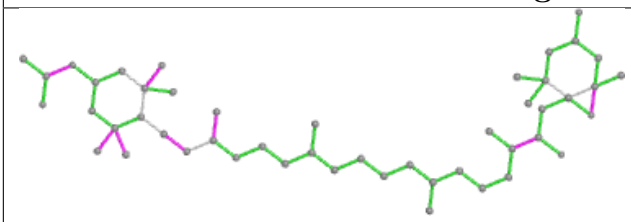

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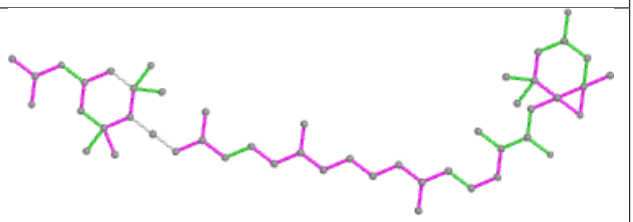

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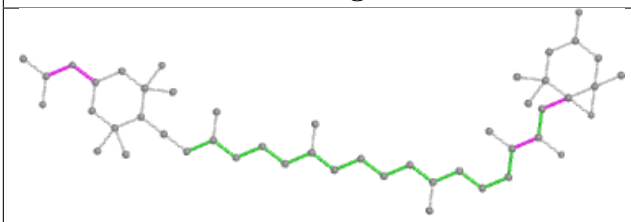

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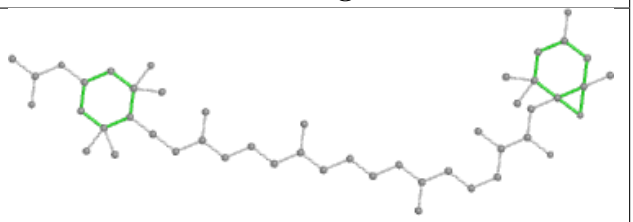

Rings

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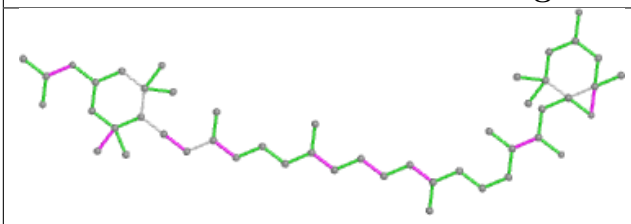

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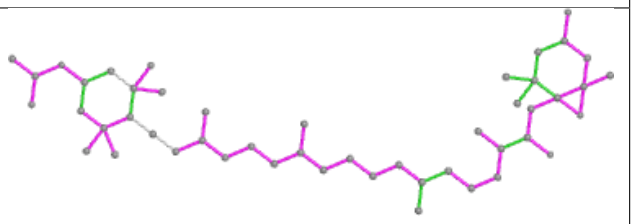

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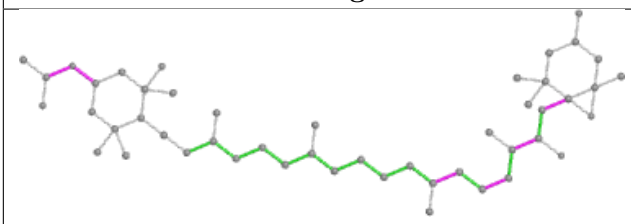

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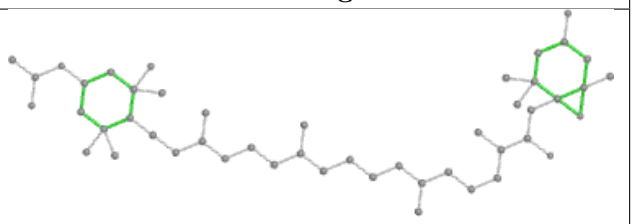
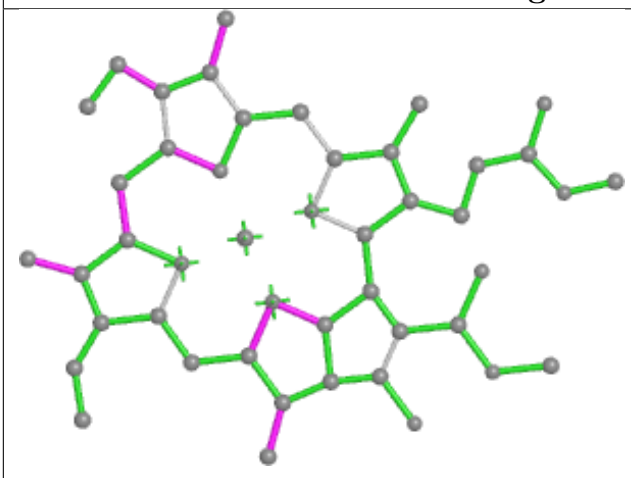


Rings

Ligand CLA 0 316



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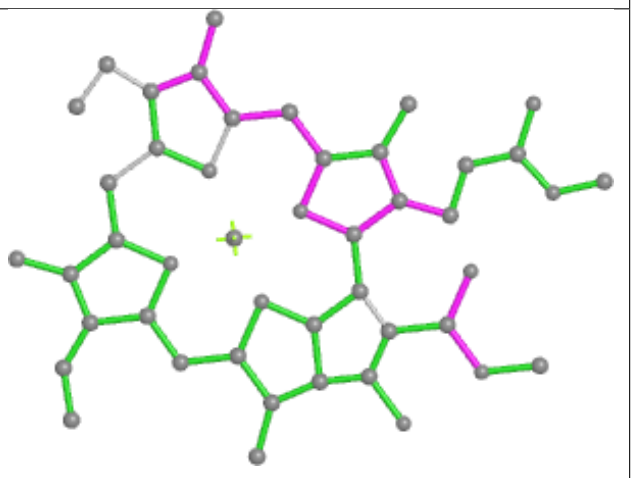

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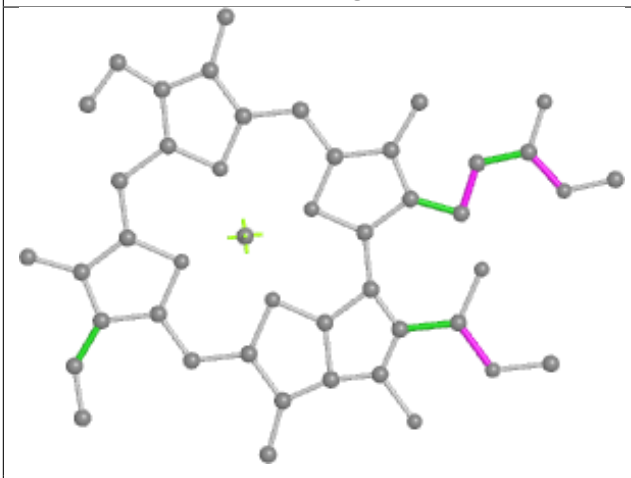

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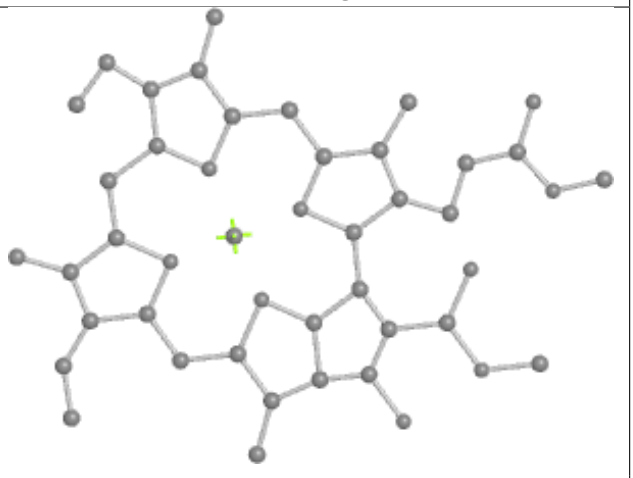
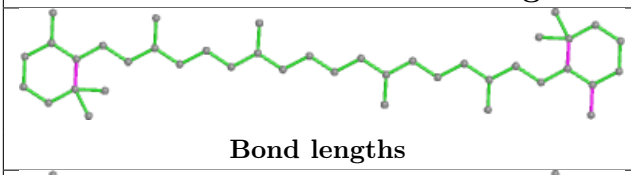


Rings

Ligand BCR B 619



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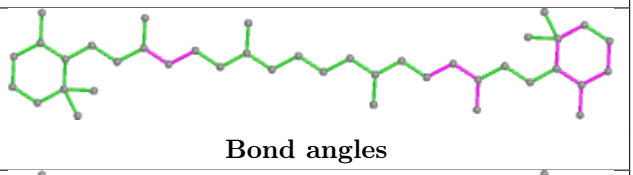

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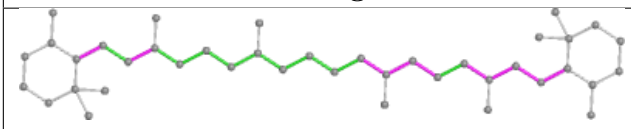

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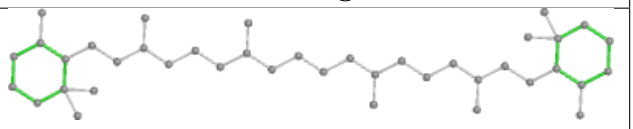
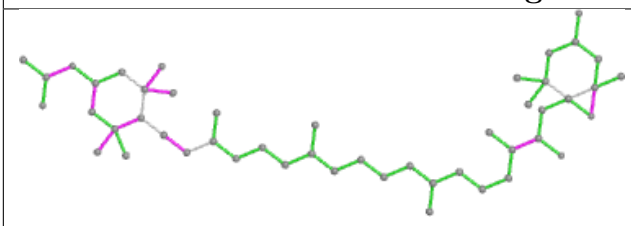


Rings

Ligand A86 17 302



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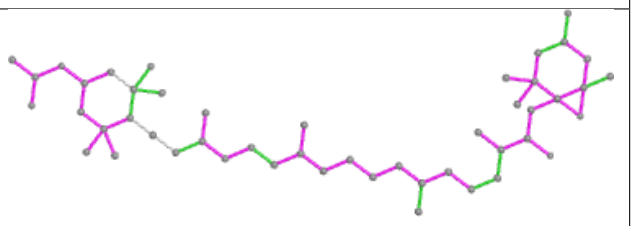
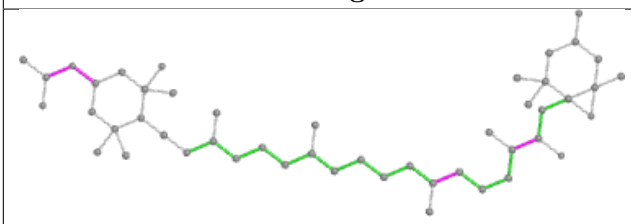


Bond angles



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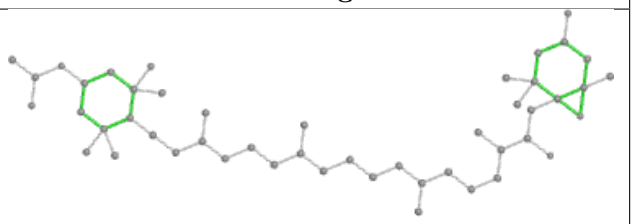
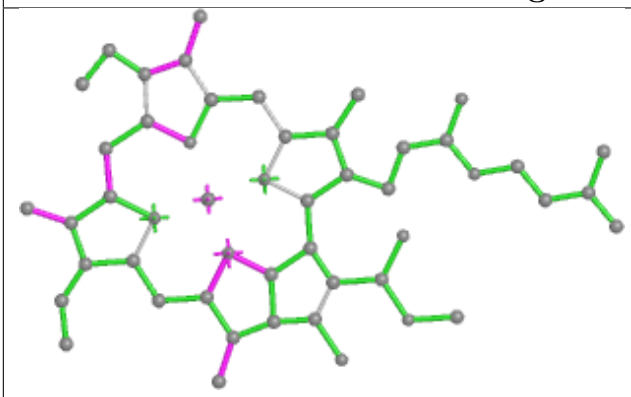


Rings

Ligand CLA 8 306



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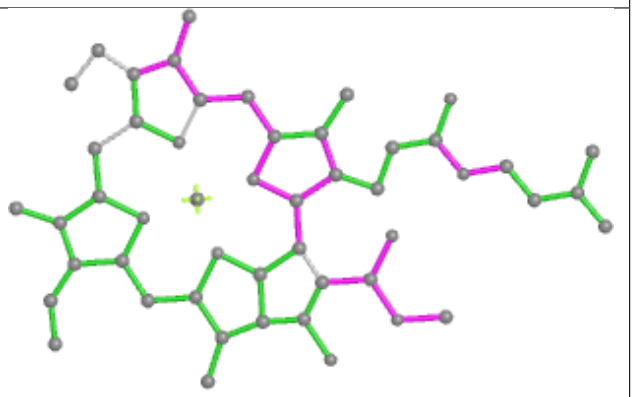

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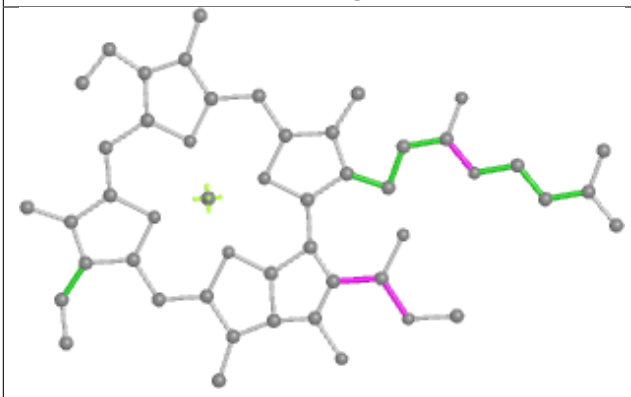
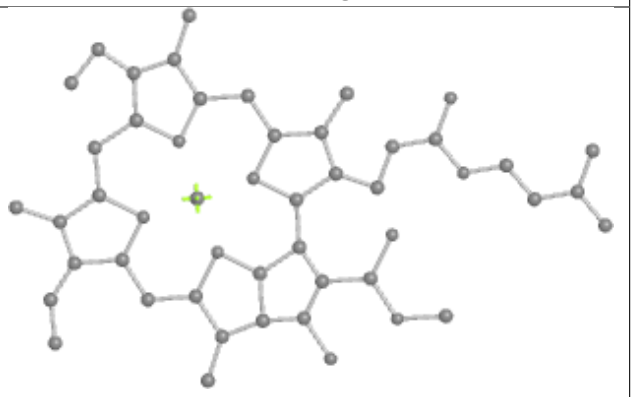
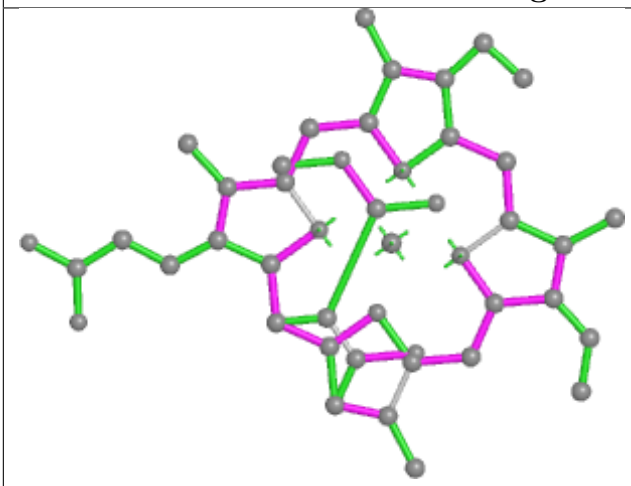


Torsions



Rings

Ligand KC1 2 313



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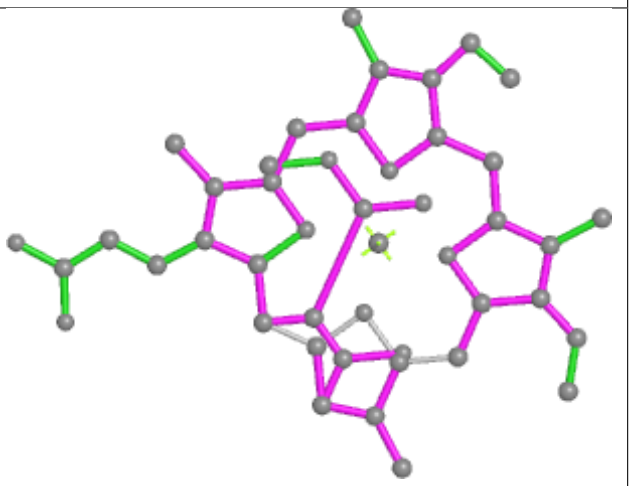

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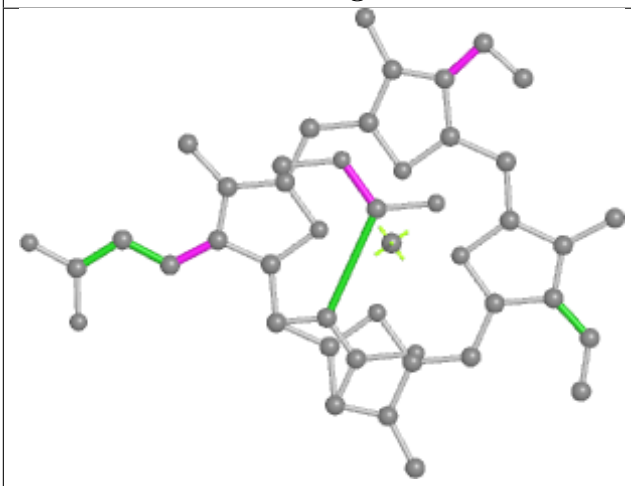

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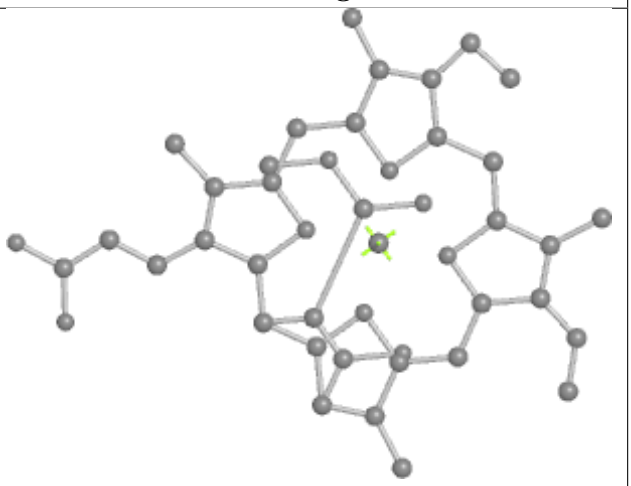
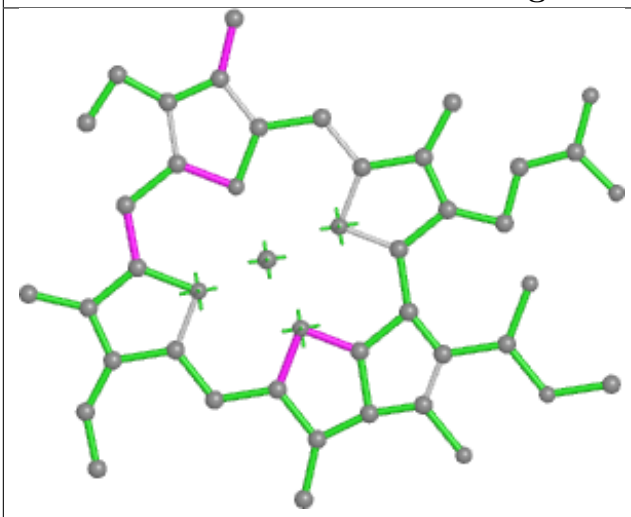


Rings

Ligand CLA 7 310



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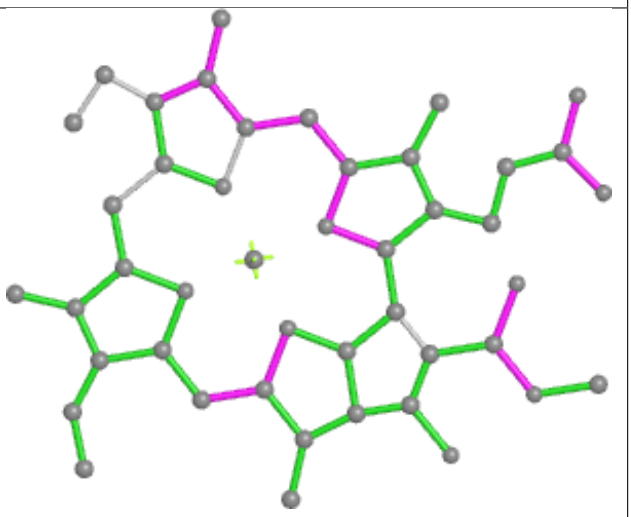

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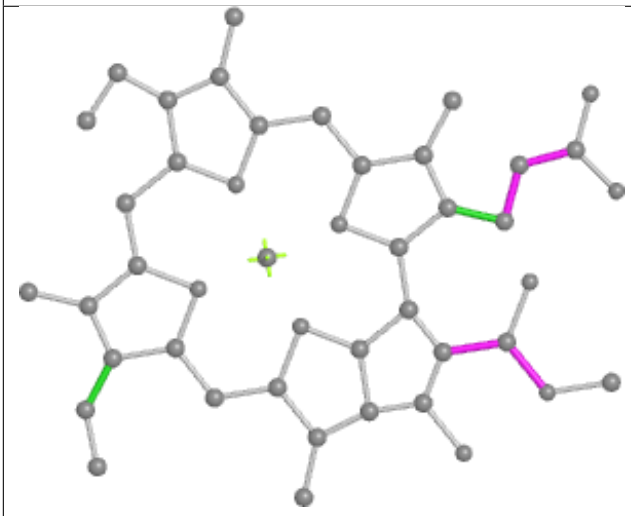

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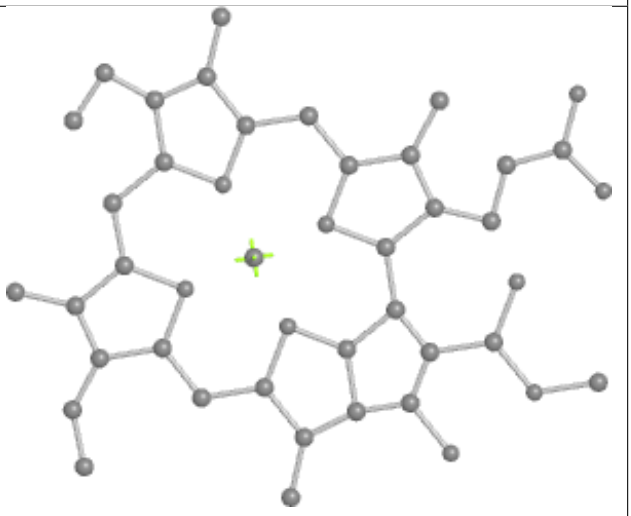
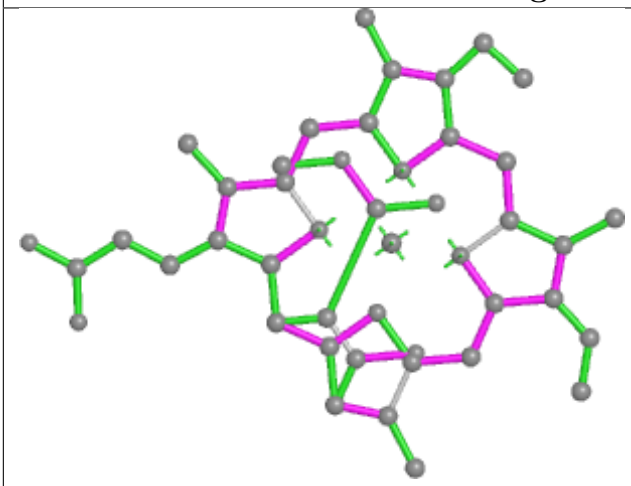


Rings

Ligand KC1 1 314



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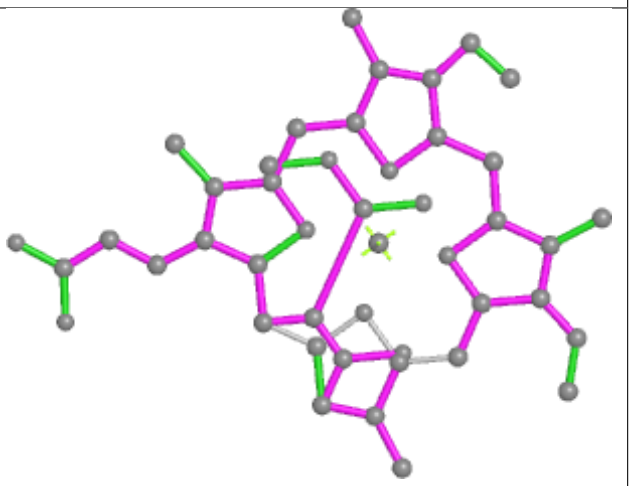

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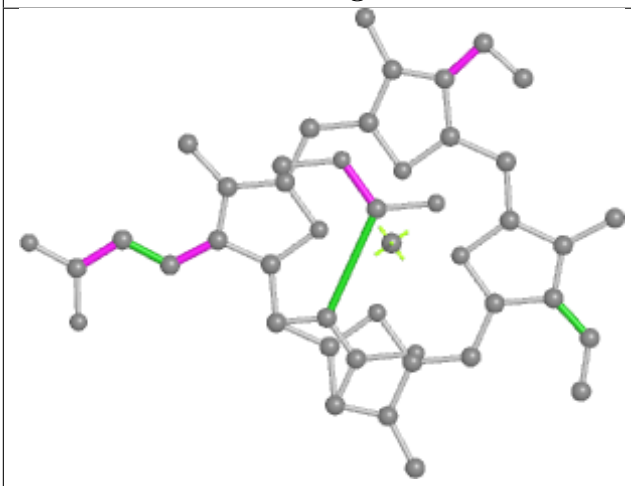

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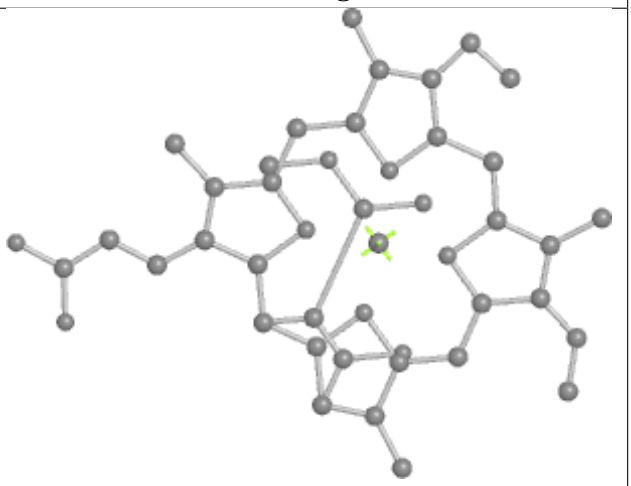
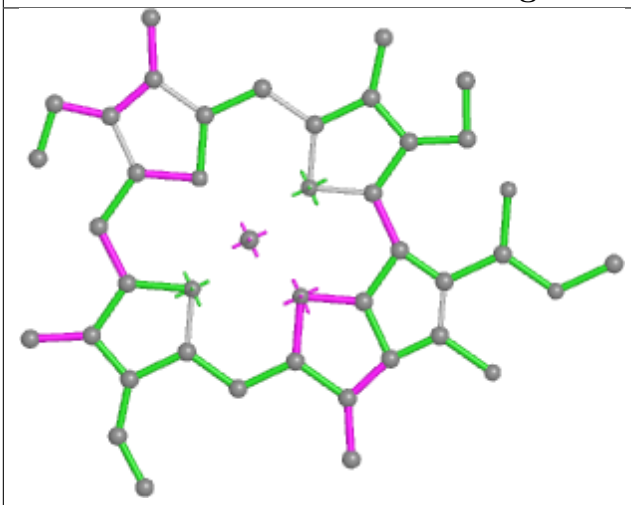


Rings

Ligand CLA 16 314



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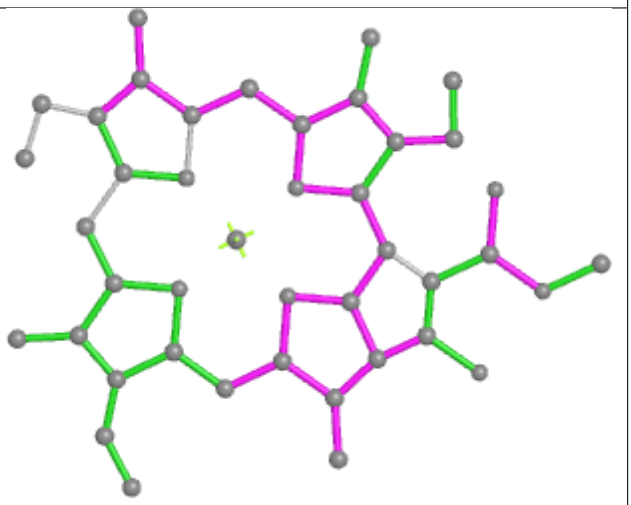

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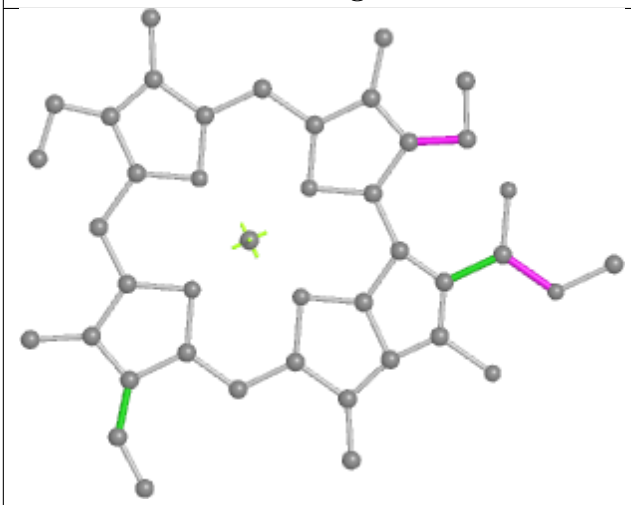

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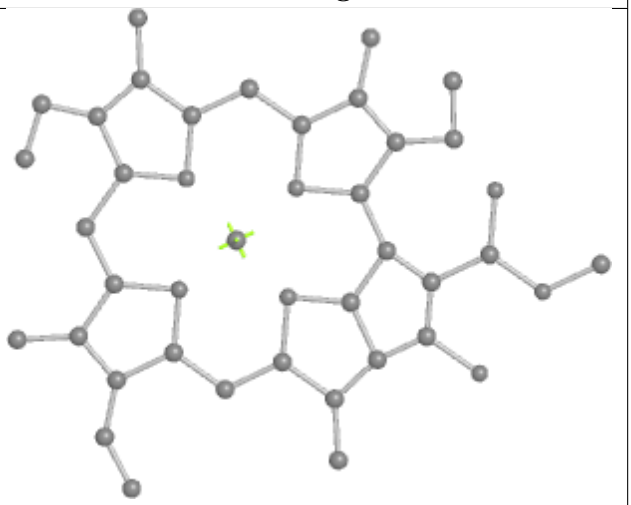
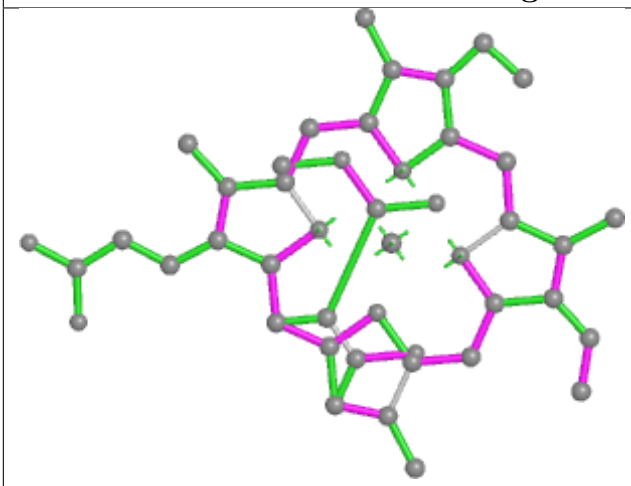


Rings

Ligand KC2 11 309



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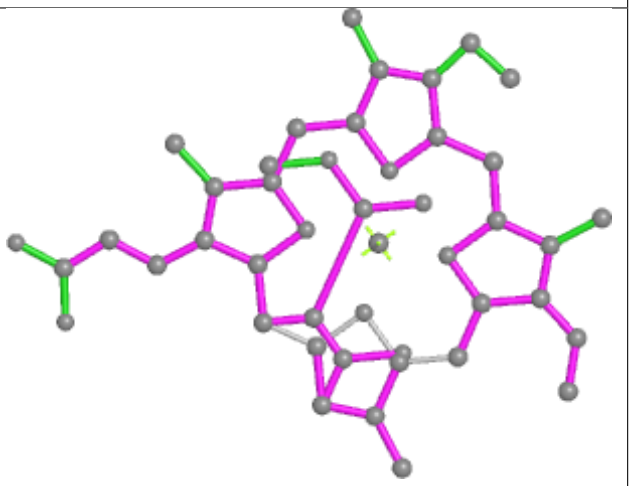

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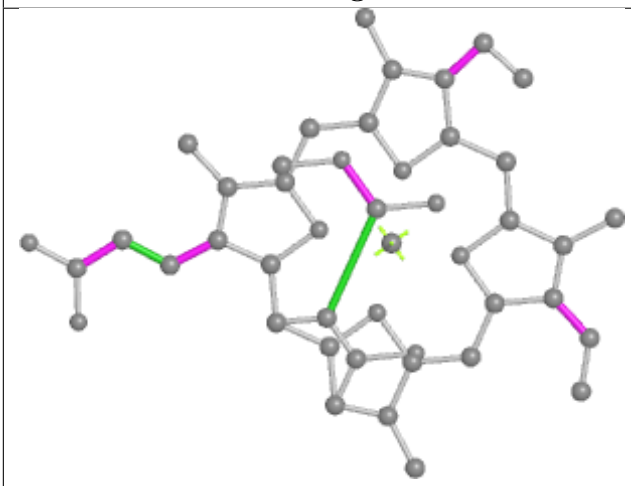

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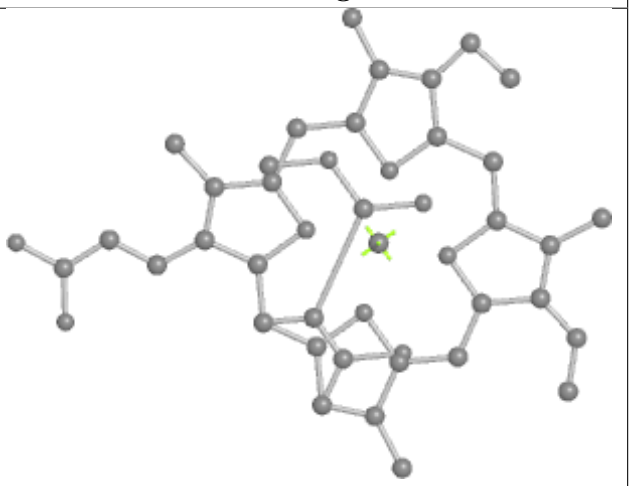
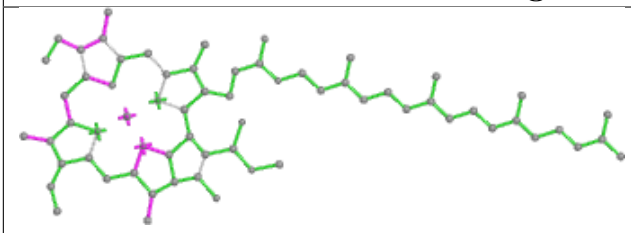


Rings

Ligand CLA d 405



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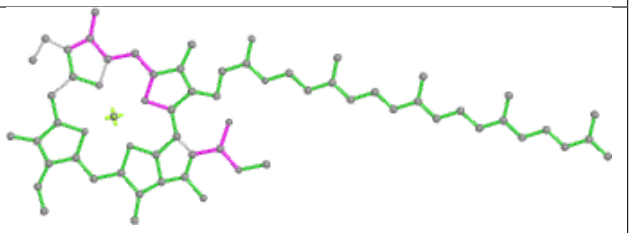

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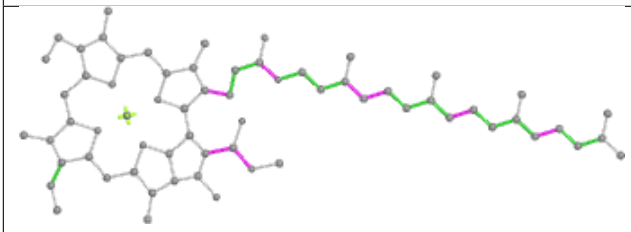

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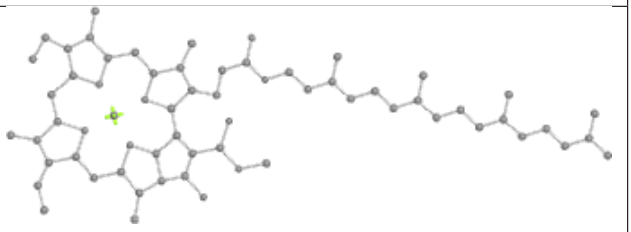
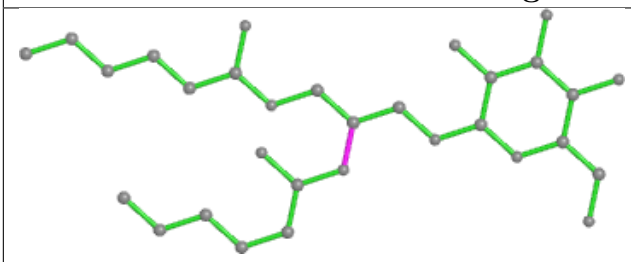


Rings

Ligand LMG p 614



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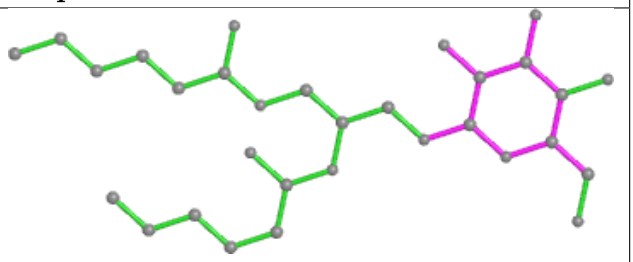

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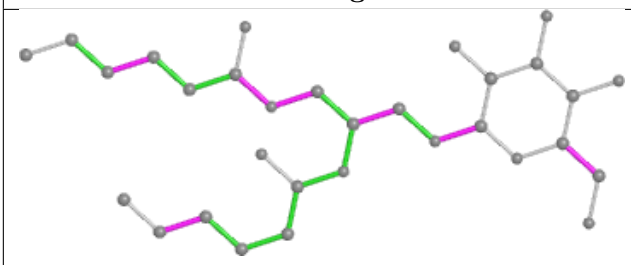

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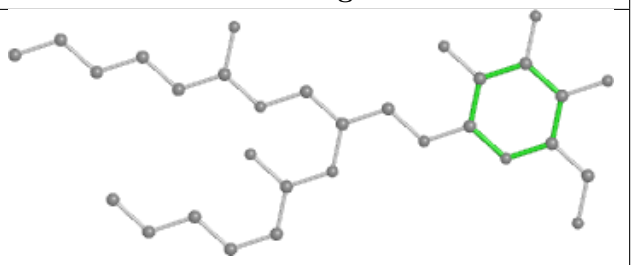
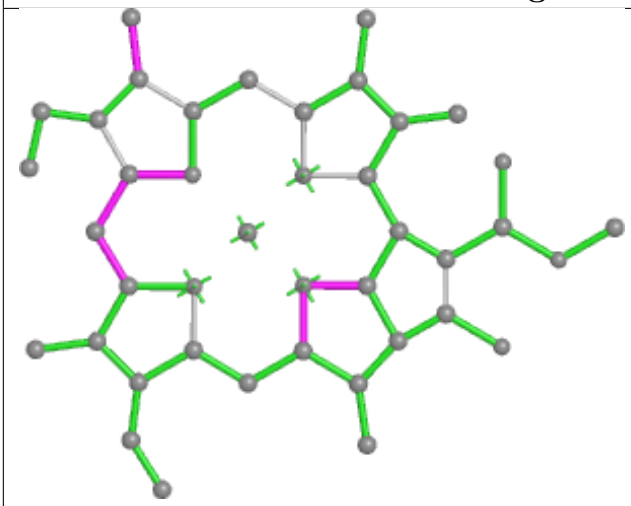


Rings

Ligand CLA 7 307



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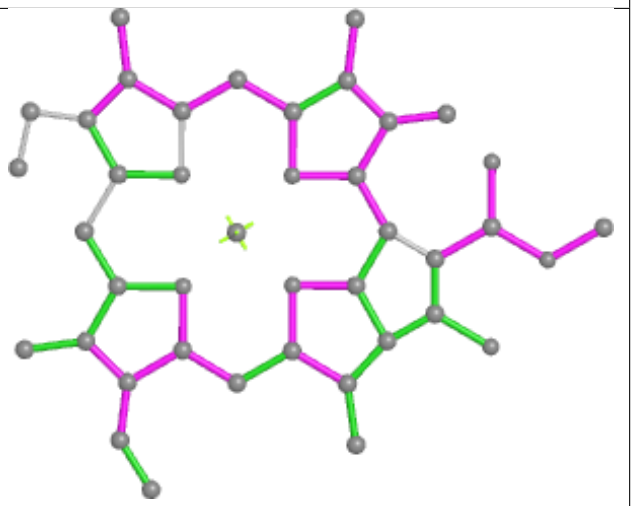

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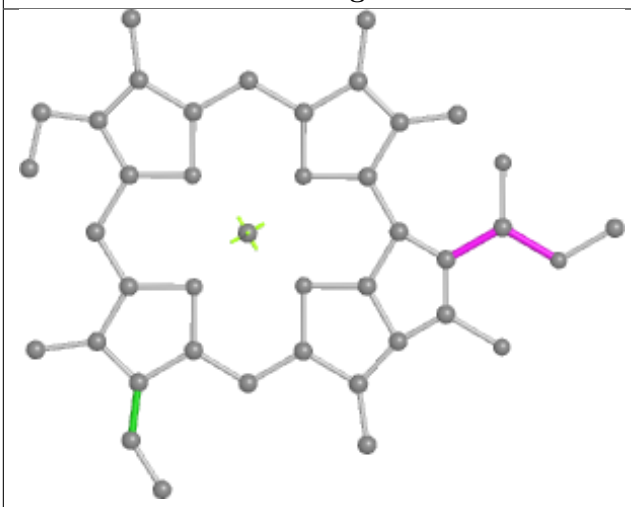

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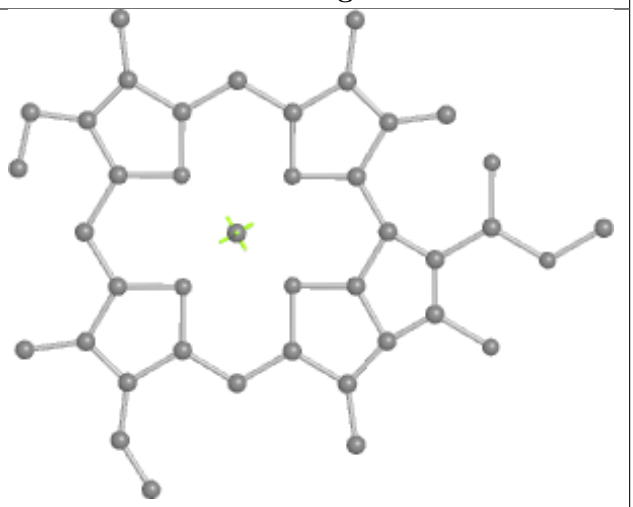

Rings

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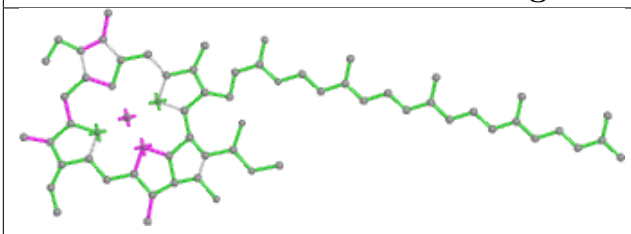

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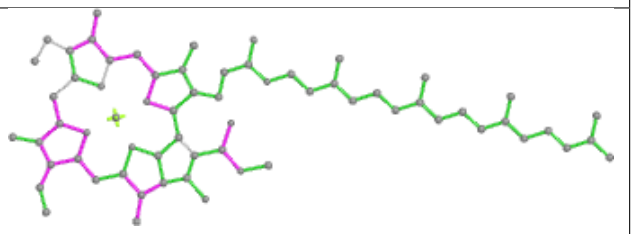

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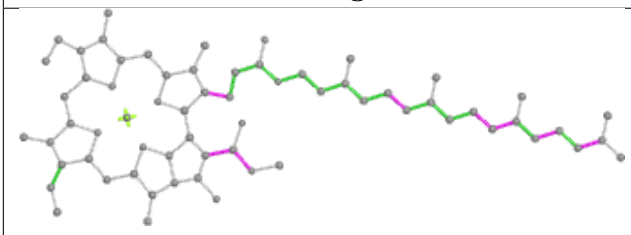

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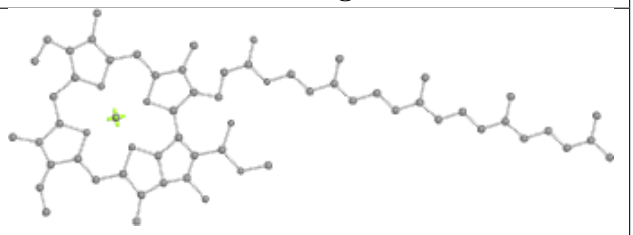
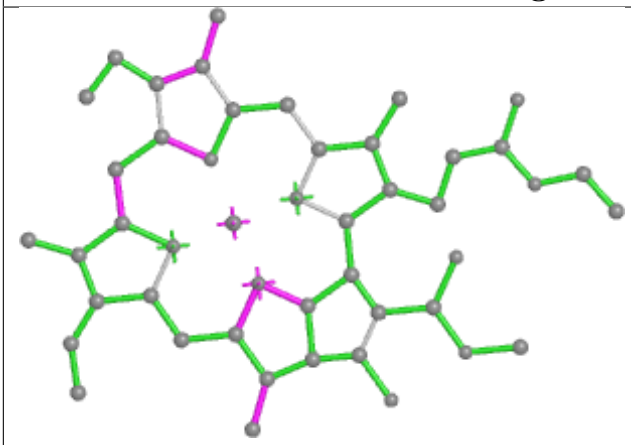


Rings

Ligand CLA r 101



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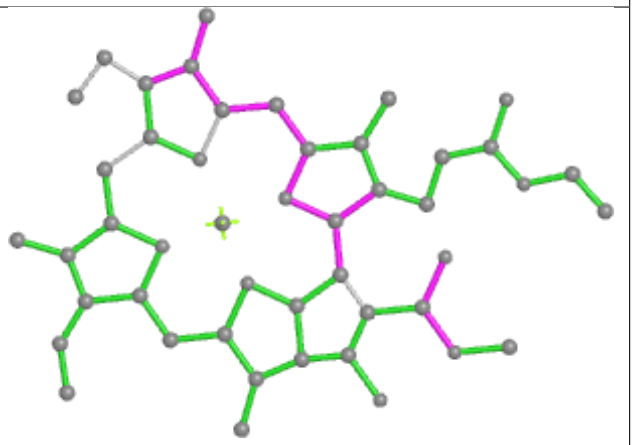

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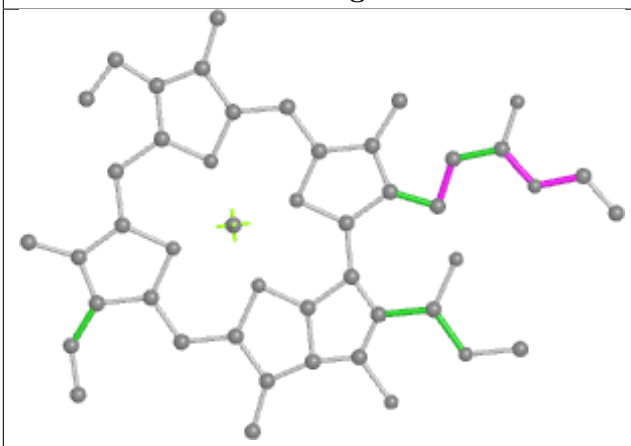

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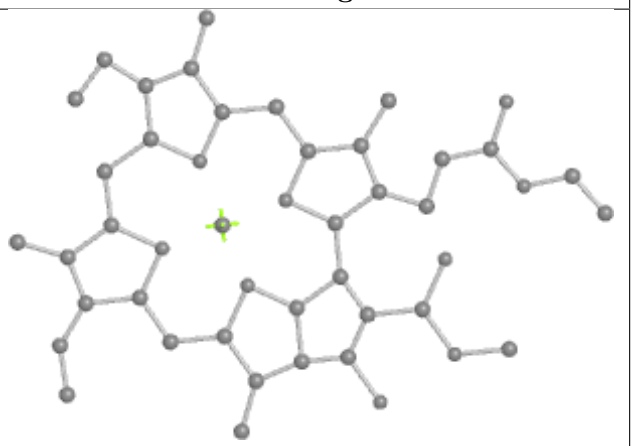
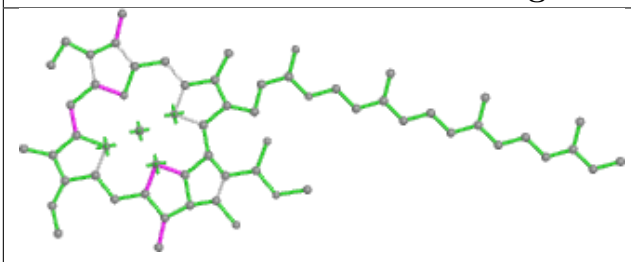
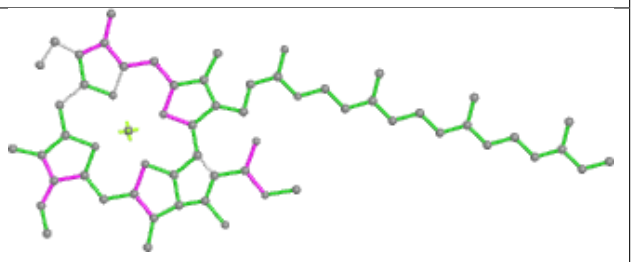
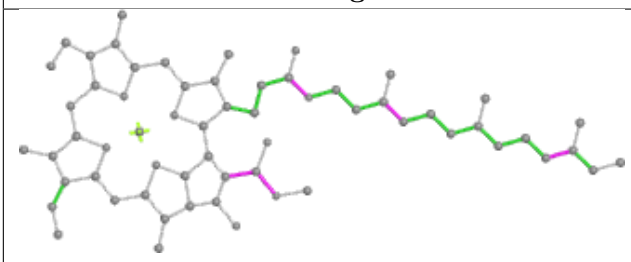
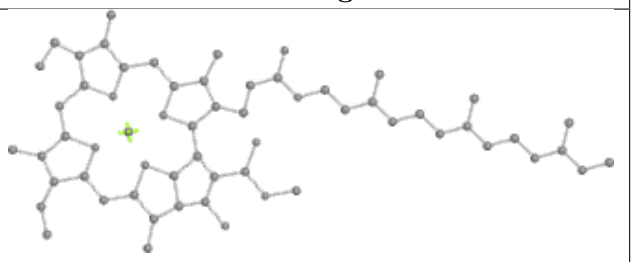
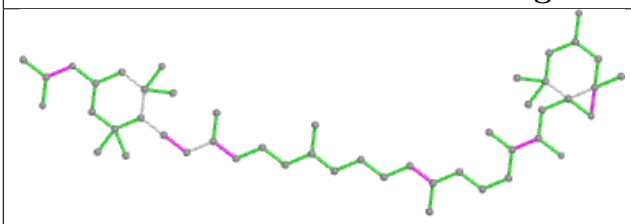
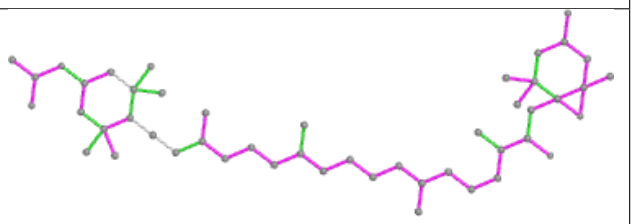
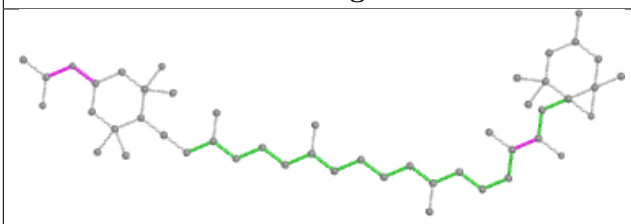
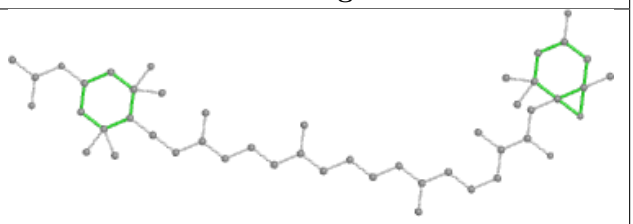
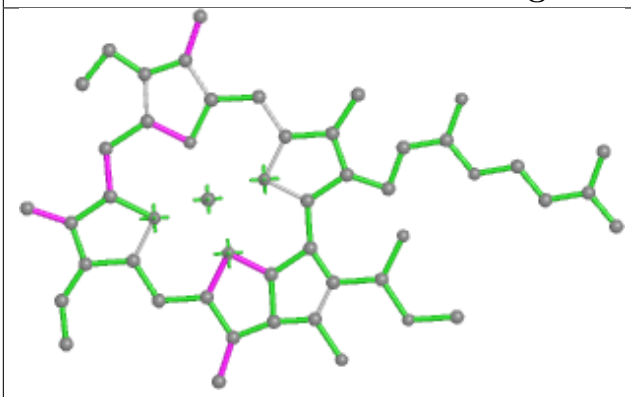


Rings

Ligand CLA 9 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 6 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 308



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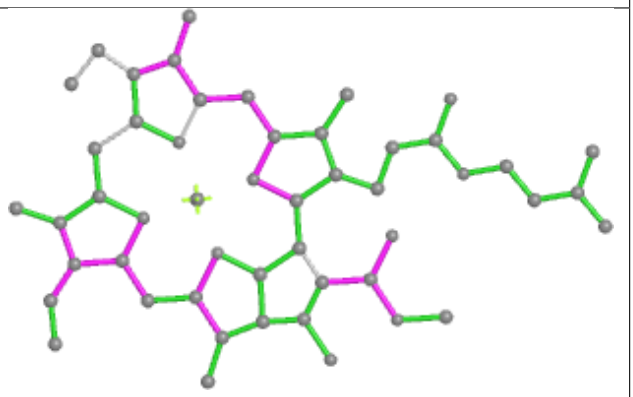
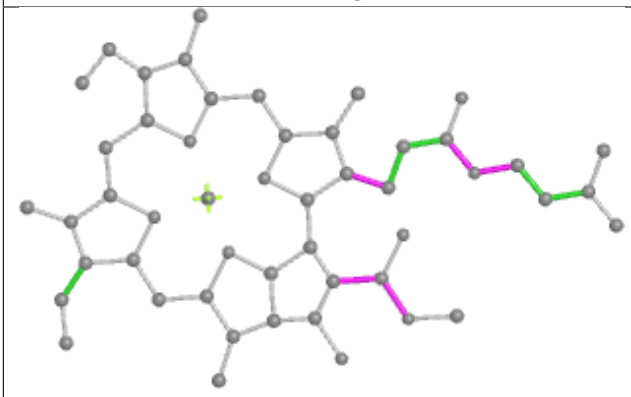
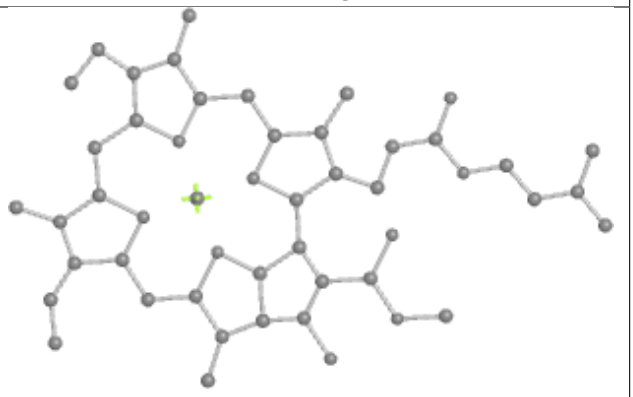


Bond angles

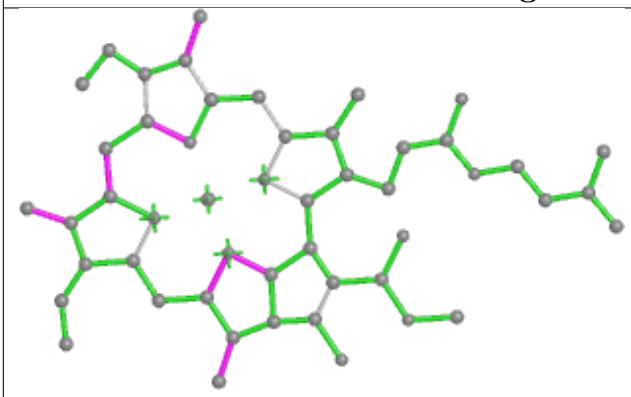


Torsions



Rings

Ligand CLA 10 308



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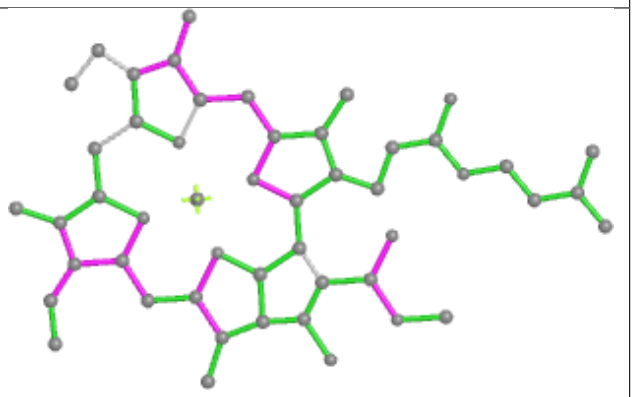

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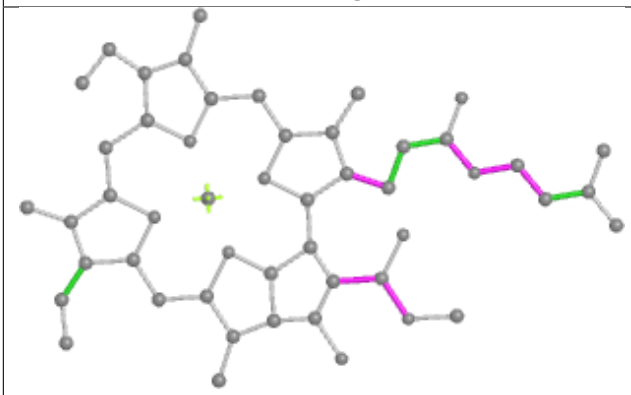
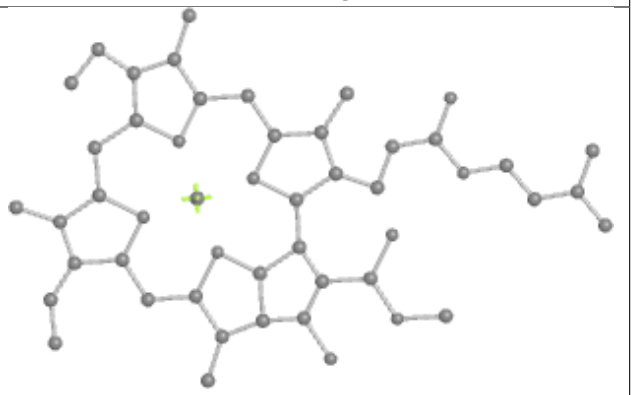
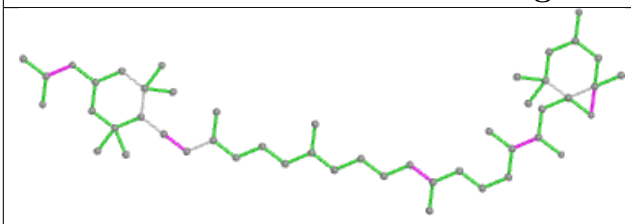


Torsions



Rings

Ligand A86 1 304



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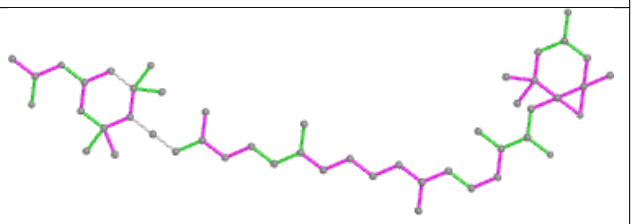

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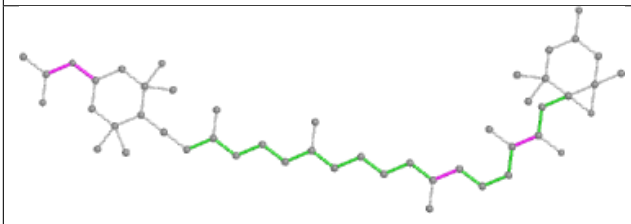

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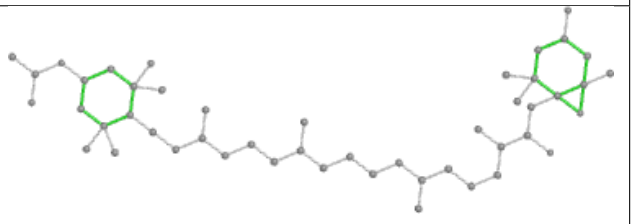
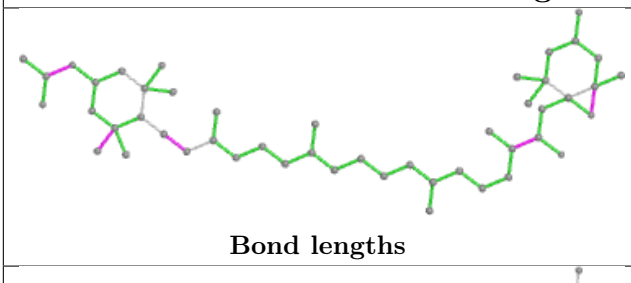


Rings

Ligand A86 5 302



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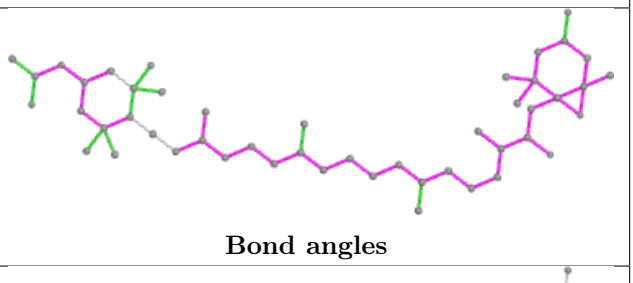

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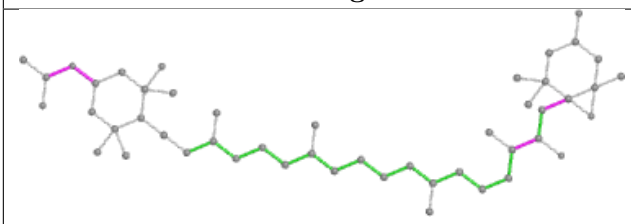

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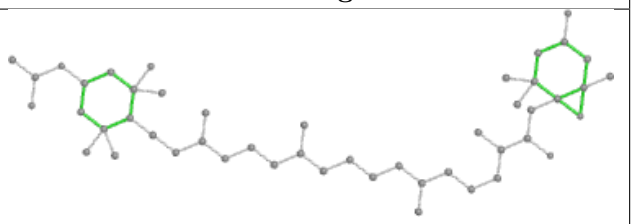
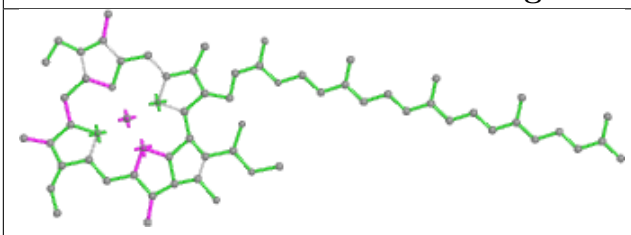


Rings

Ligand CLA B 613



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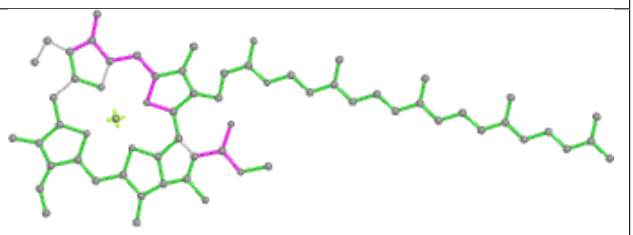

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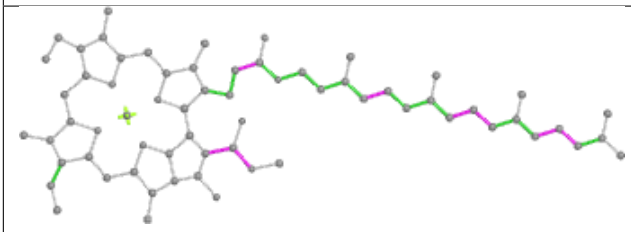

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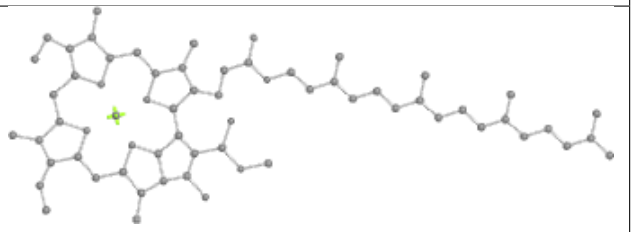
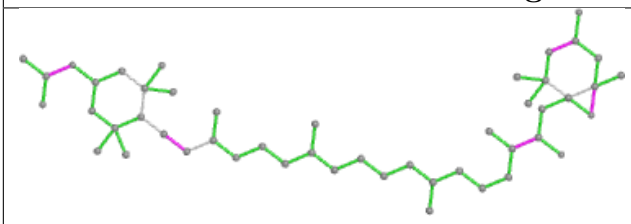


Rings

Ligand A86 15 303



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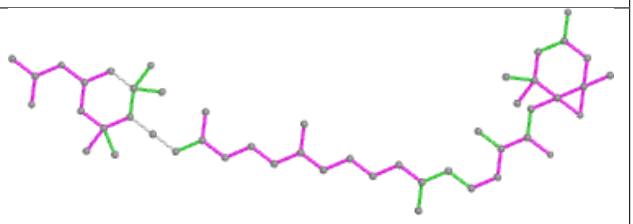

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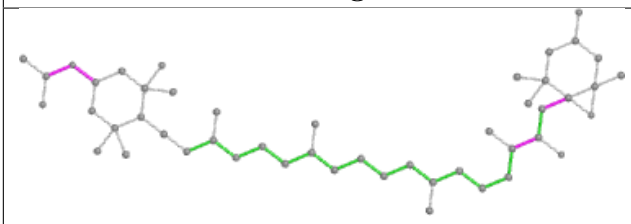

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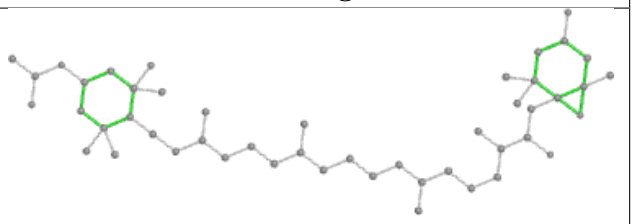
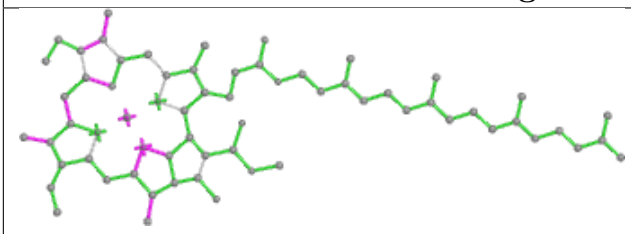


Rings

Ligand CLA W 202



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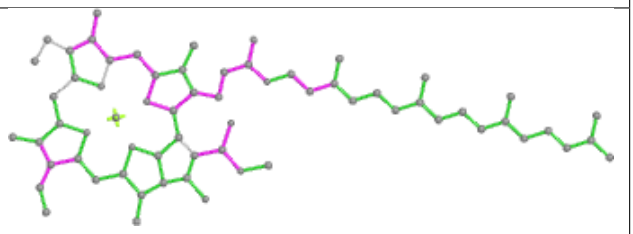

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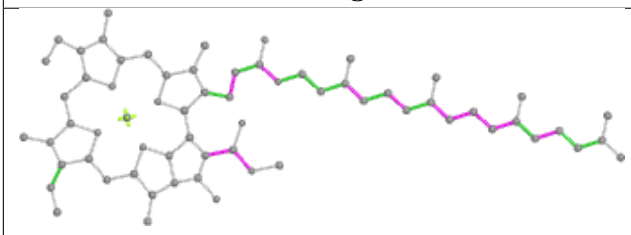

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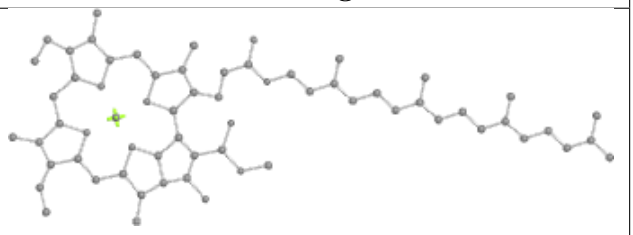
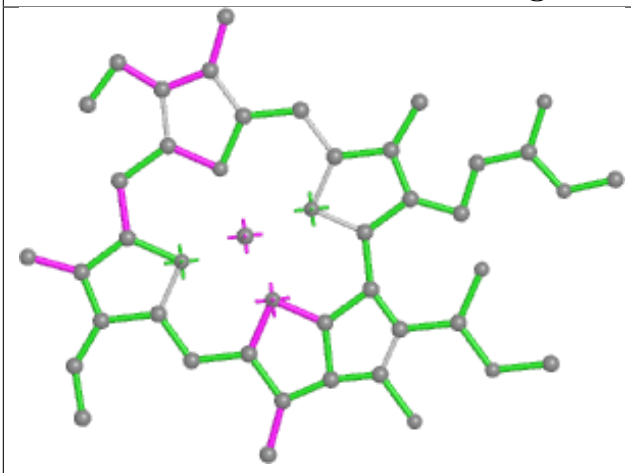


Rings

Ligand CLA 8 311



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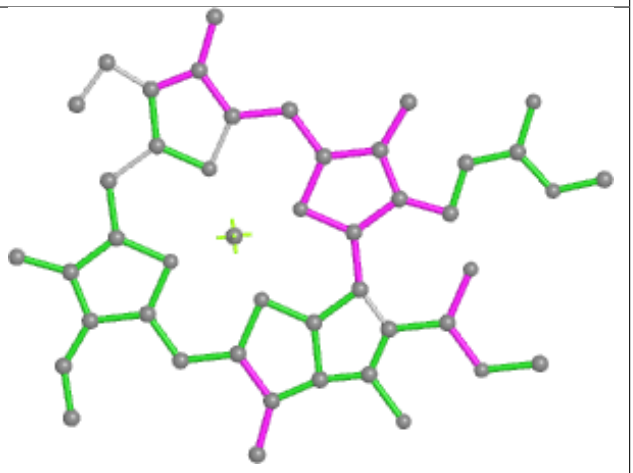

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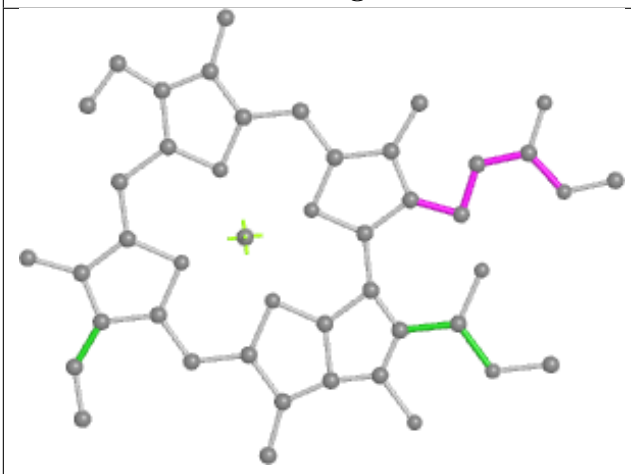

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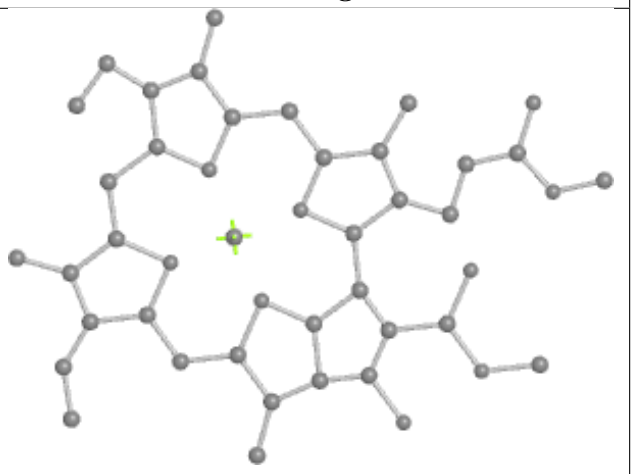
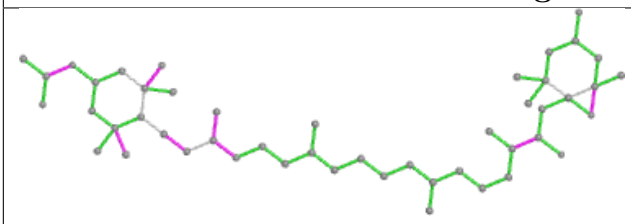


Rings

Ligand A86 0 306



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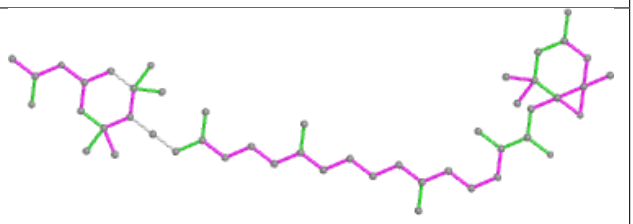

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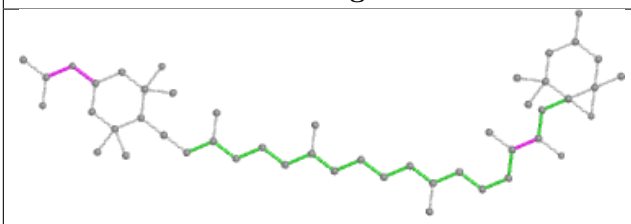

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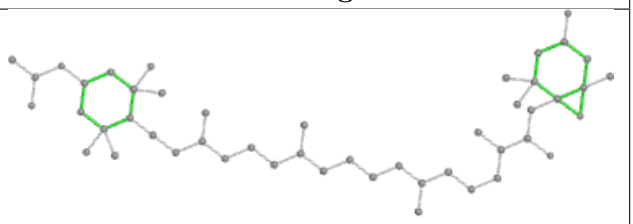
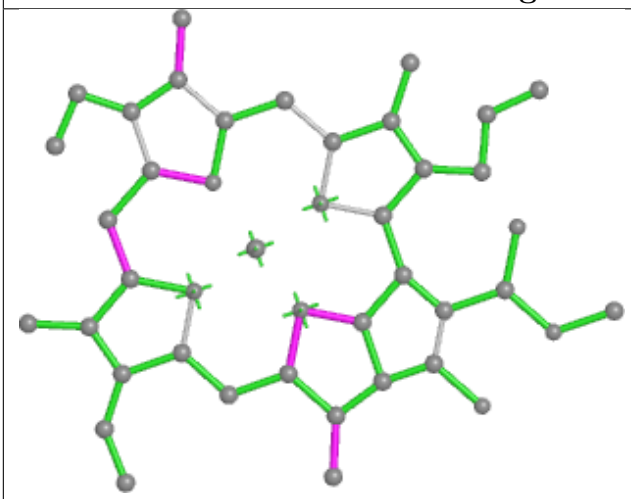


Rings

Ligand CLA 16 316



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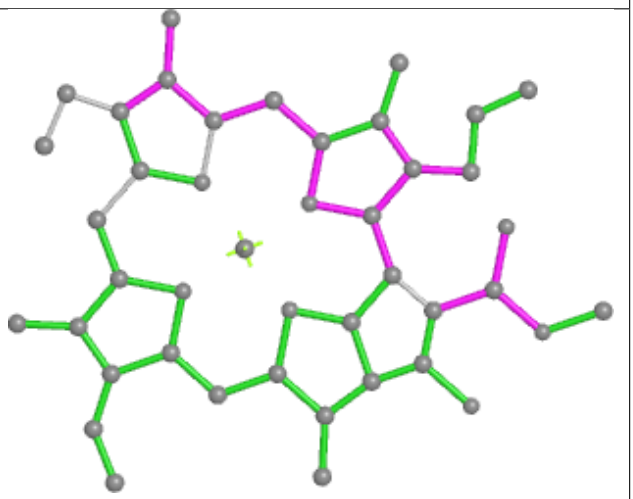

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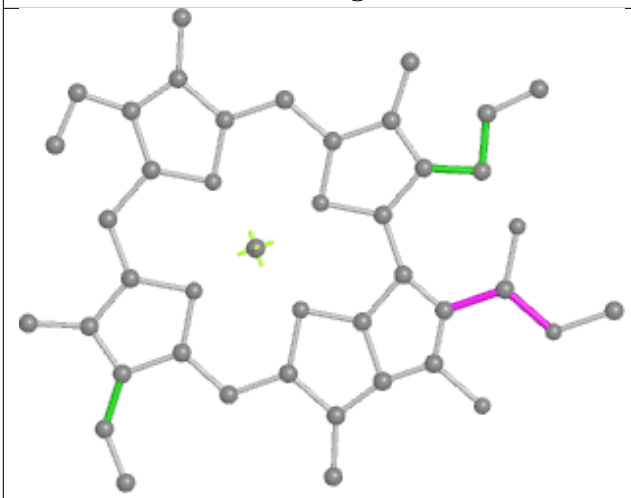

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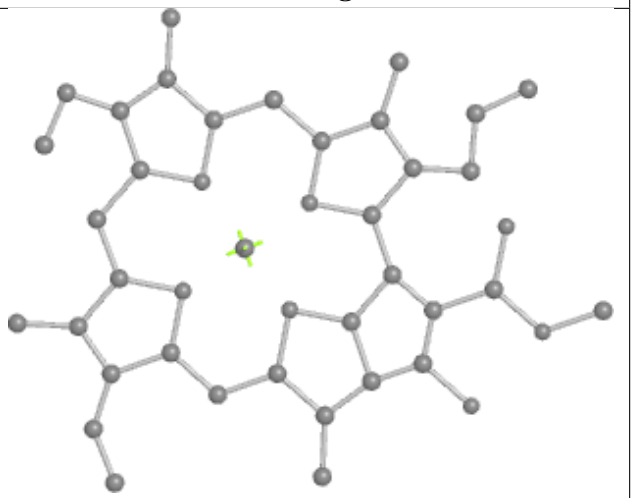
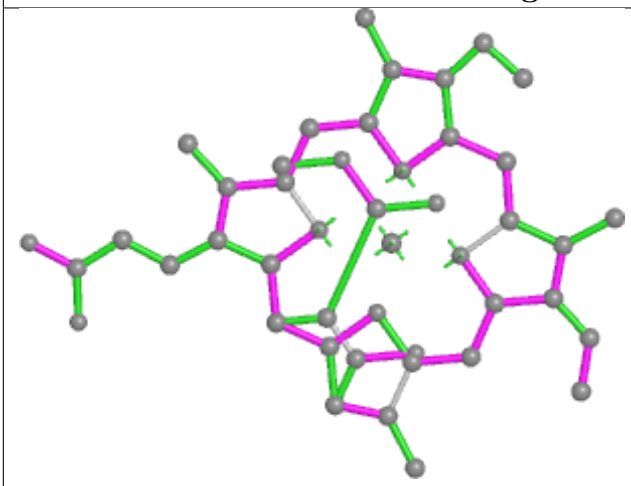


Rings

Ligand KC2 15 310



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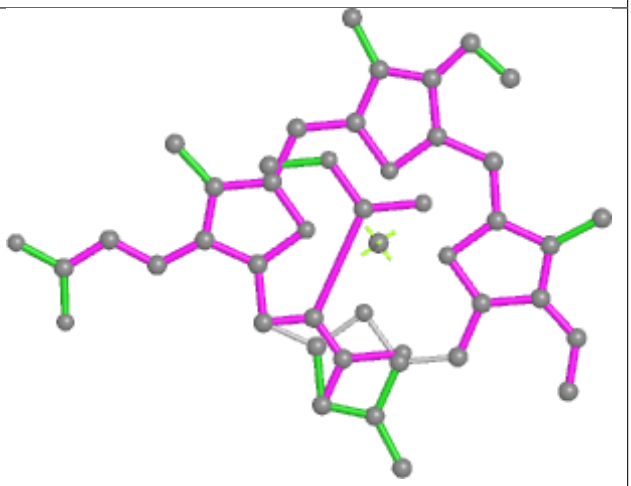

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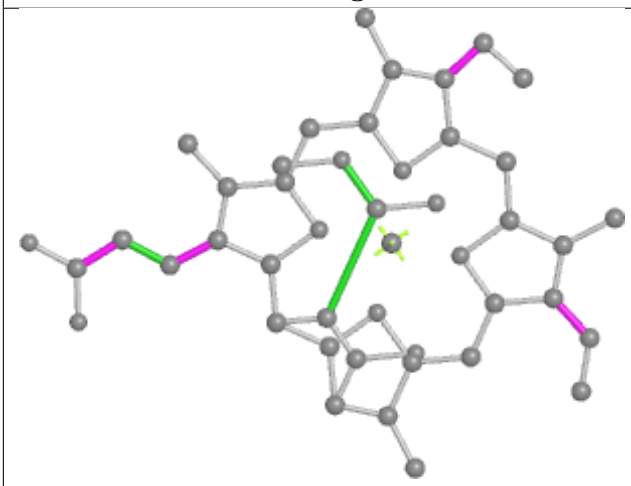

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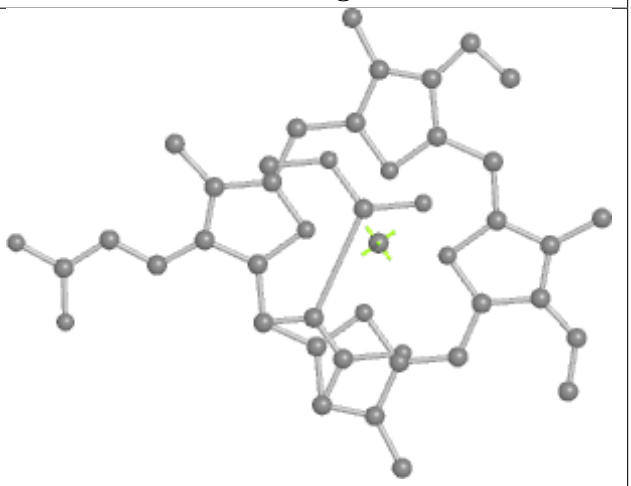
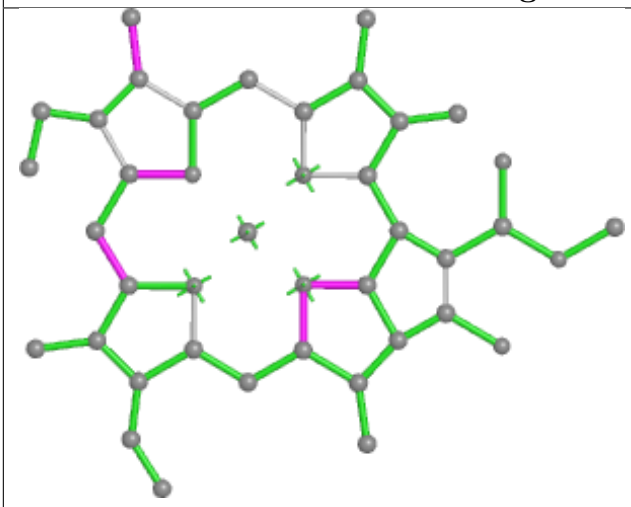


Rings

Ligand CLA 17 307



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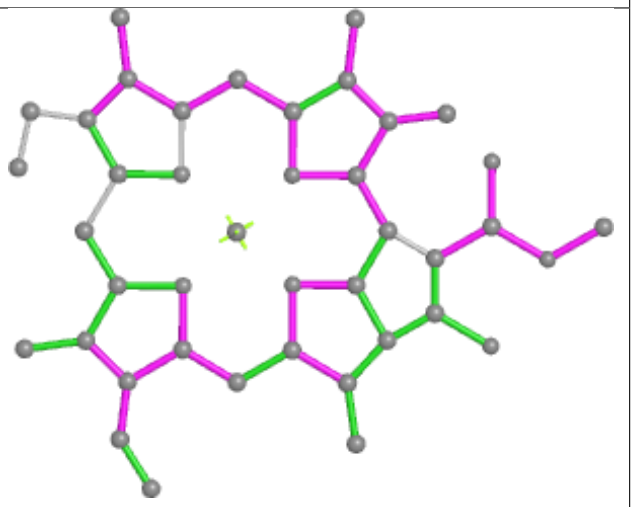

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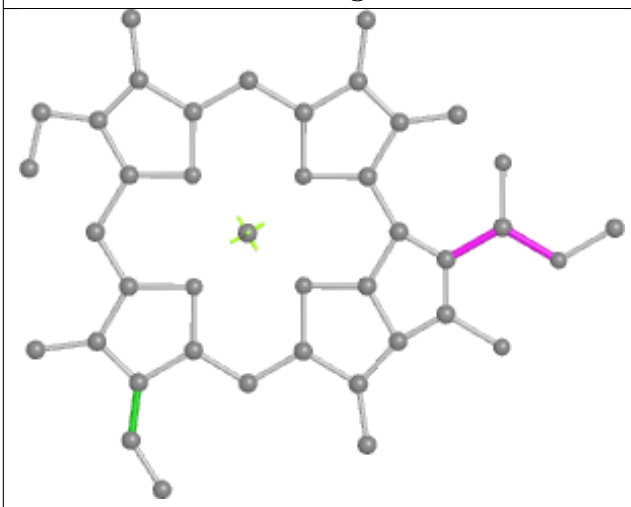

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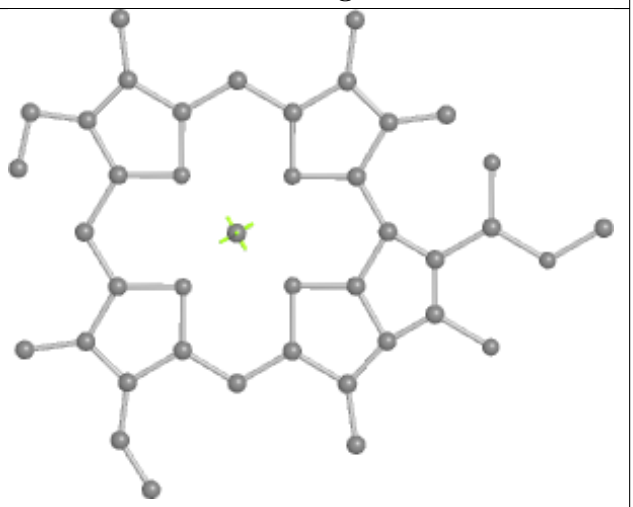

Rings

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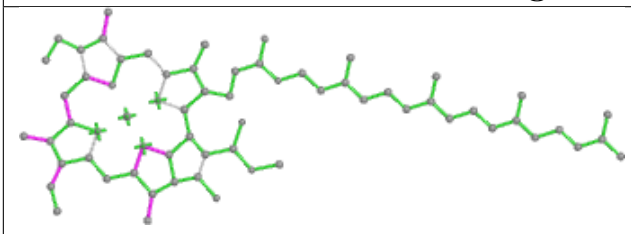

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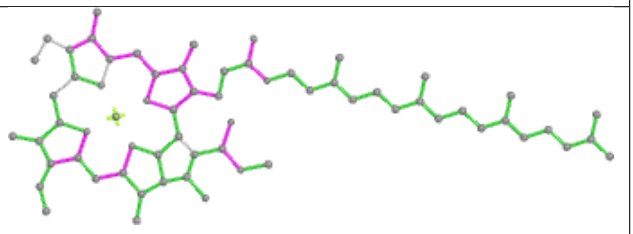
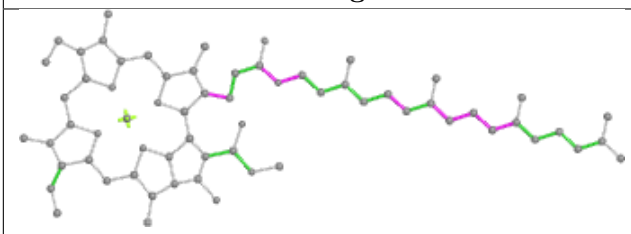


Bond angles



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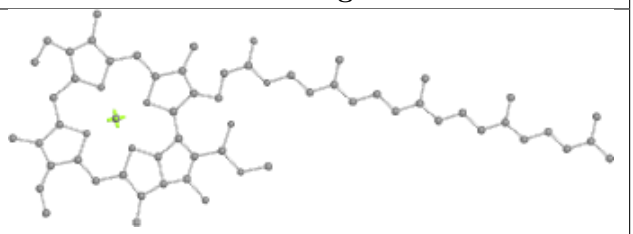
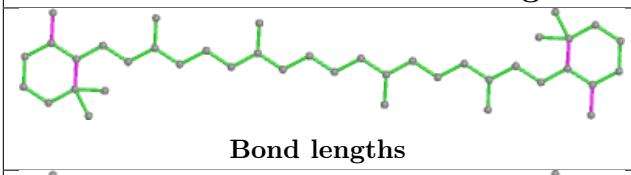


Rings

Ligand BCR Y 101



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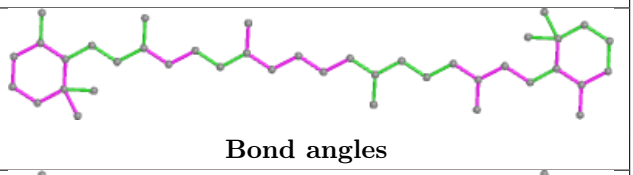
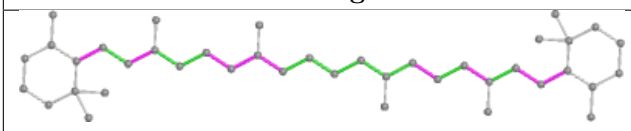


Bond angles



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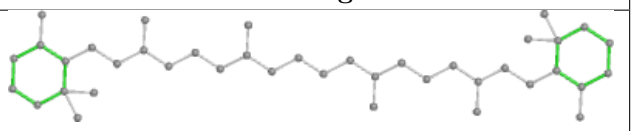
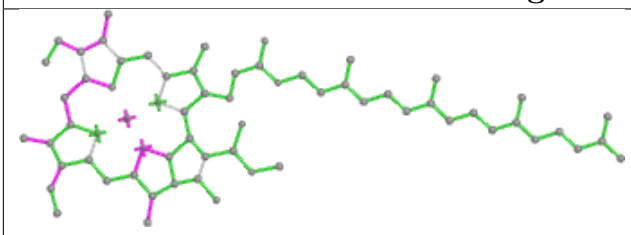


Rings

Ligand CLA b 607



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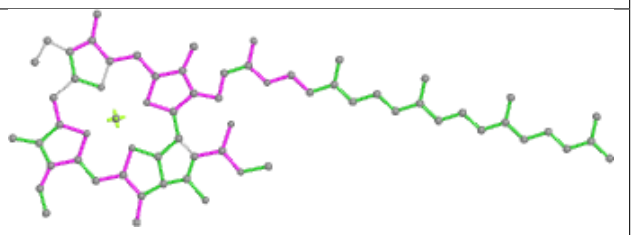
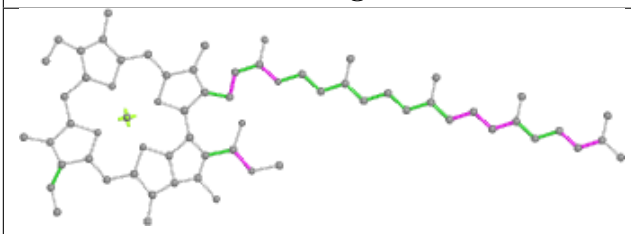


Bond angles



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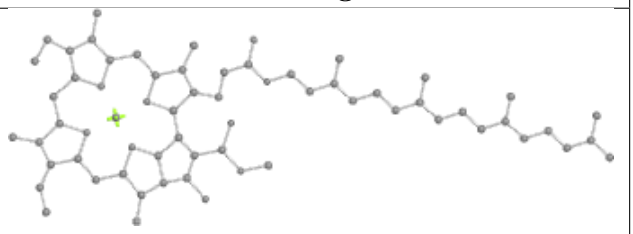
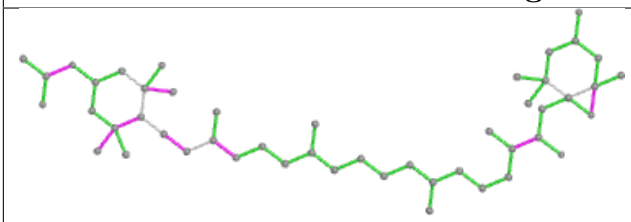


Rings

Ligand A86 17 301



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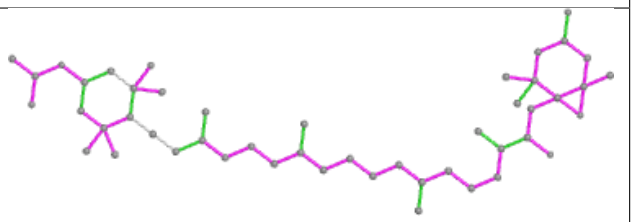

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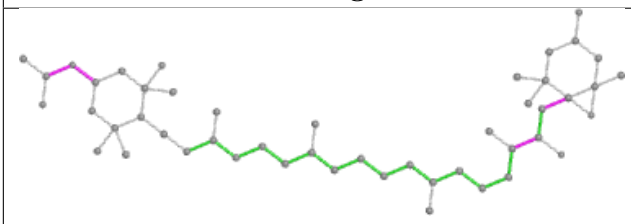

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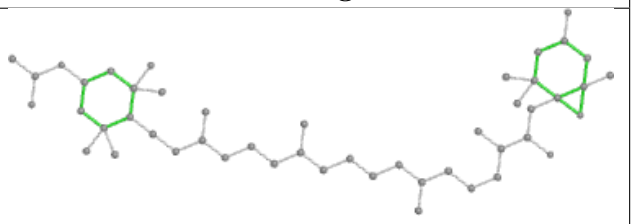
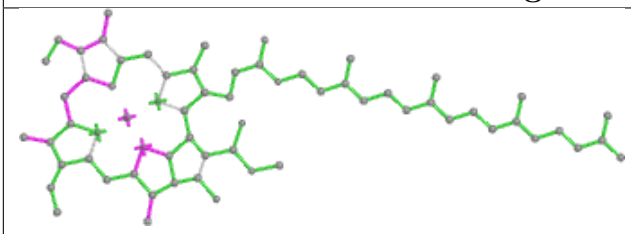


Rings

Ligand CLA B 607



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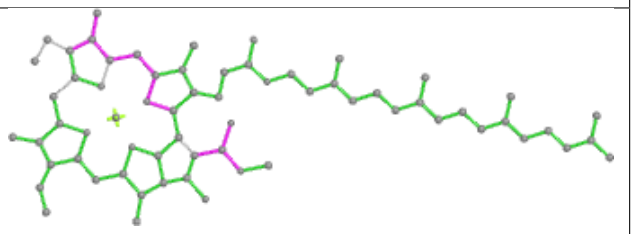

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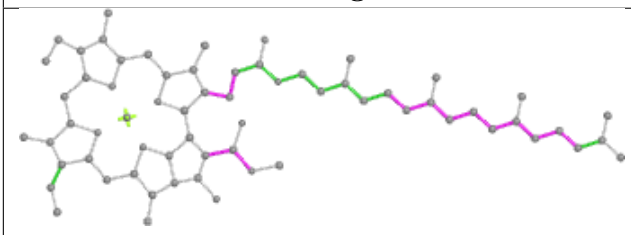

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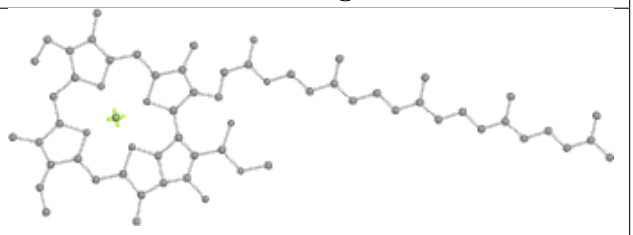
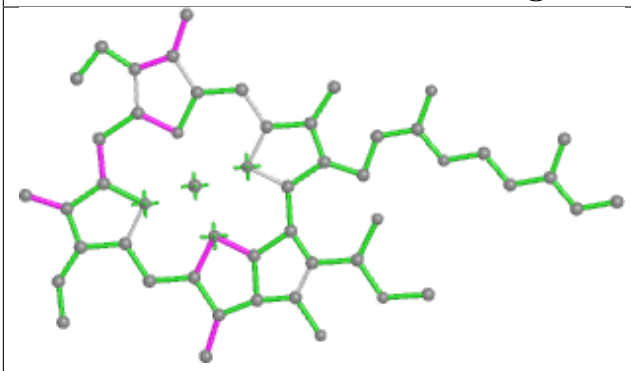


Rings

Ligand CLA p 608



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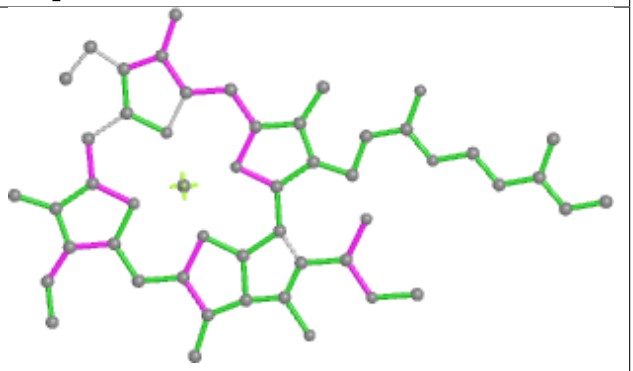

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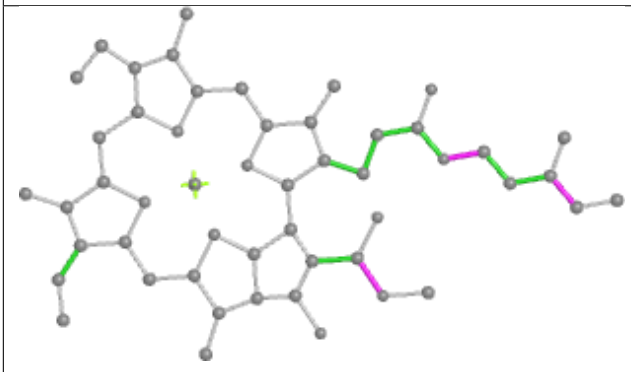

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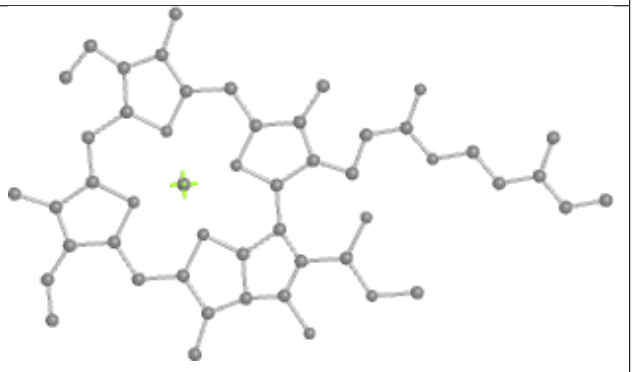
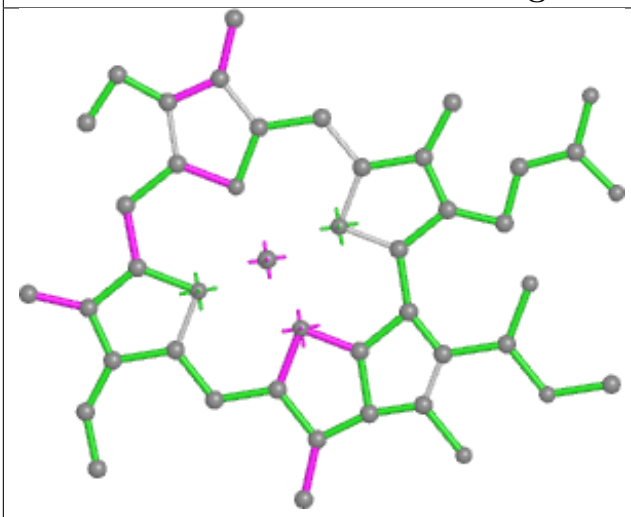


Rings

Ligand CLA 2 311



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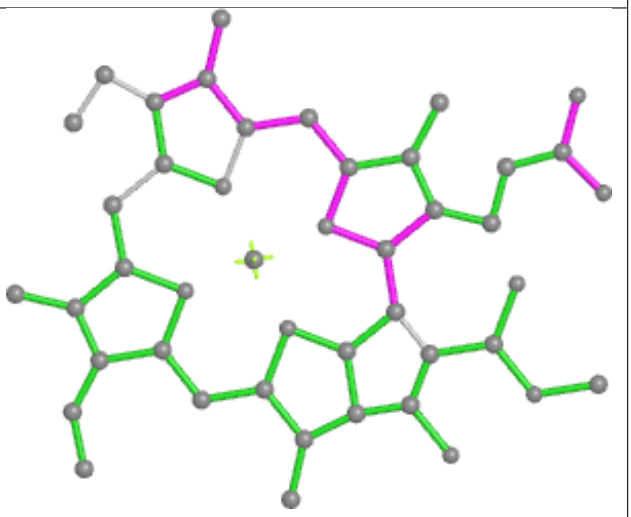

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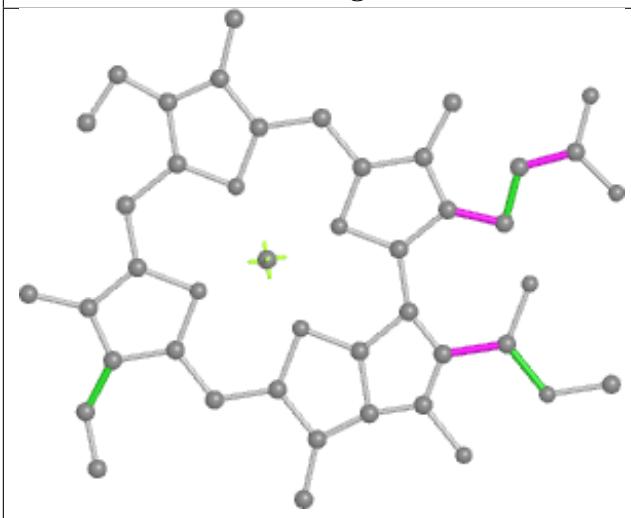

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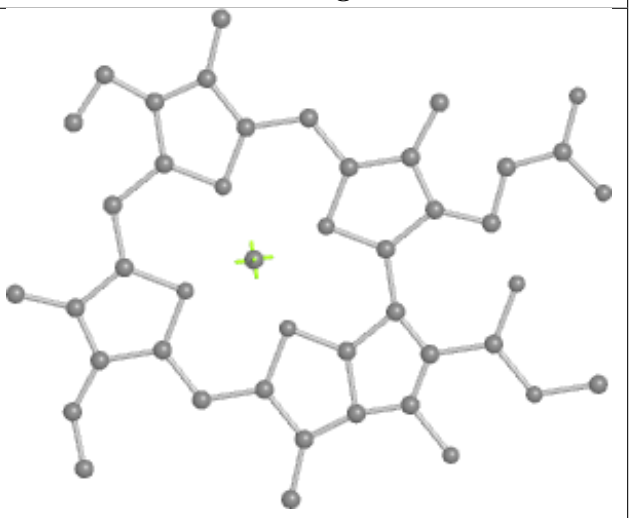
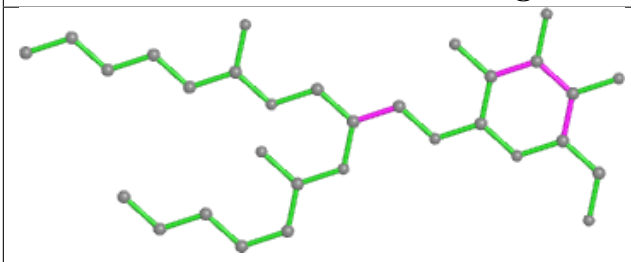


Rings

Ligand LMG 10 319



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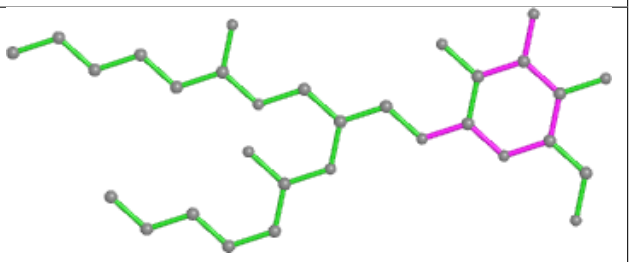

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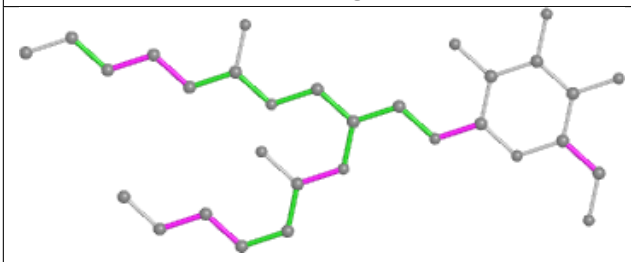

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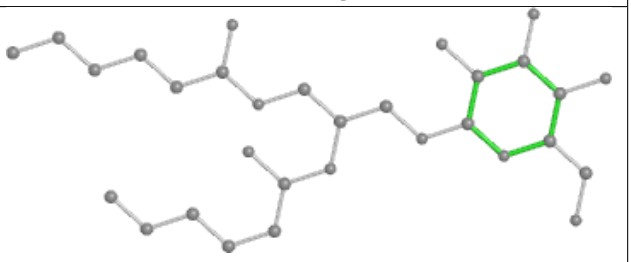
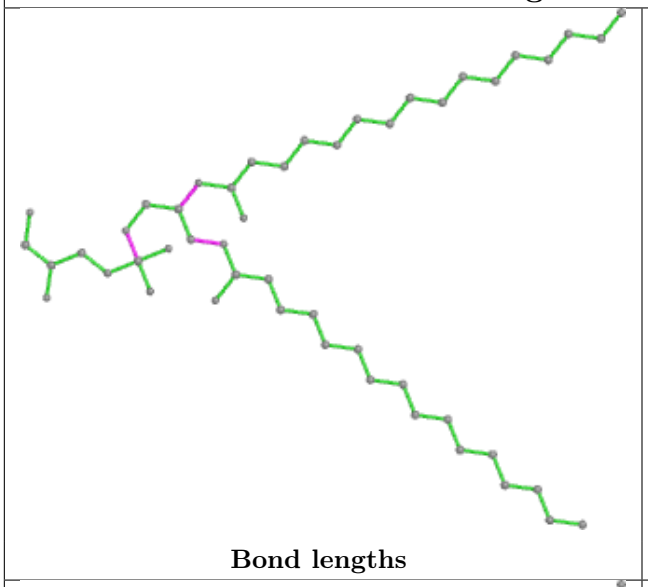


Rings

Ligand LHG L 101



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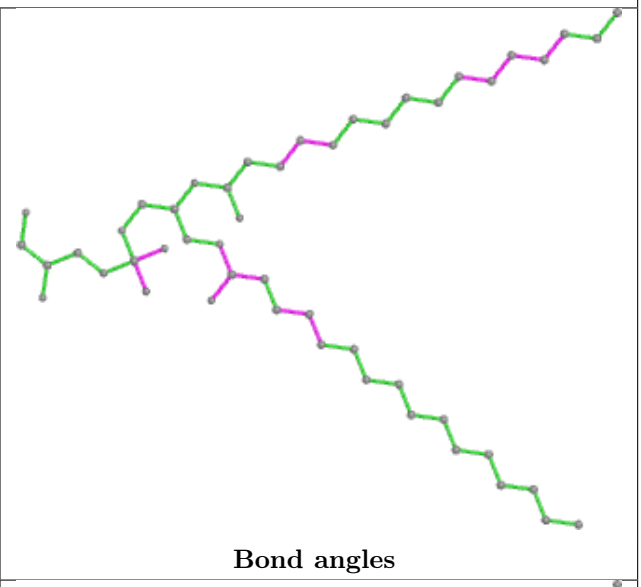

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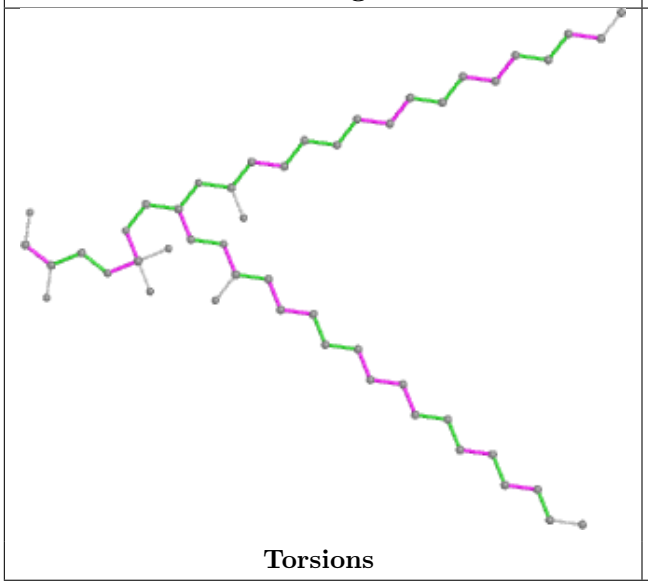

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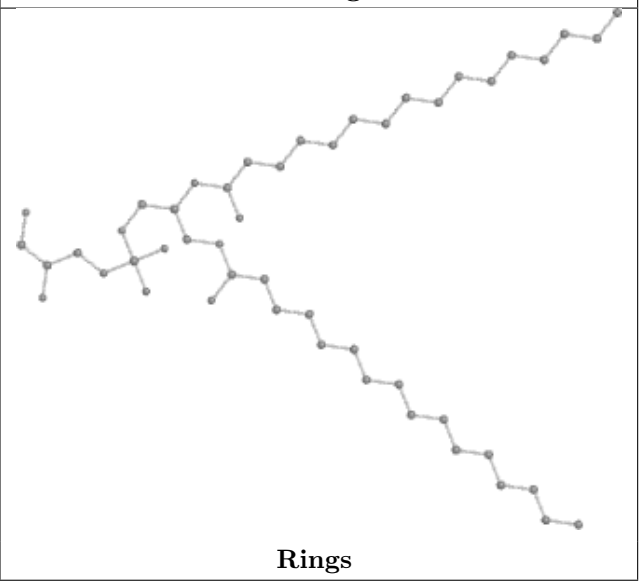

Rings

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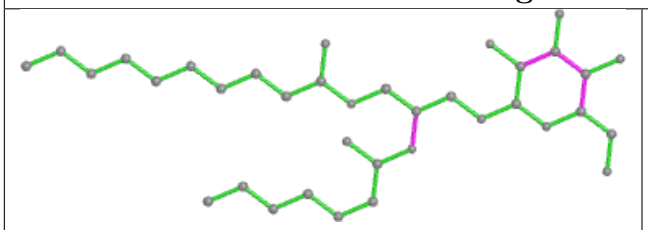

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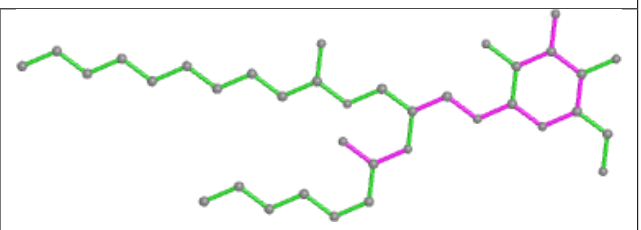

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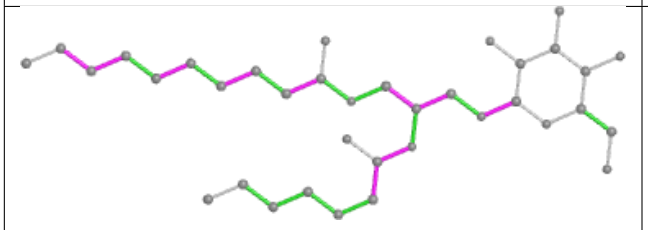

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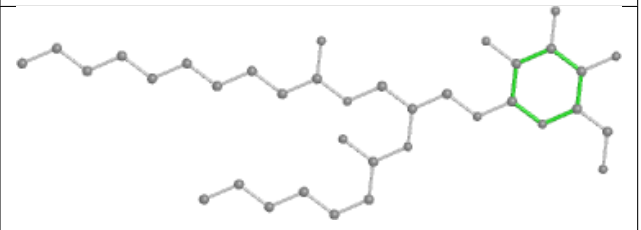
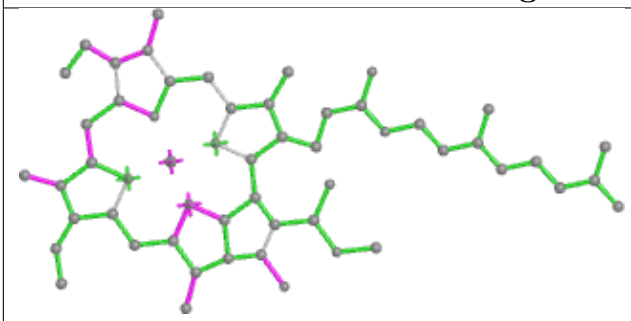


Rings

Ligand CLA 18 312



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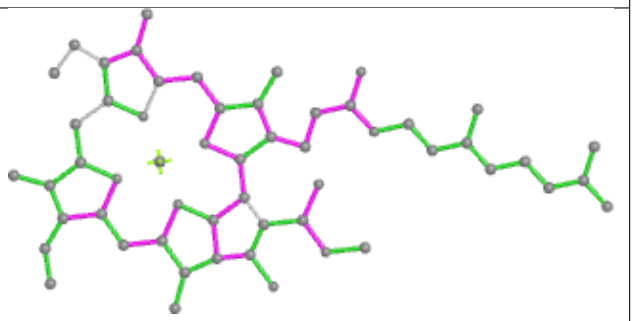

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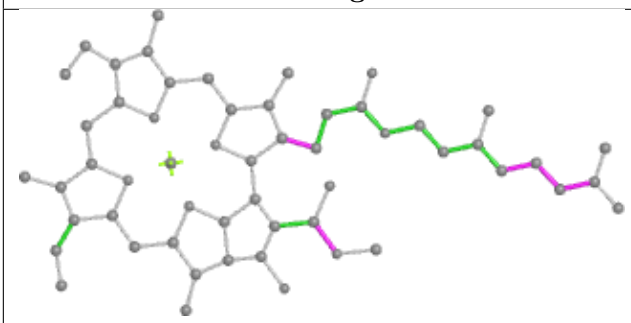

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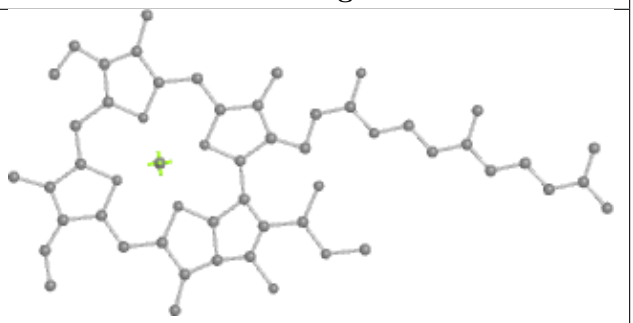
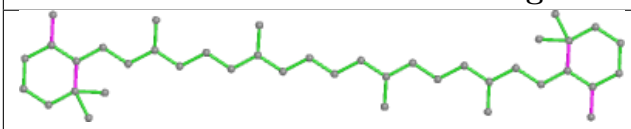


Rings

Ligand BCR y 101



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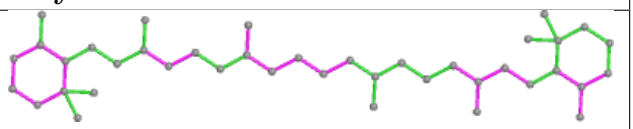

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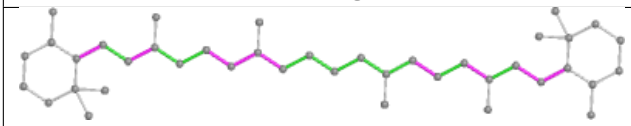

Torsions

Rings

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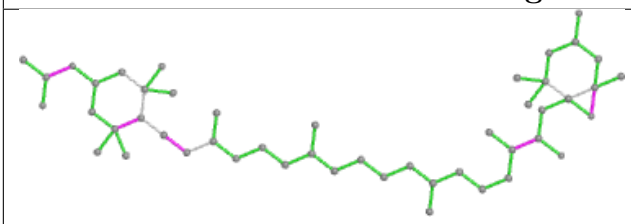

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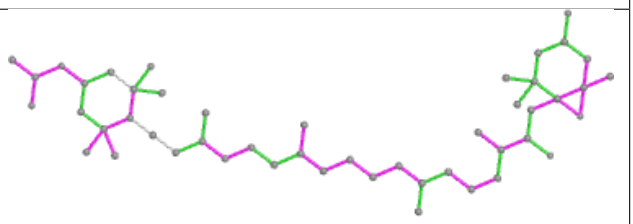

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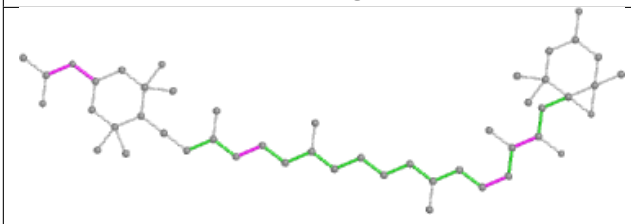

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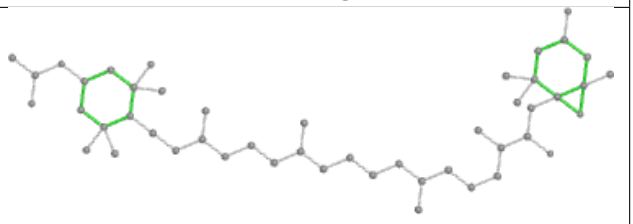
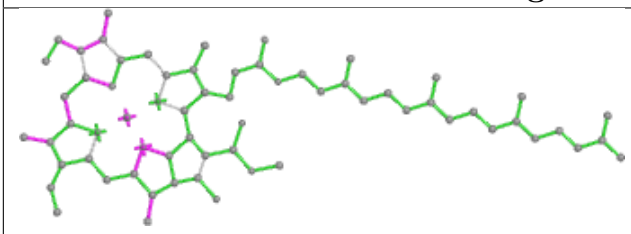


Rings

Ligand CLA p 601



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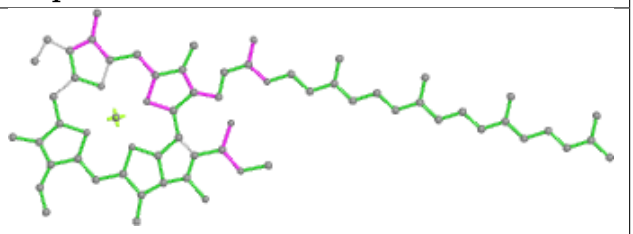

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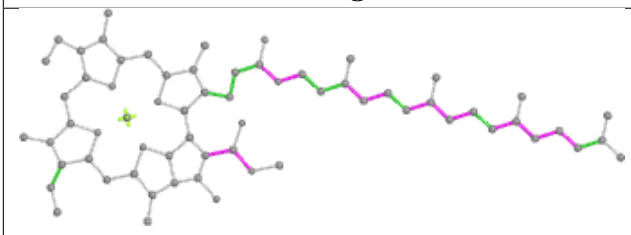

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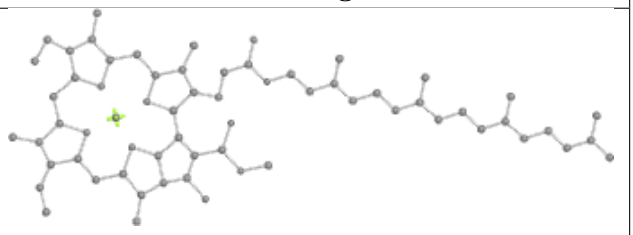
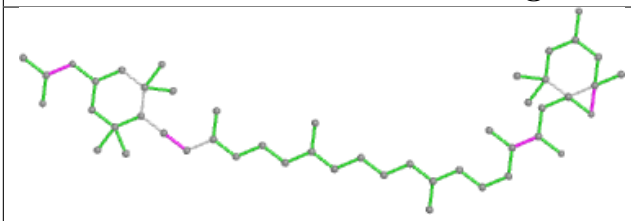


Rings

Ligand A86 11 319



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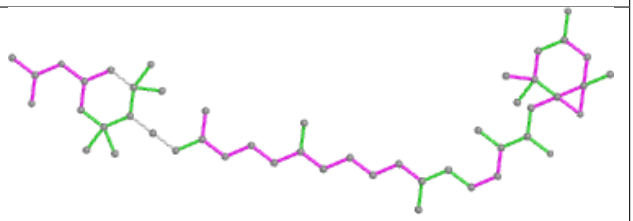

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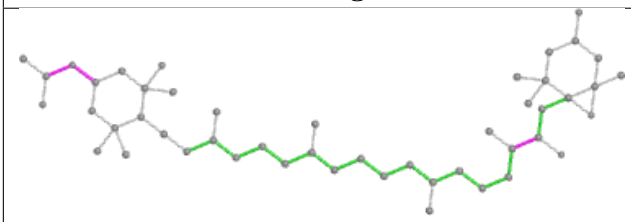

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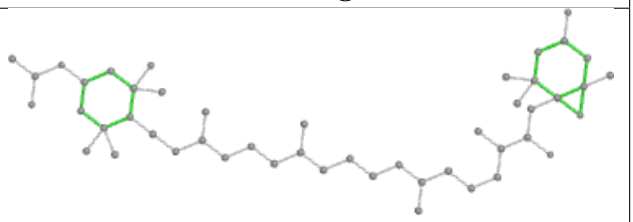
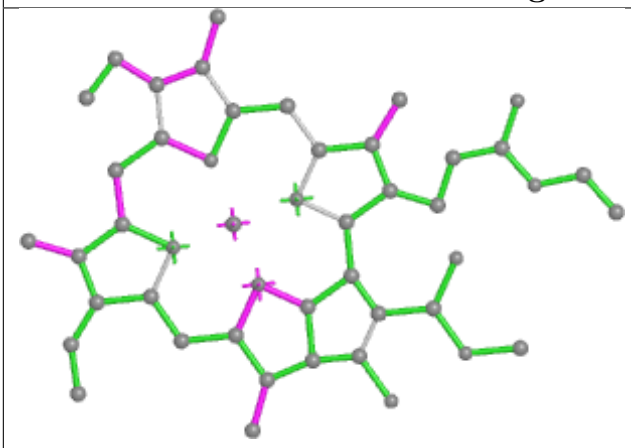


Rings

Ligand CLA 5 312



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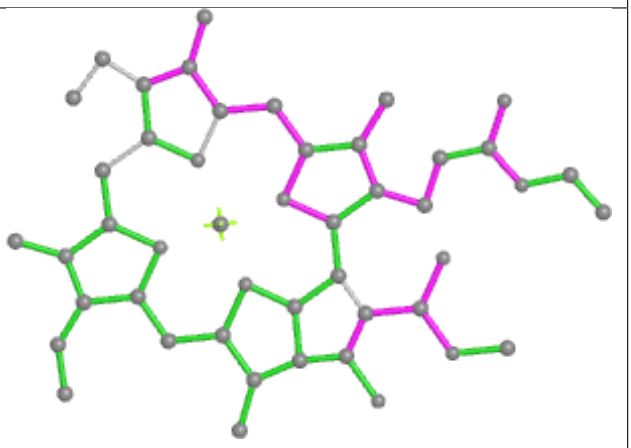

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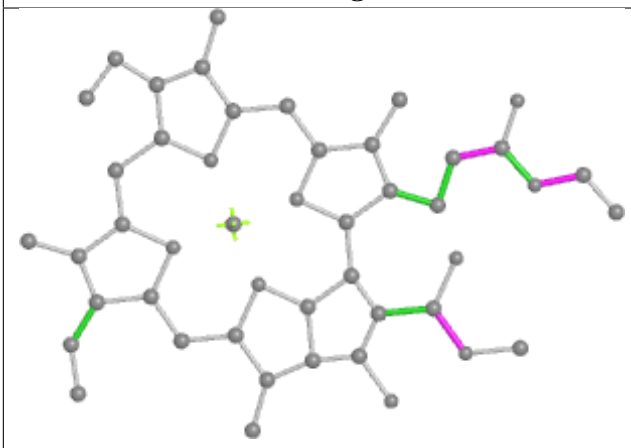

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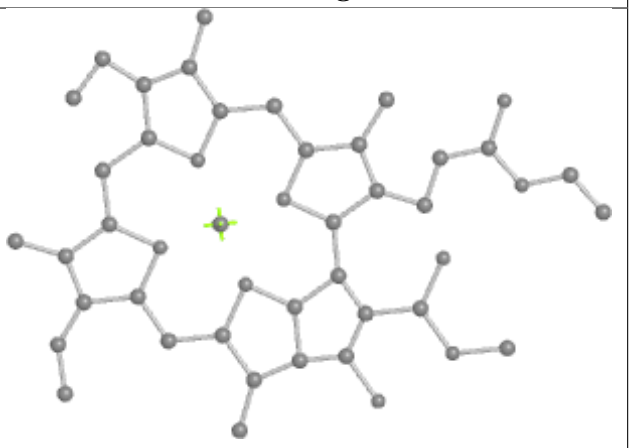
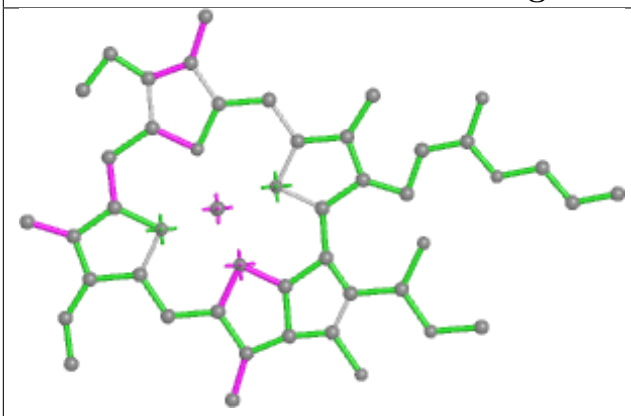


Rings

Ligand CLA 2 312



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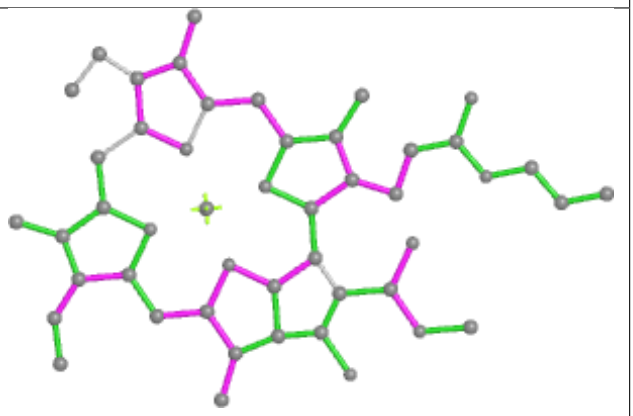

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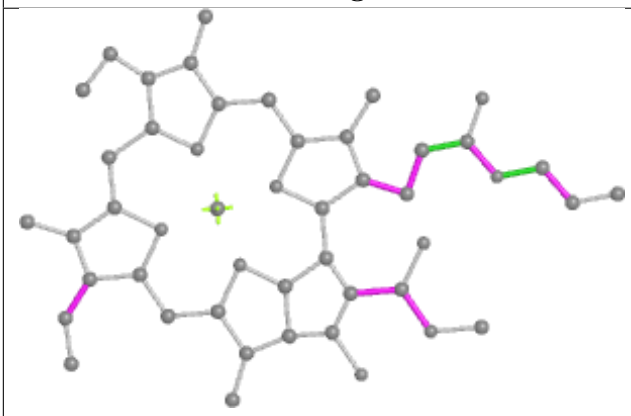

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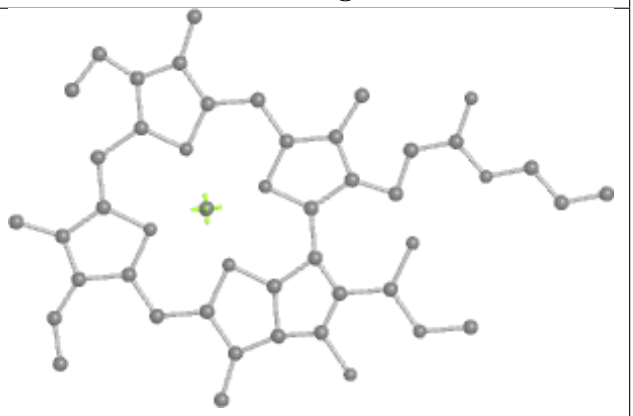
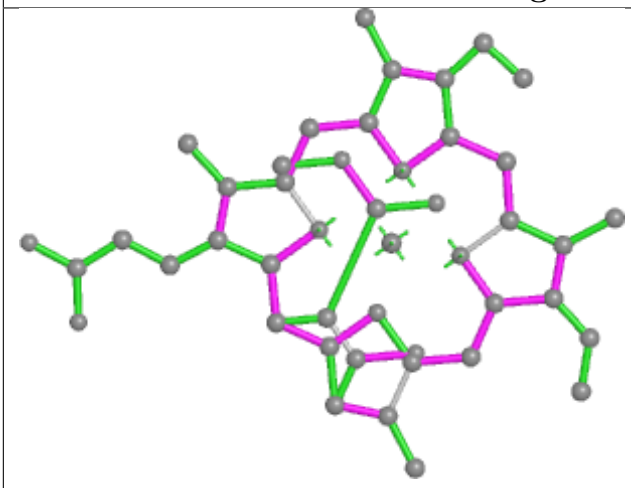
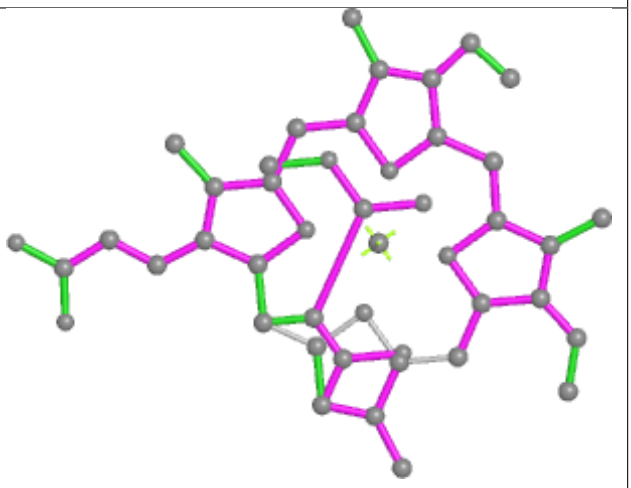


Rings

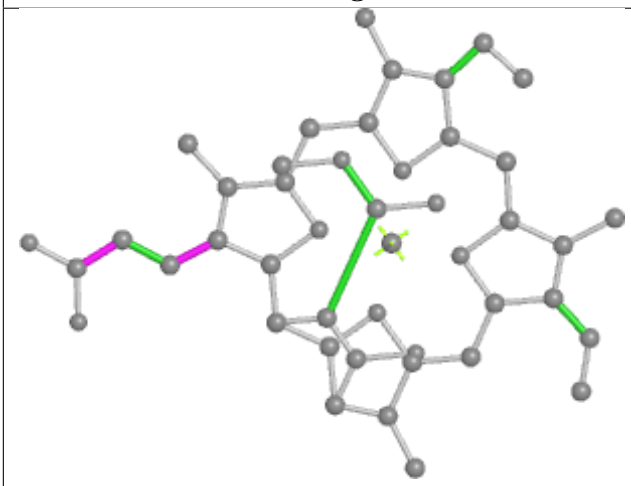
Ligand KC1 0 315



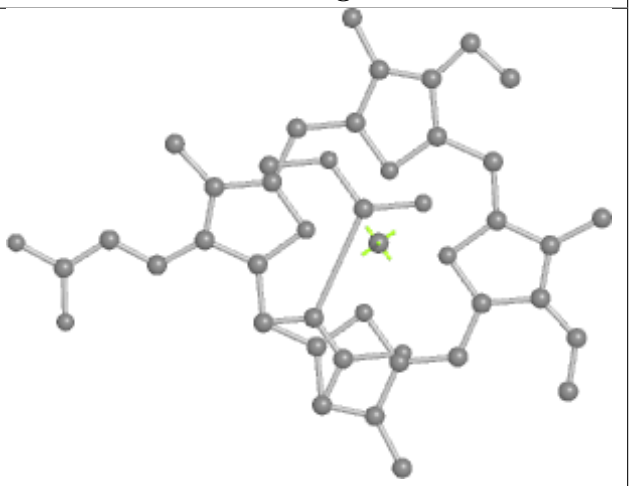
Bond lengths



Bond angles

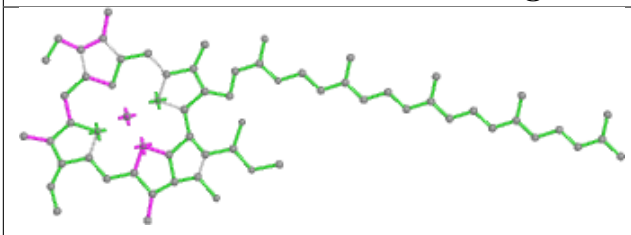


Torsions



Rings

Ligand CLA B 601



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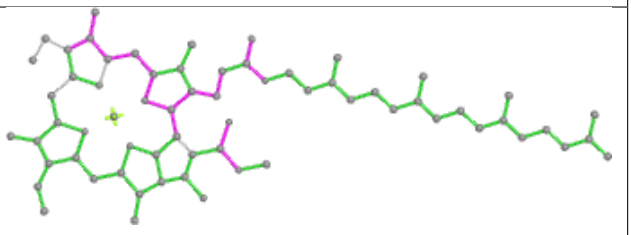
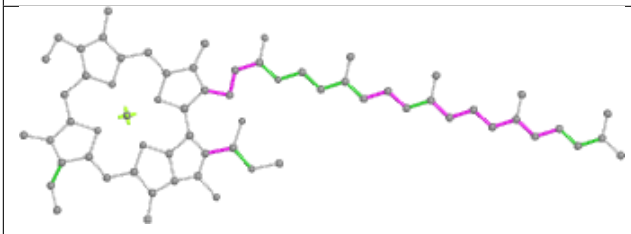


Bond angles



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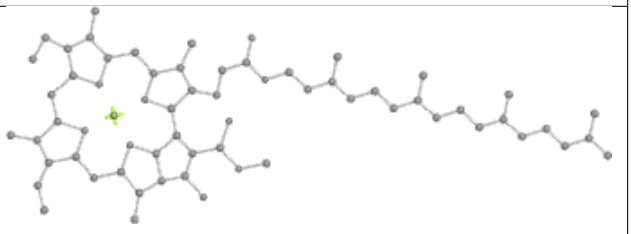
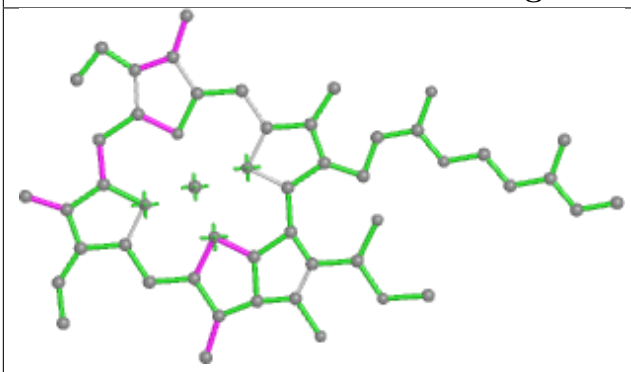


Rings

Ligand CLA P 608



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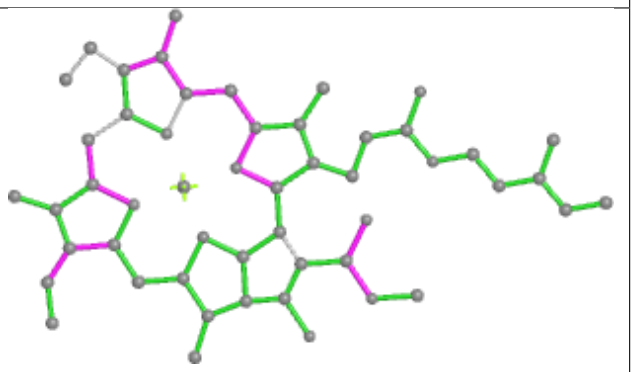
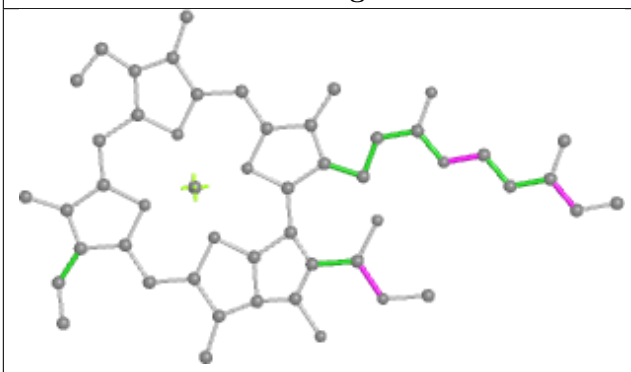


Bond angles



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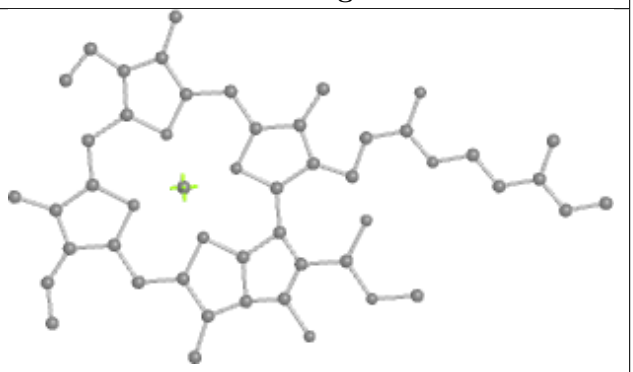
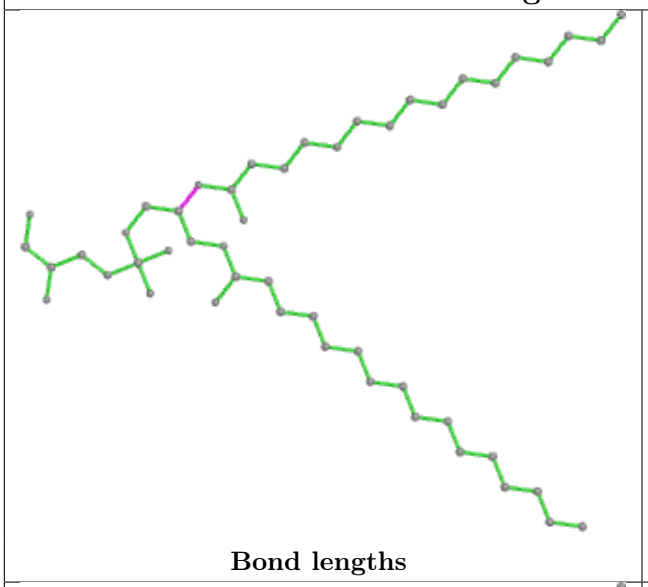


Rings

Ligand LHG D 407



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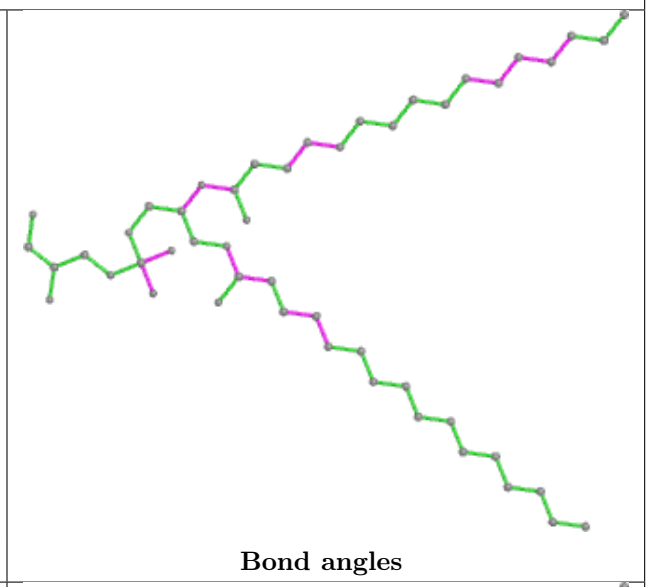
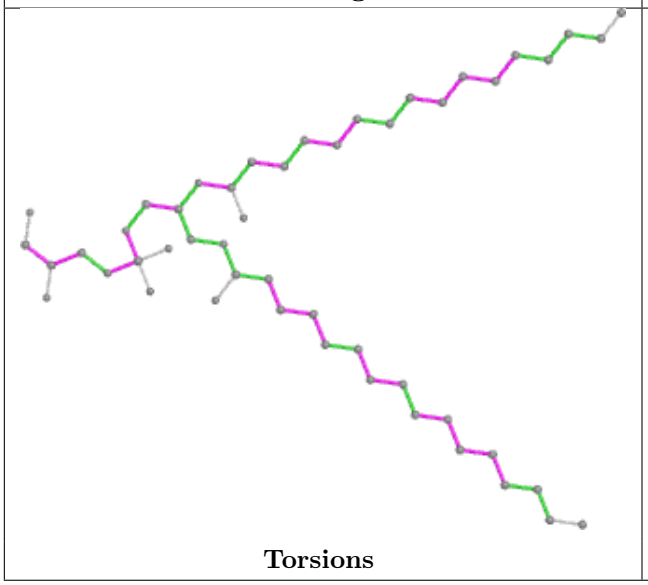


Bond angles



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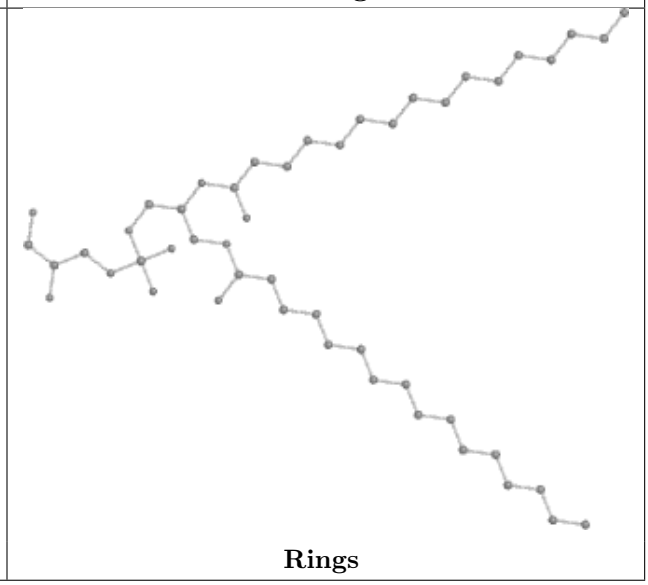
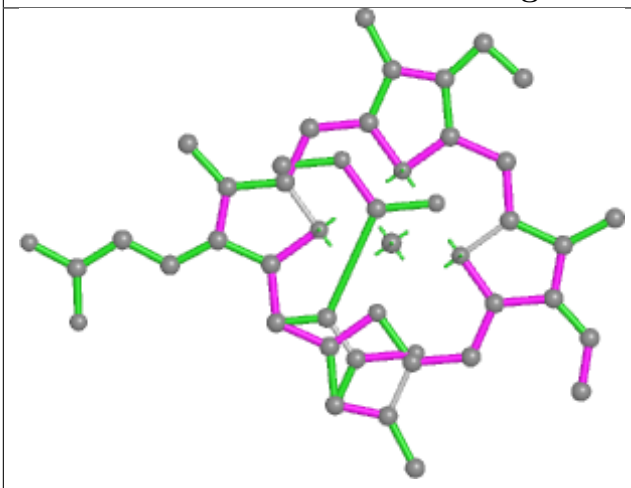


Rings

Ligand KC2 17 311



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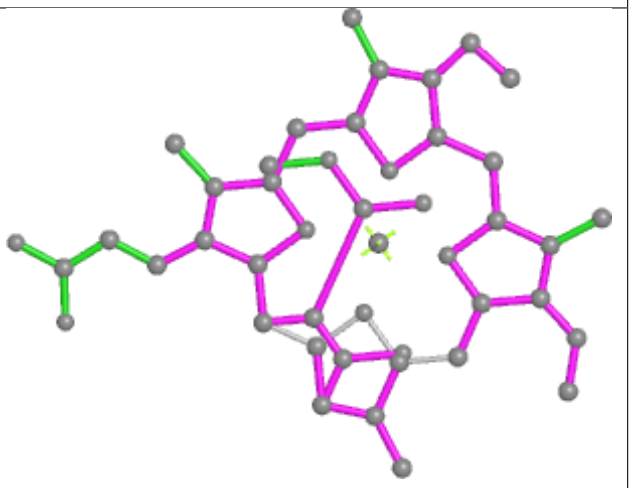

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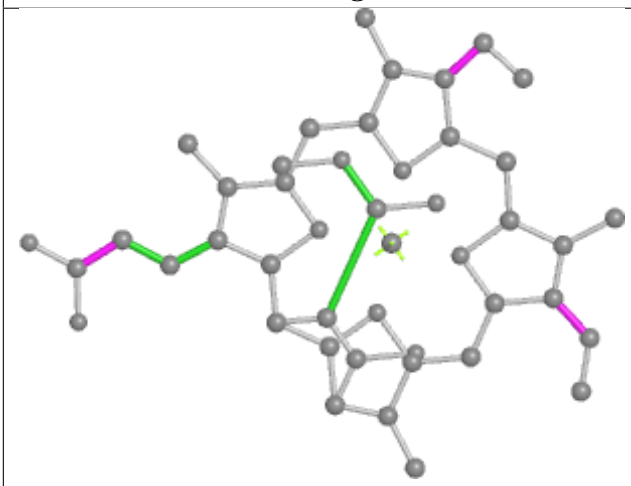

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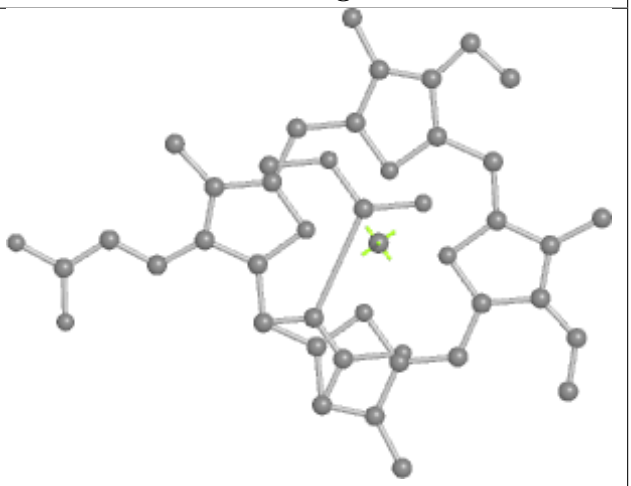
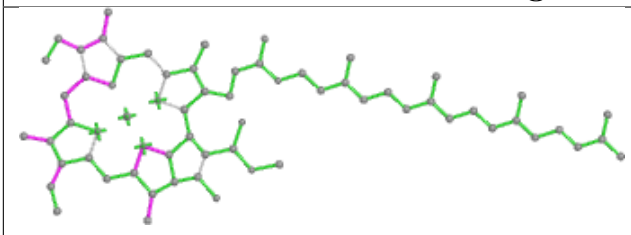


Rings

Ligand CLA b 616



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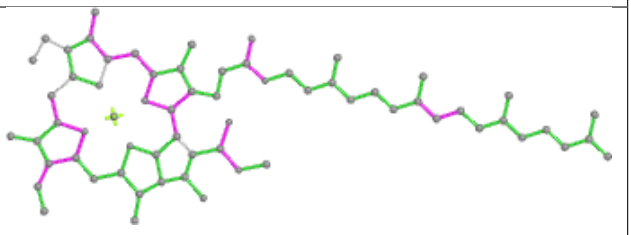
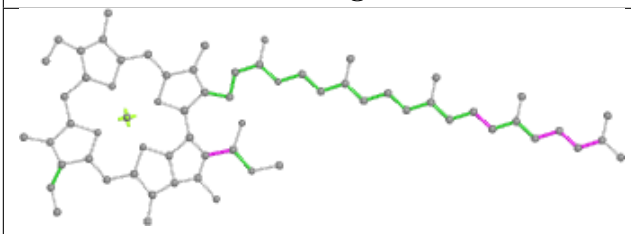


Bond angles



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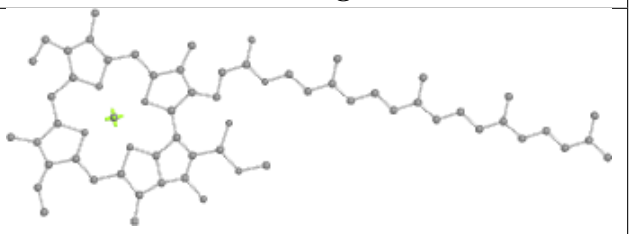
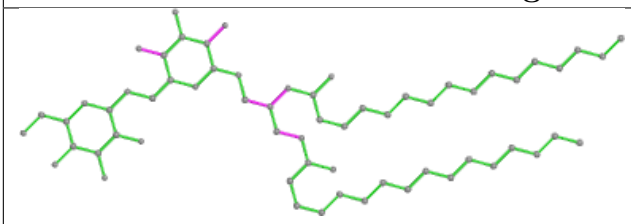


Rings

Ligand DGD h 102



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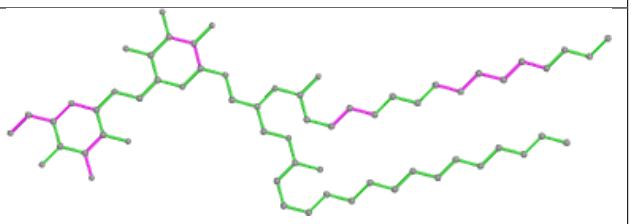

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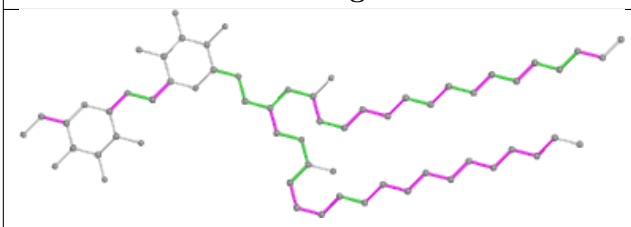

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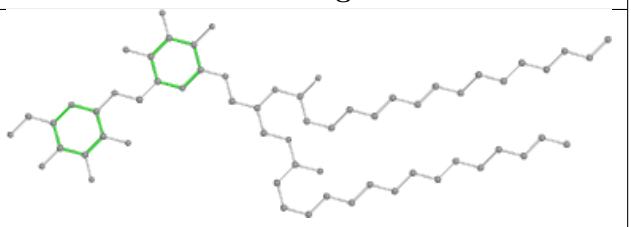
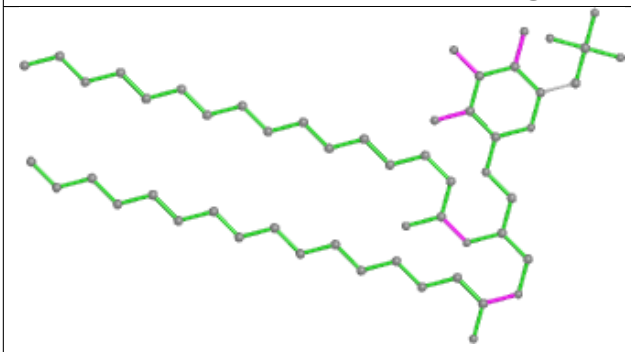


Rings

Ligand SQD B 623



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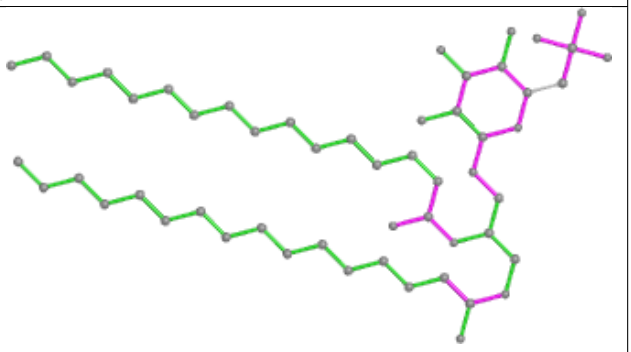

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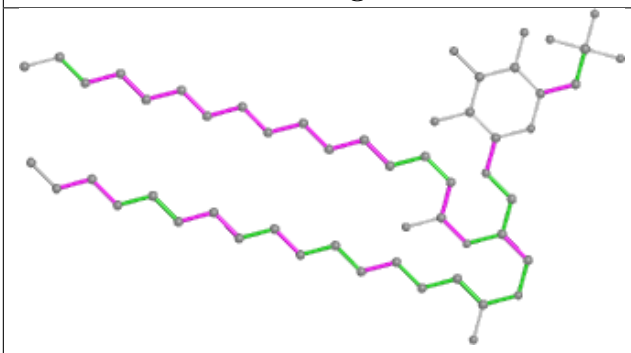

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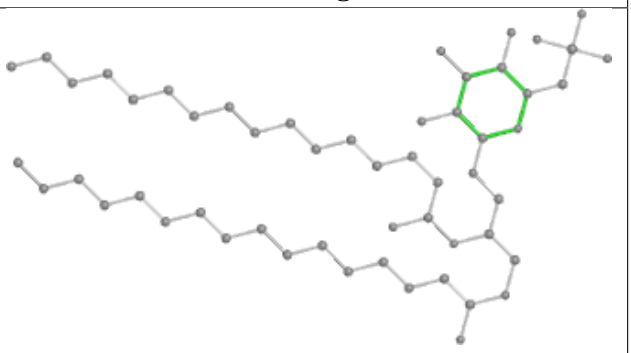
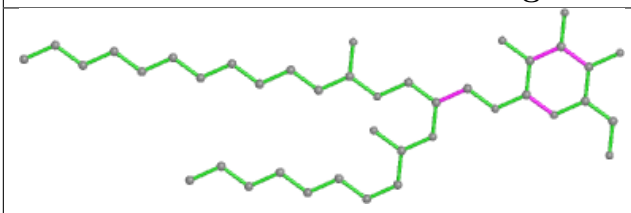


Rings

Ligand LMG d 403



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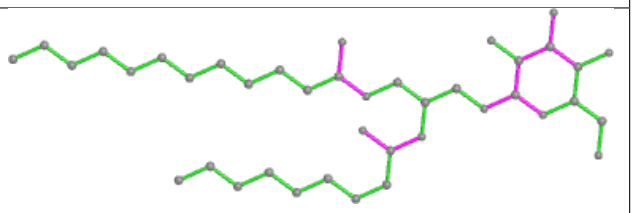

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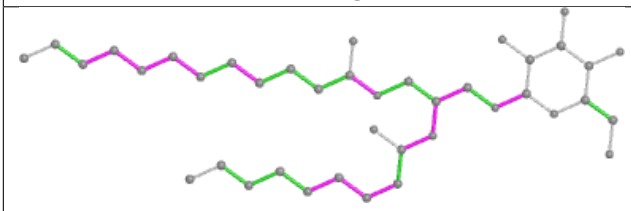
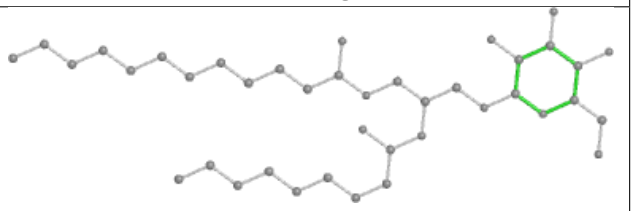
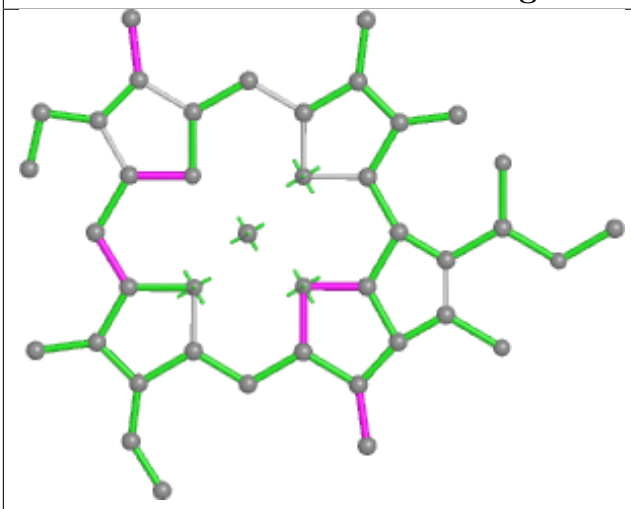


Torsions



Rings

Ligand CLA 16 311



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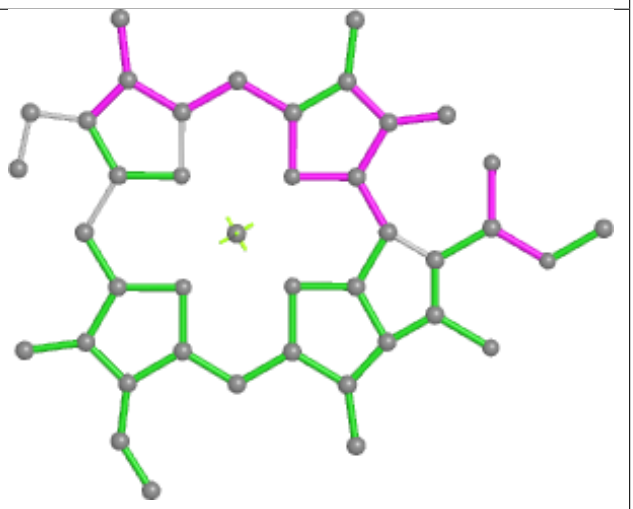

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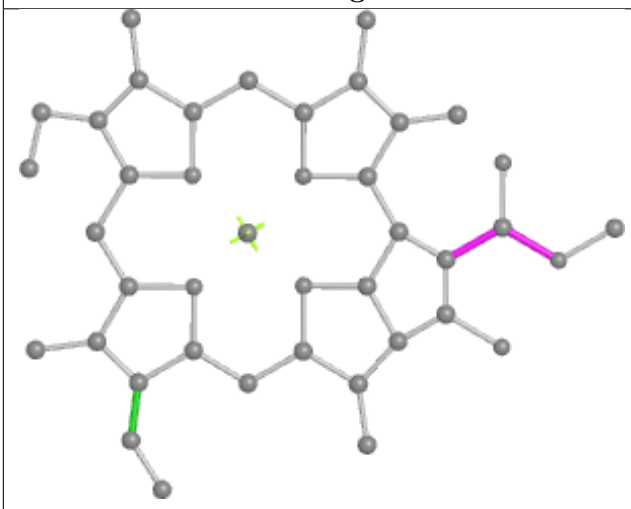

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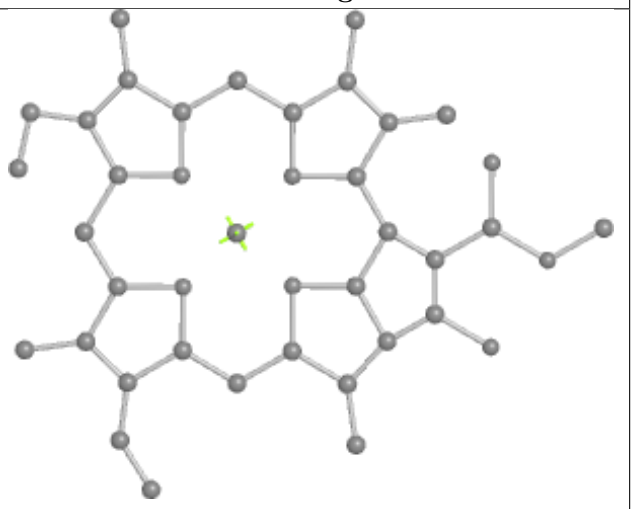
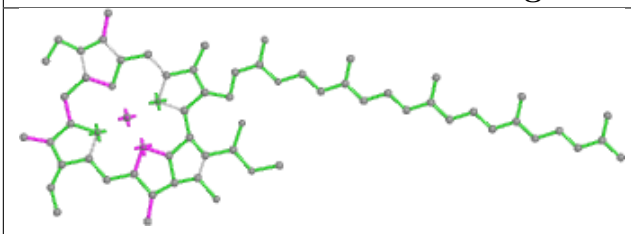


Rings

Ligand CLA B 614



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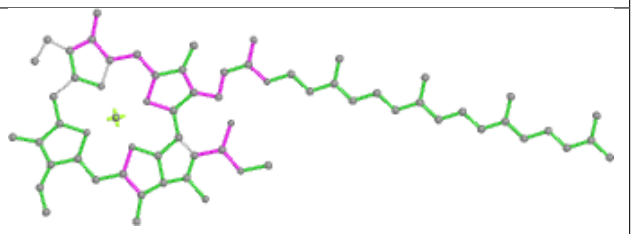
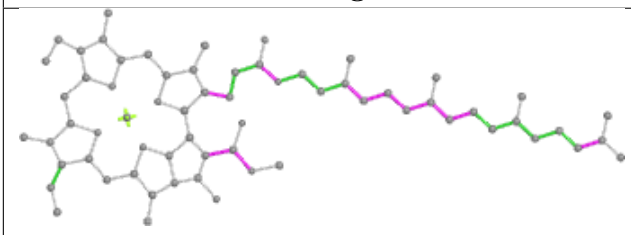


Bond angles



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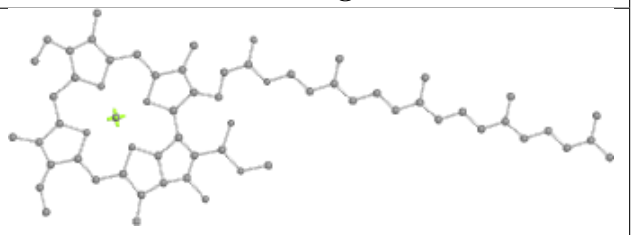
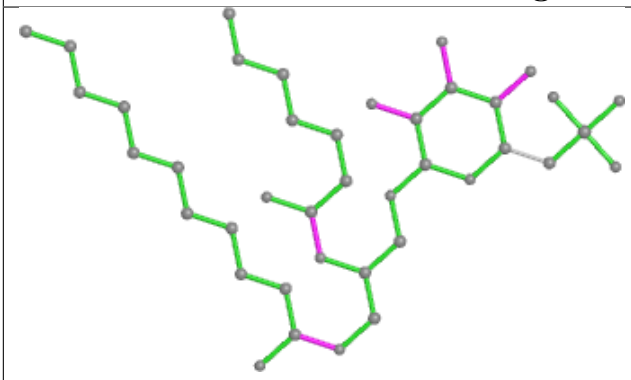


Rings

Ligand SQD i 101



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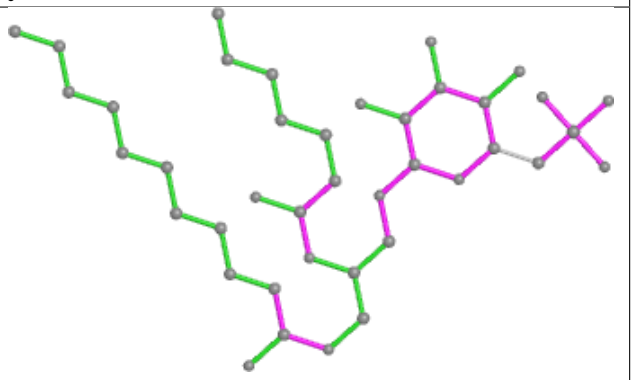
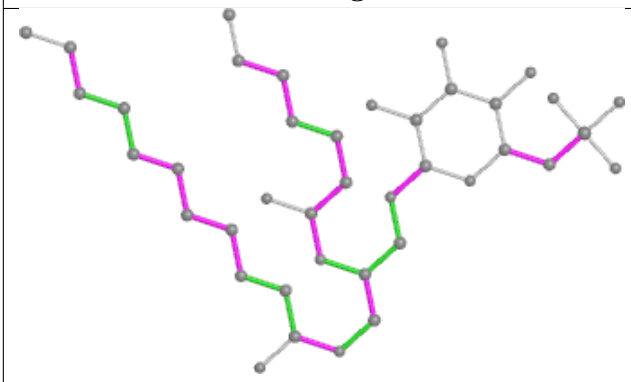


Bond angles



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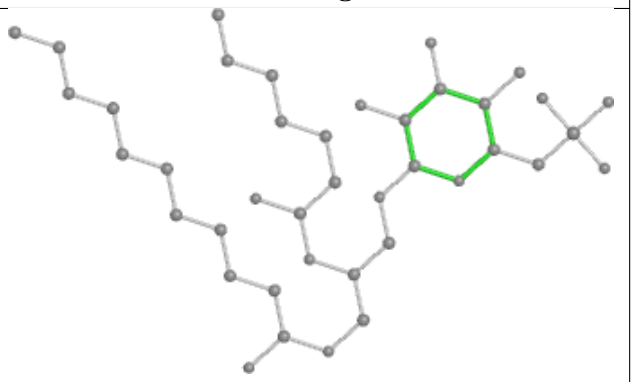
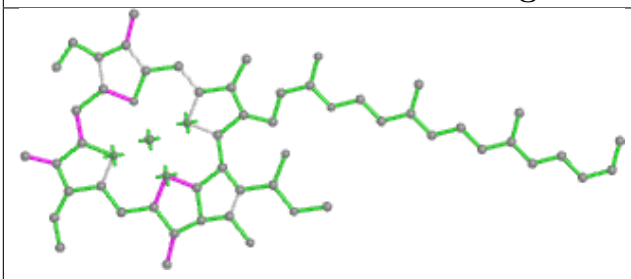


Rings

Ligand CLA 10 309



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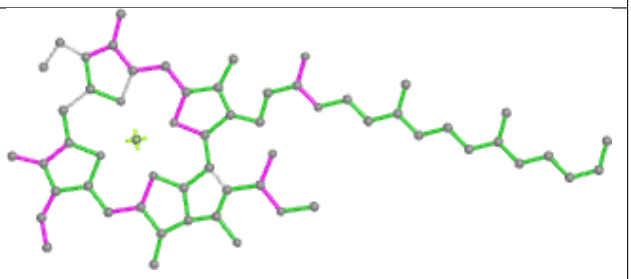
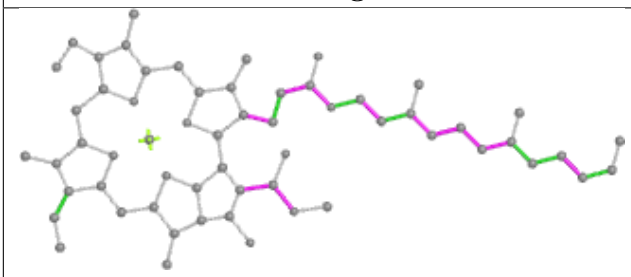


Bond angles



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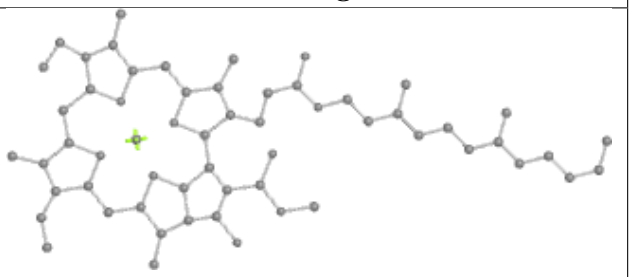
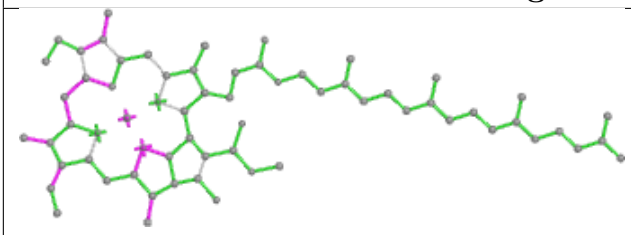
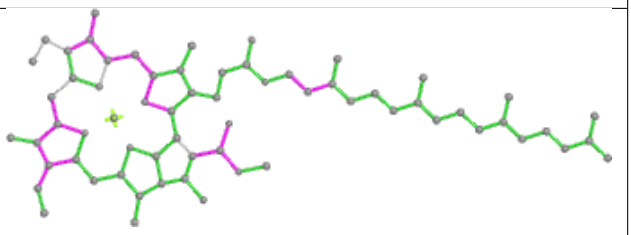


Rings

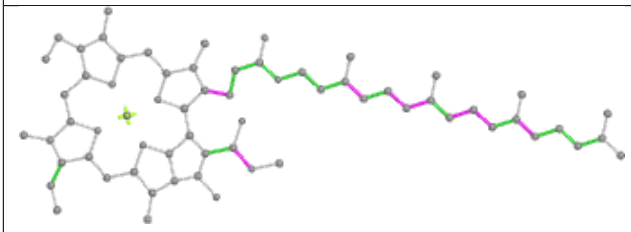
Ligand CLA b 612



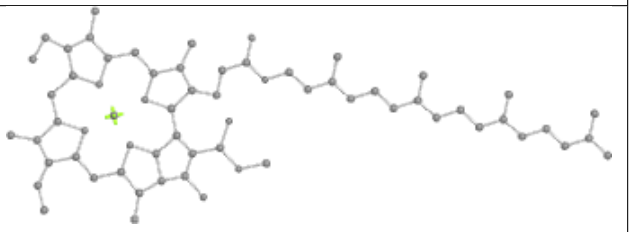
Bond lengths



Bond angles

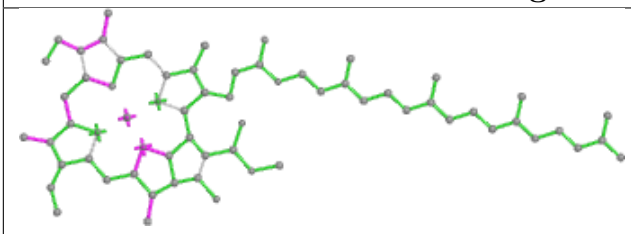


Torsions



Rings

Ligand CLA c 508



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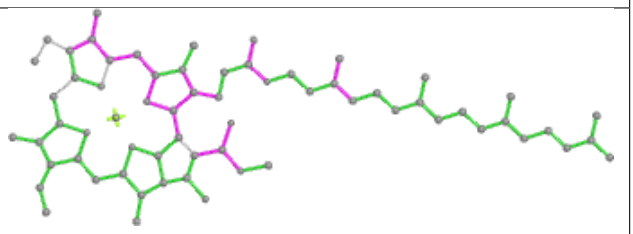

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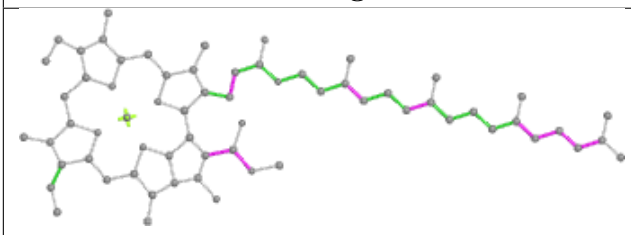
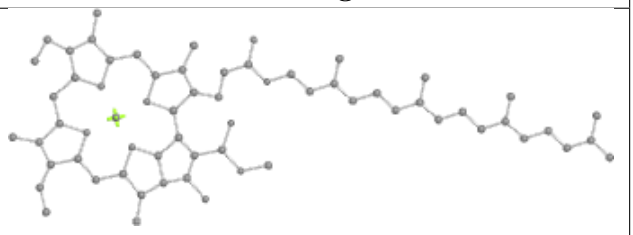
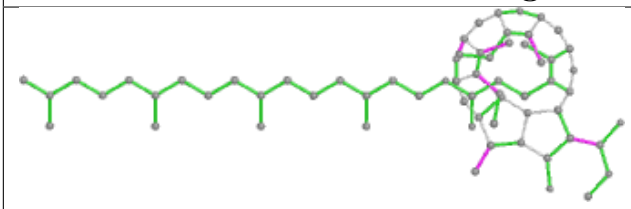


Torsions



Rings

Ligand PHO A 405



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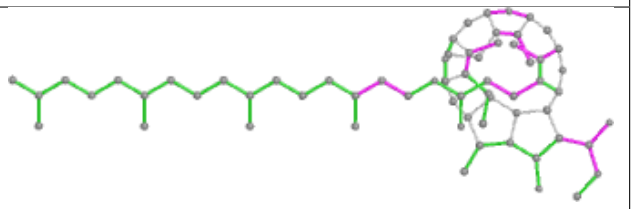

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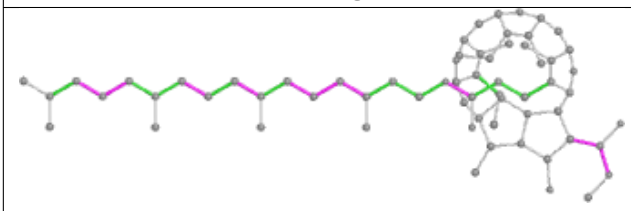

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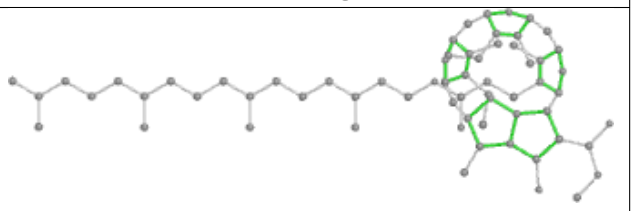
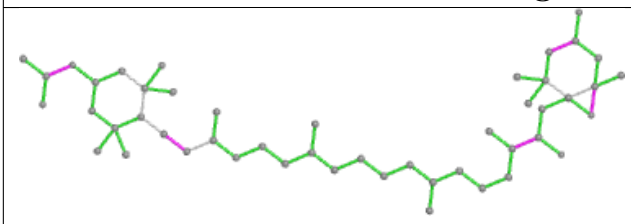


Rings

Ligand A86 2 303



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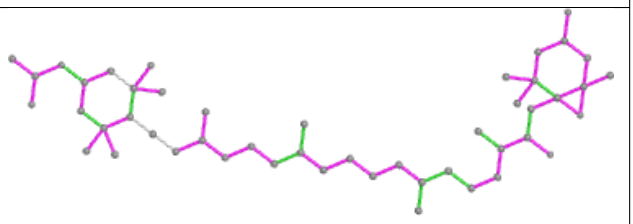

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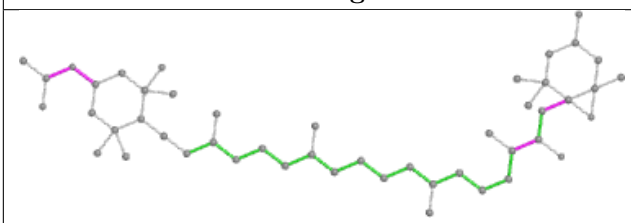

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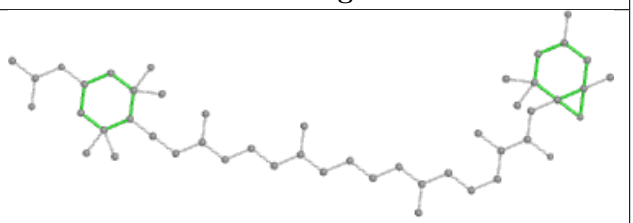
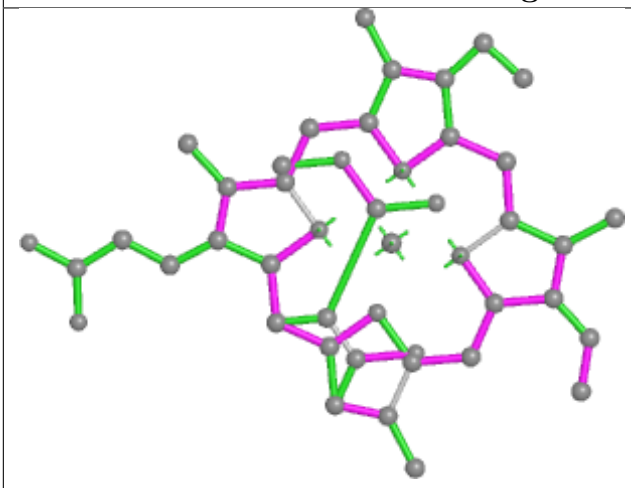


Rings

Ligand KC2 16 310



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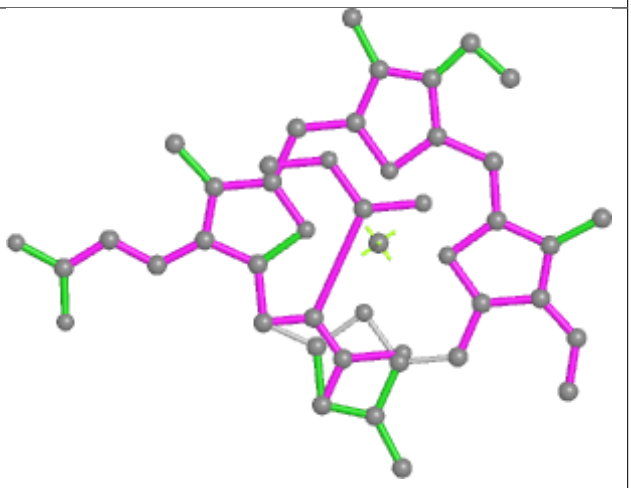

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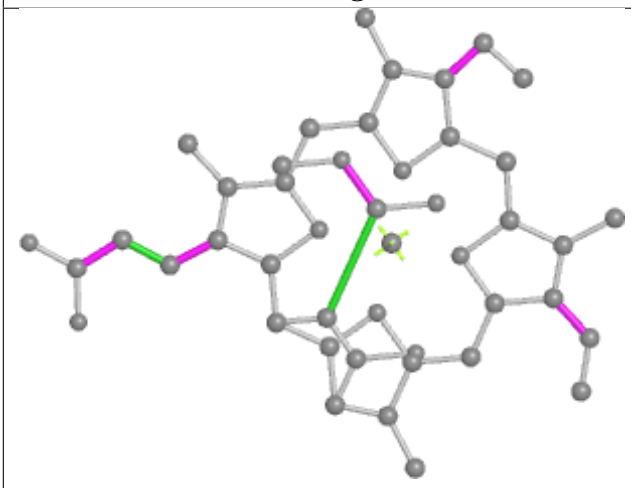

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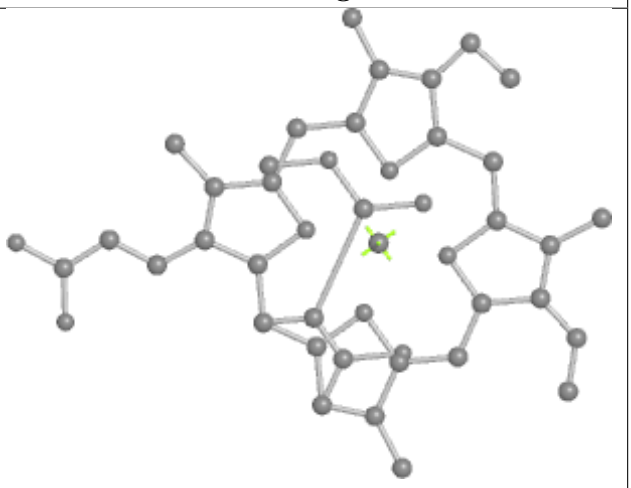
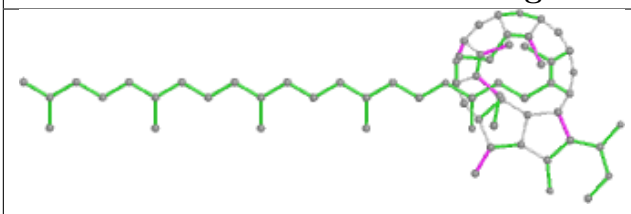


Rings

Ligand PHO d 402



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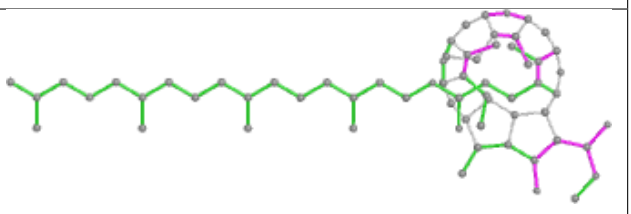

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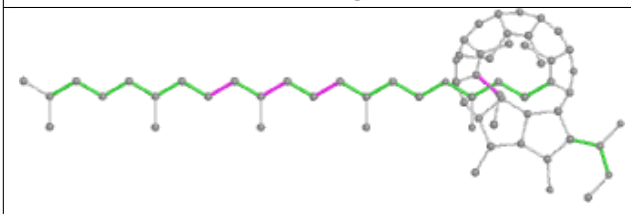

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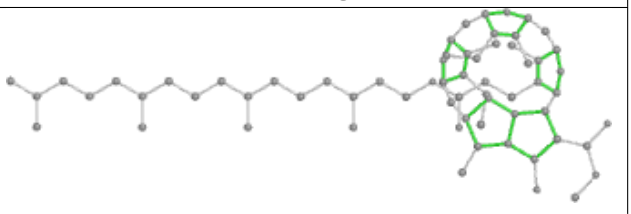
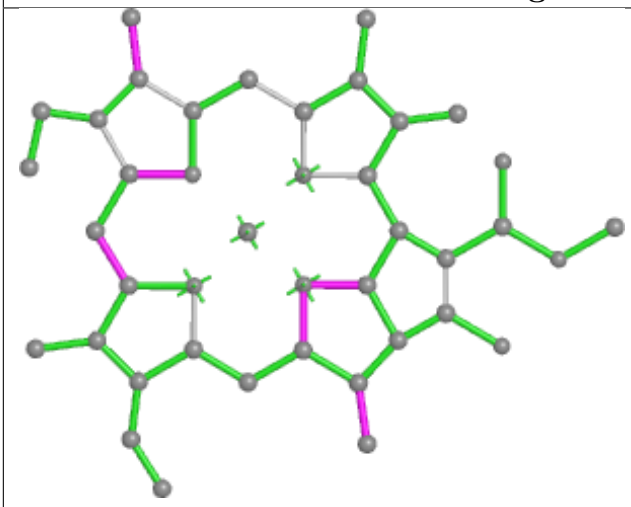


Rings

Ligand CLA 7 315



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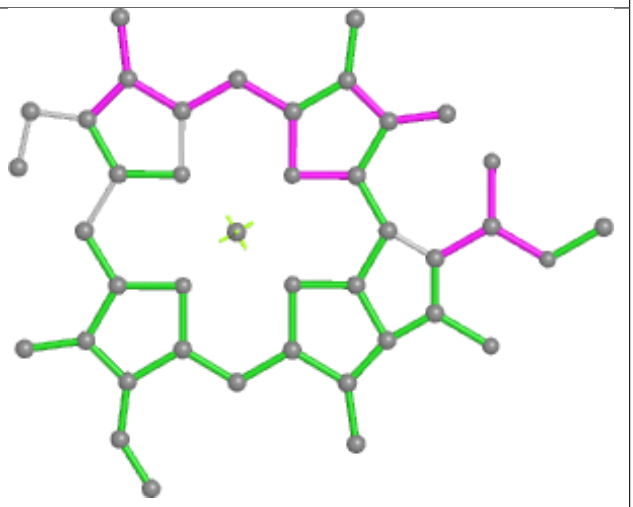

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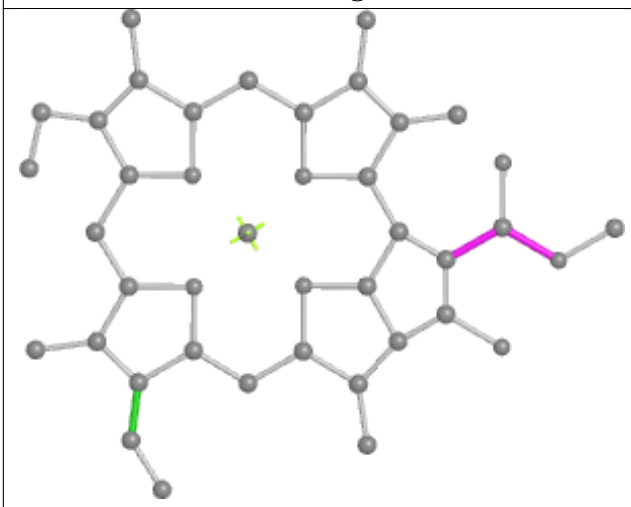

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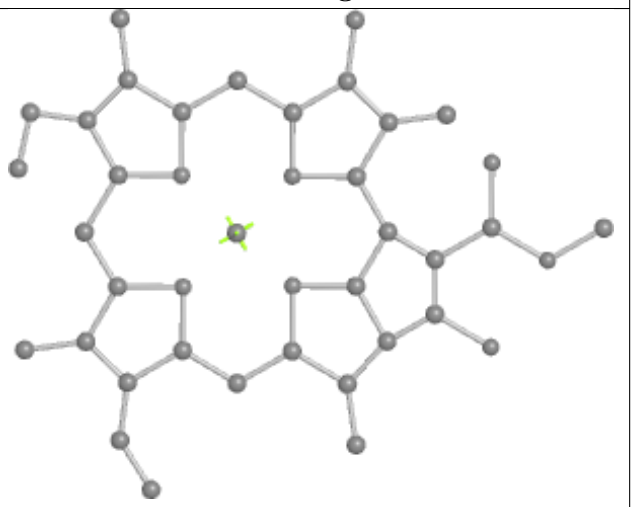
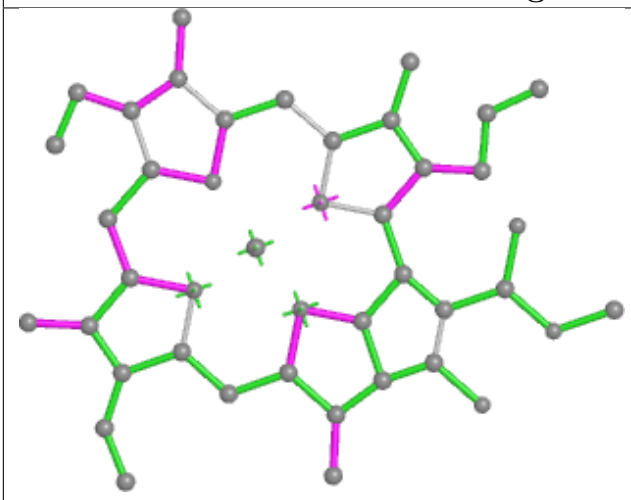


Rings

Ligand CLA p 606



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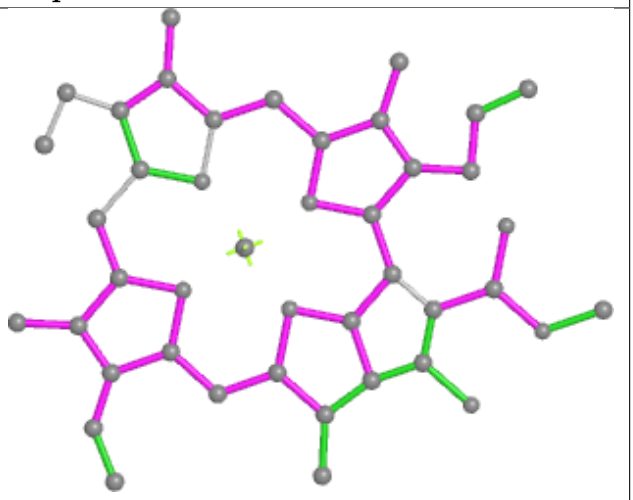

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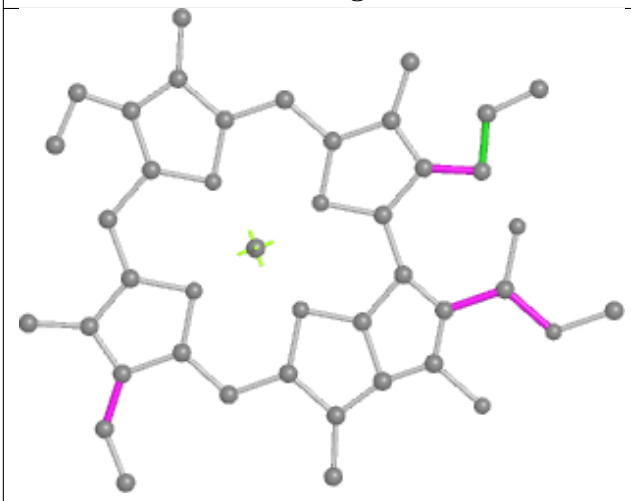

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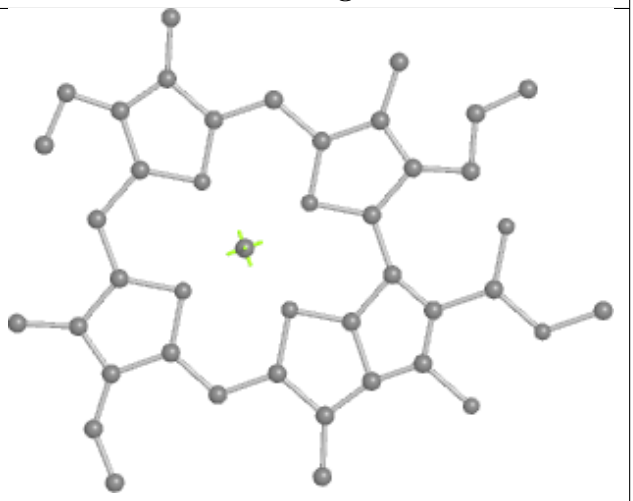
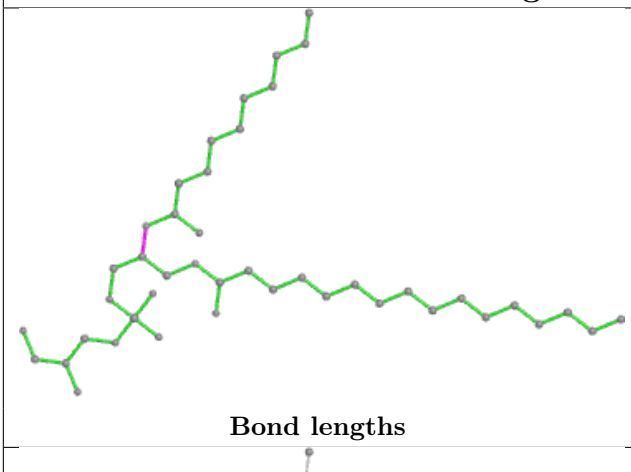


Rings

Ligand LHG B 622



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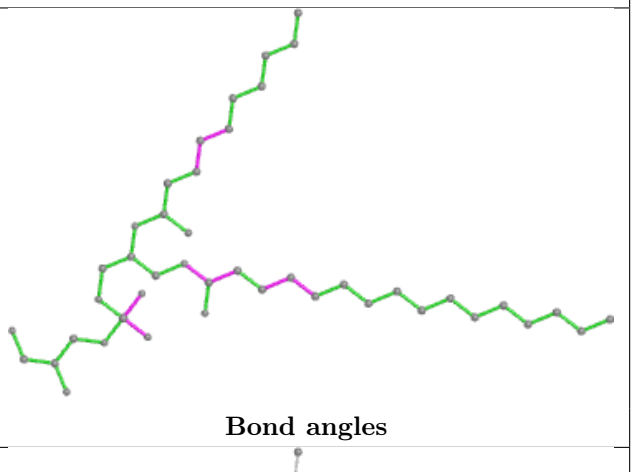

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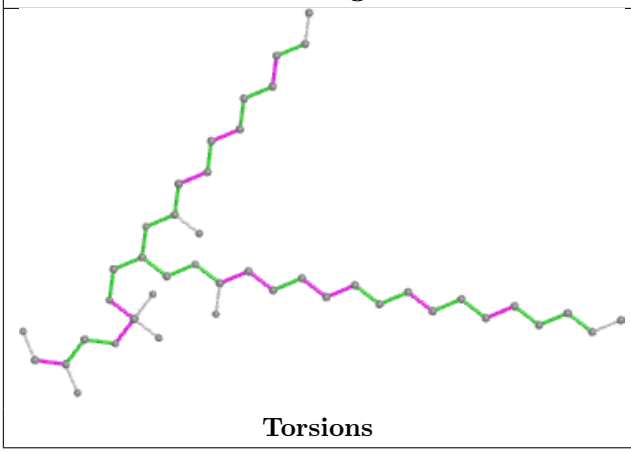

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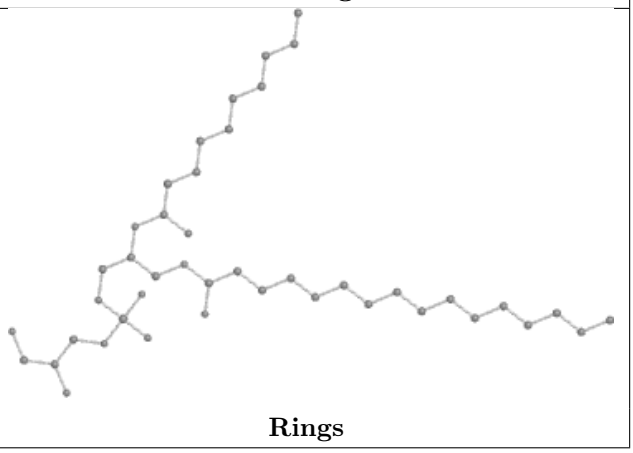
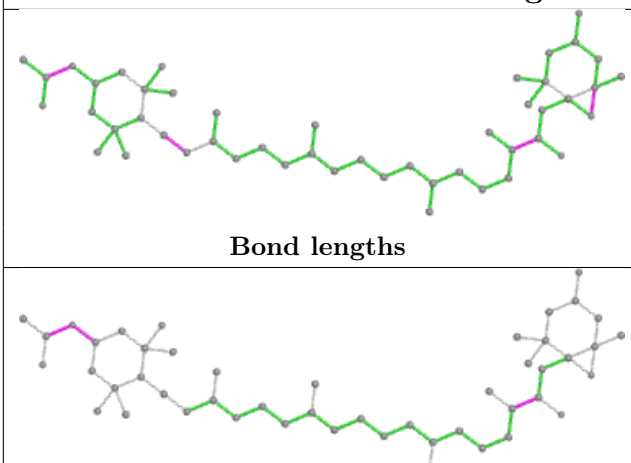


Rings

Ligand A86 10 306



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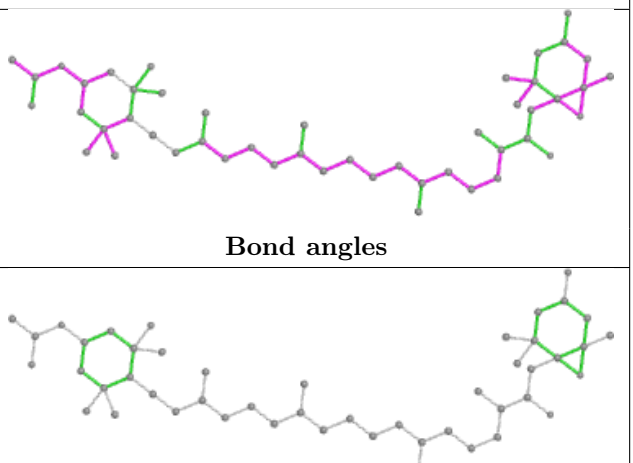

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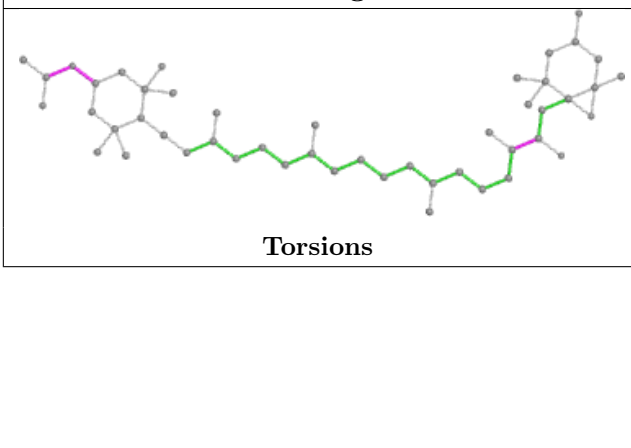

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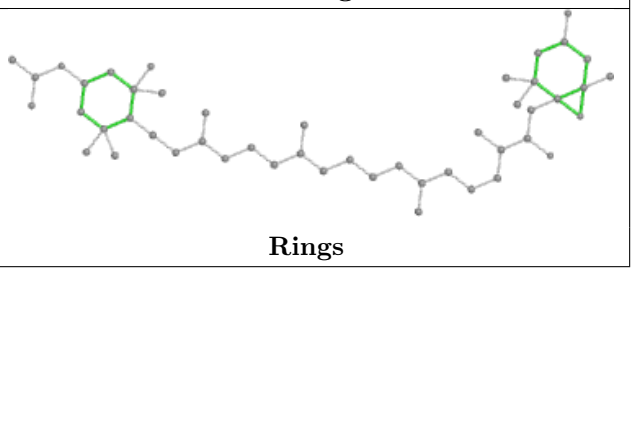
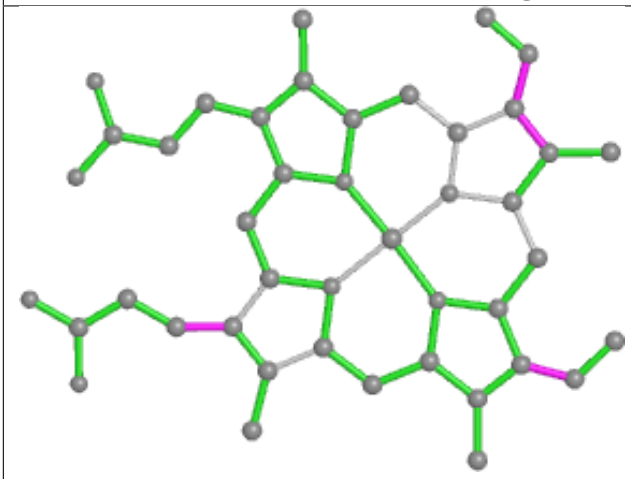


Rings

Ligand HEM V 201



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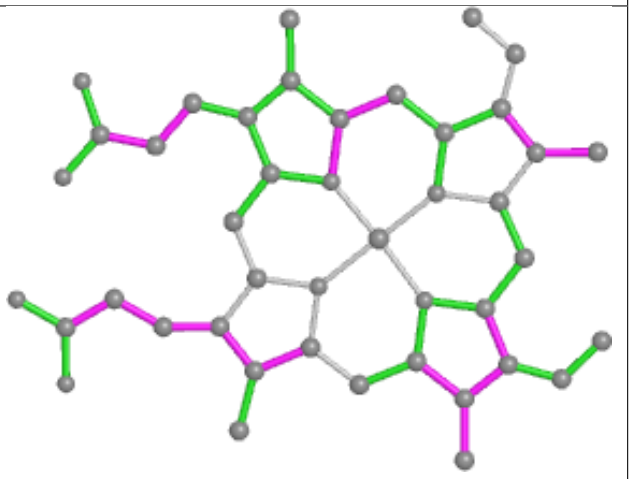

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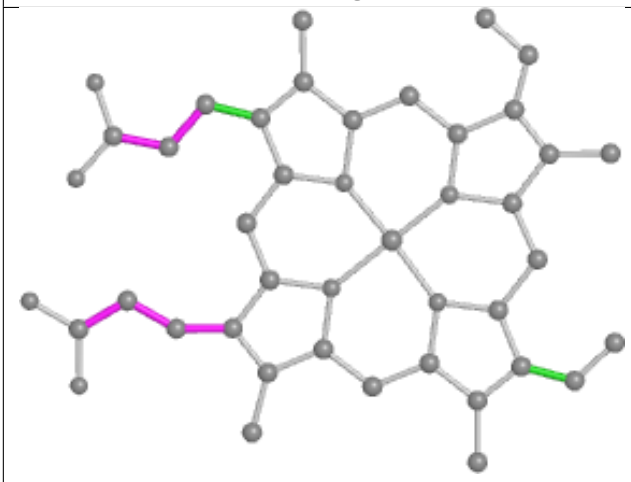

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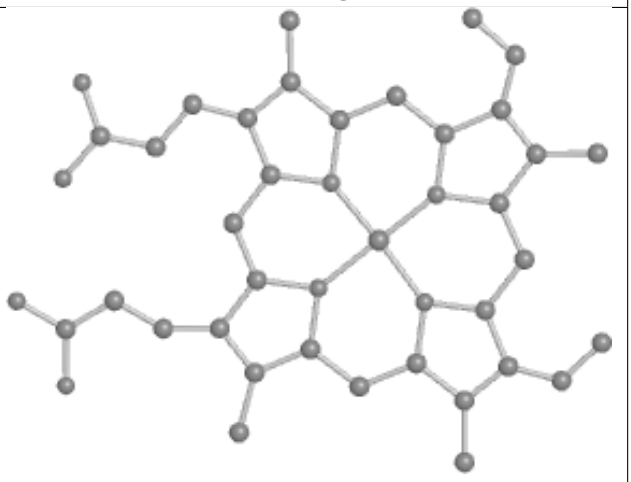
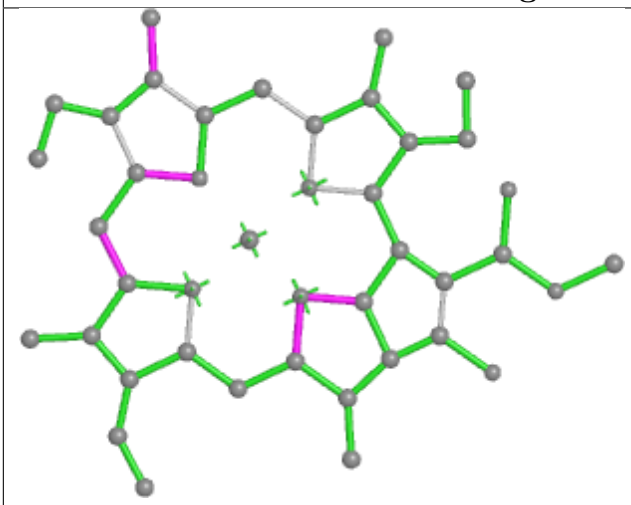


Rings

Ligand CLA 13 307



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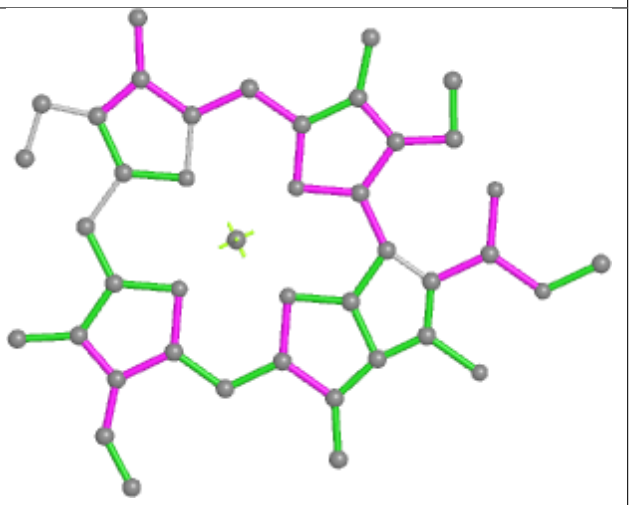

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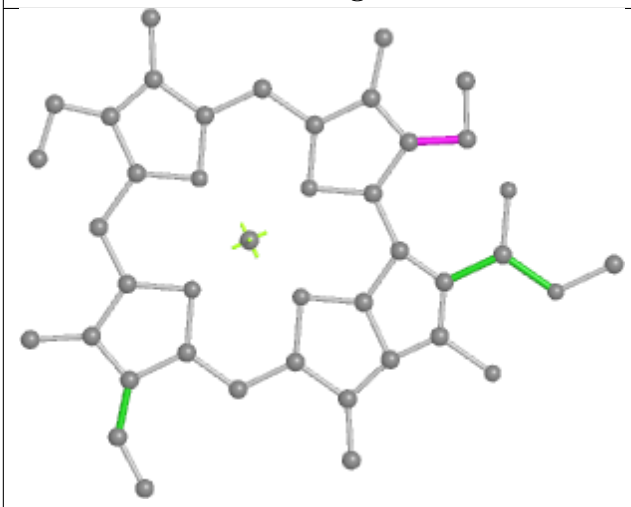

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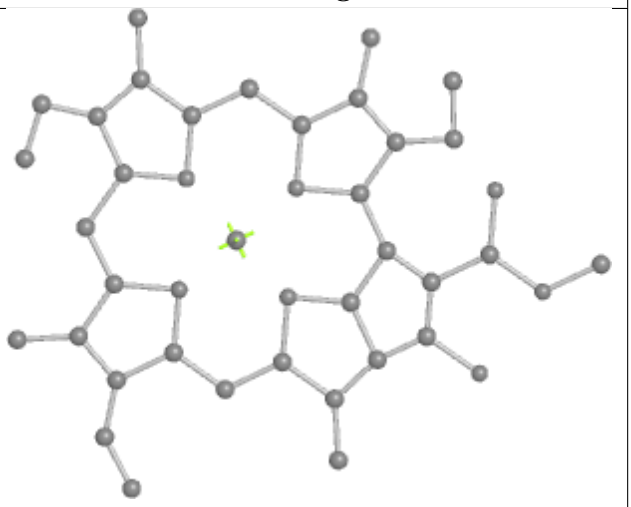
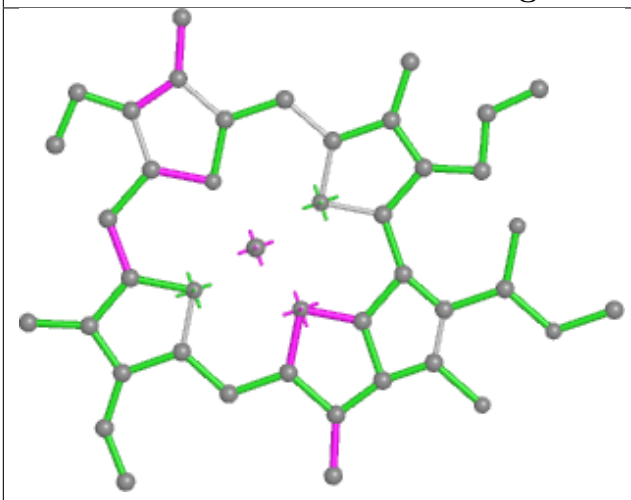


Rings

Ligand CLA 18 314



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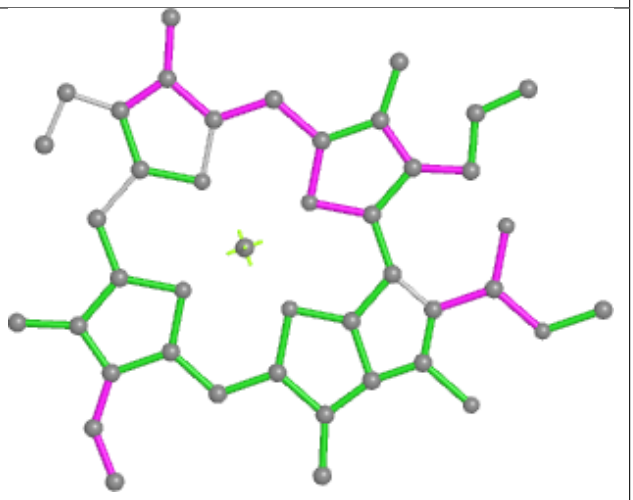

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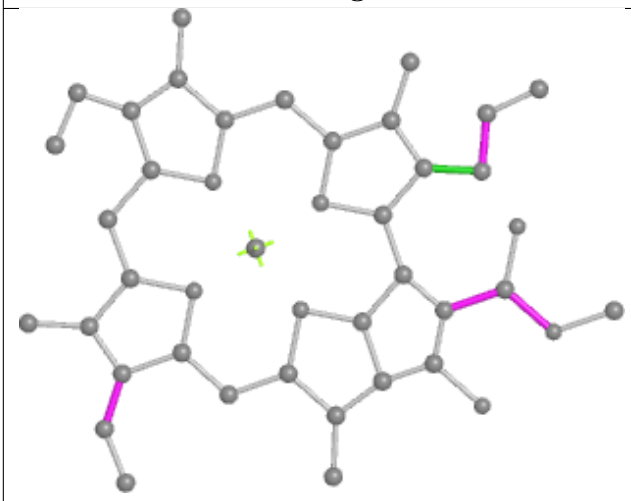

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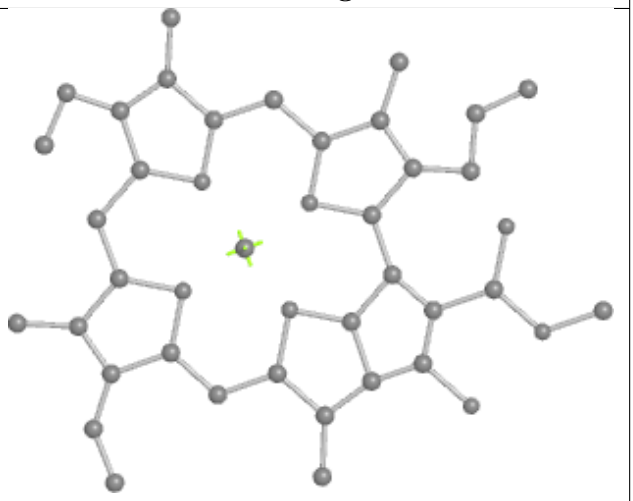
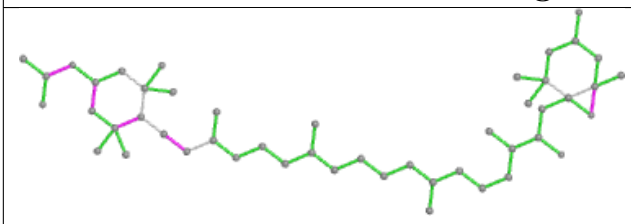


Rings

Ligand A86 7 305



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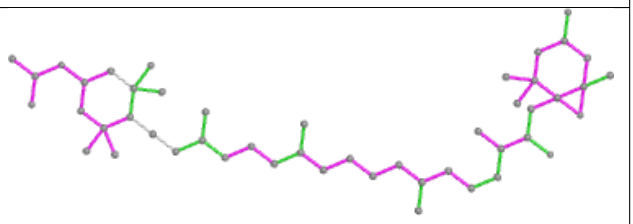

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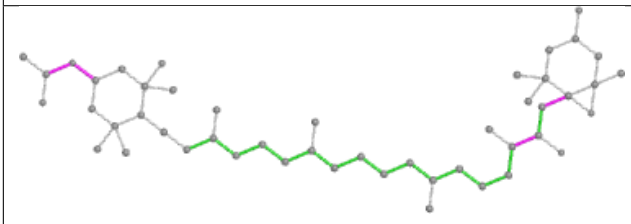

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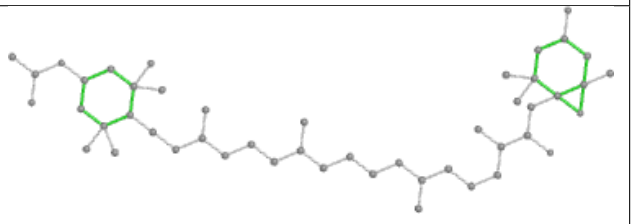
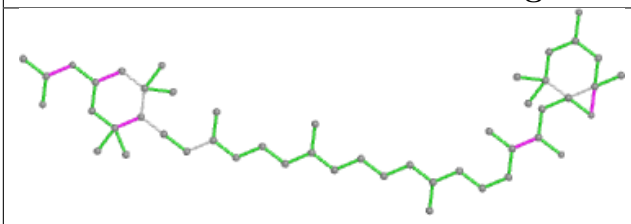


Rings

Ligand A86 14 304



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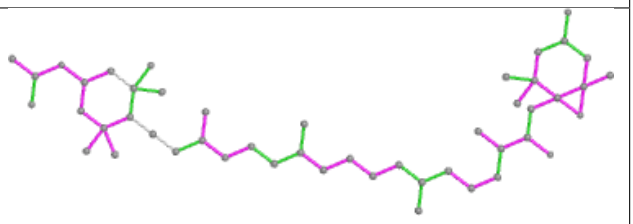
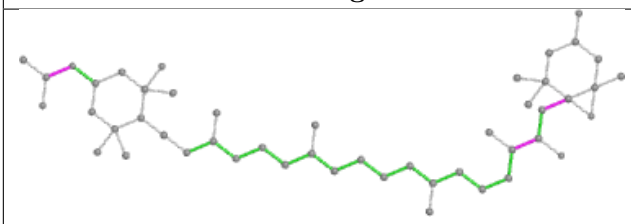


Bond angles



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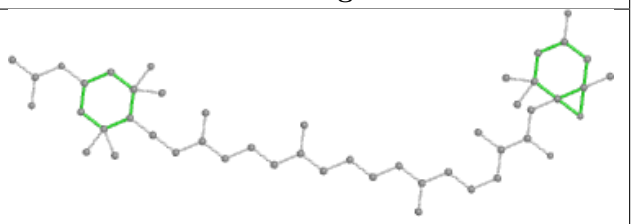
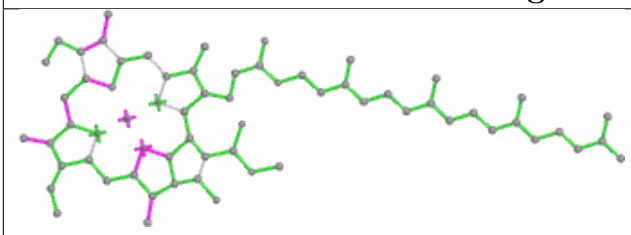


Rings

Ligand CLA b 609



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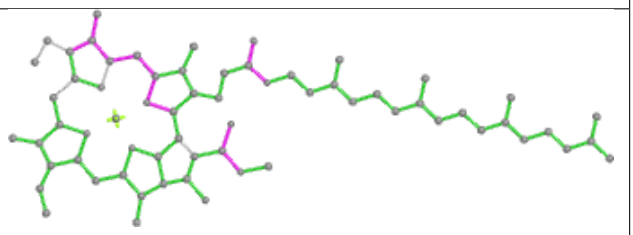

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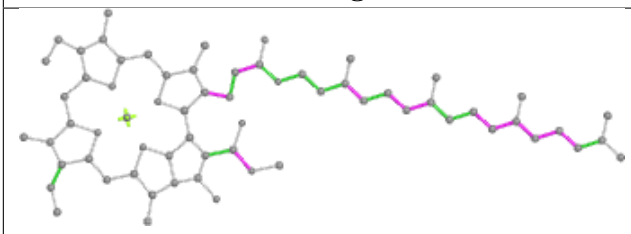

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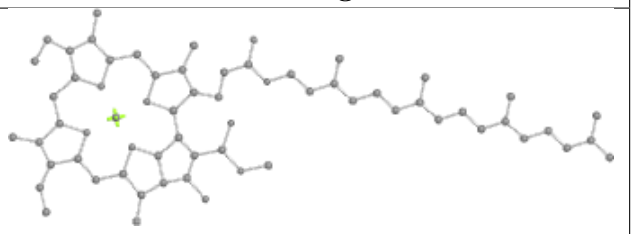
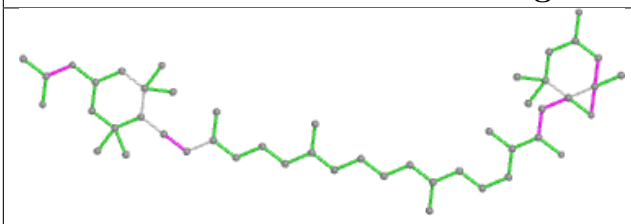


Rings

Ligand A86 9 305



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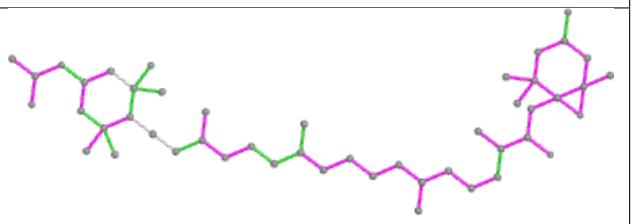

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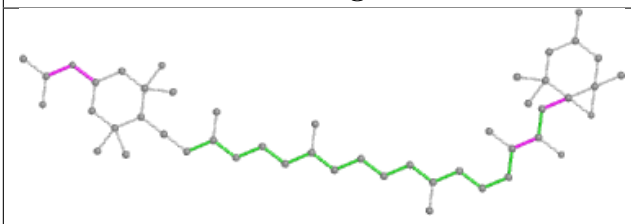

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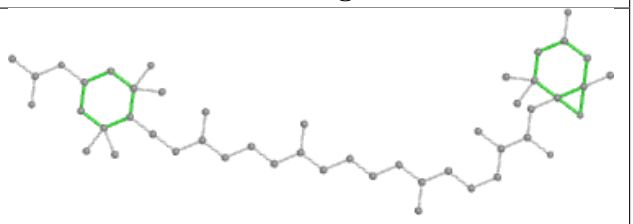
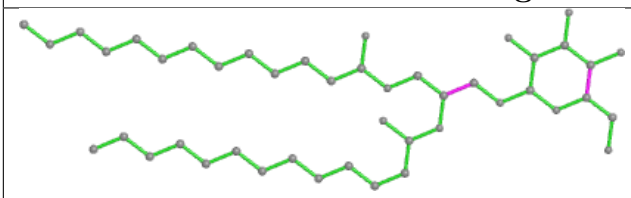


Rings

Ligand LMG 11 317



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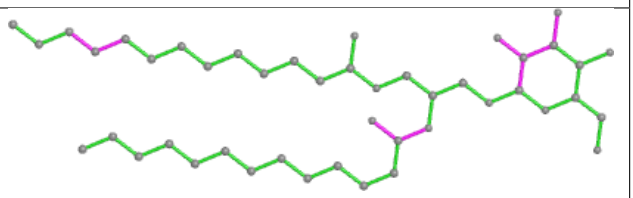

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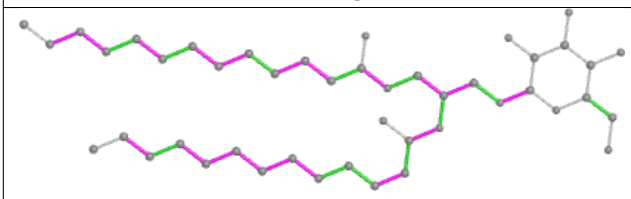

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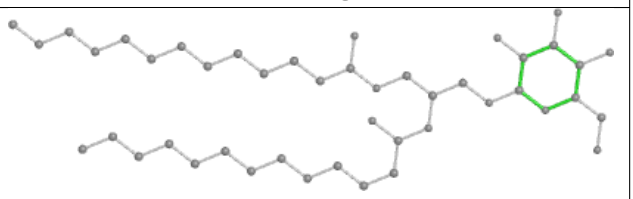
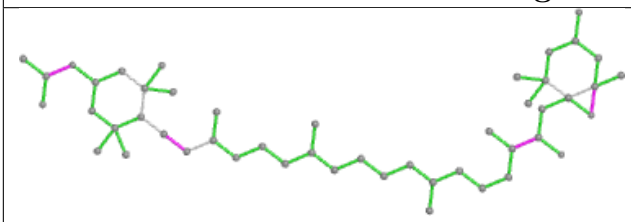


Rings

Ligand A86 9 302



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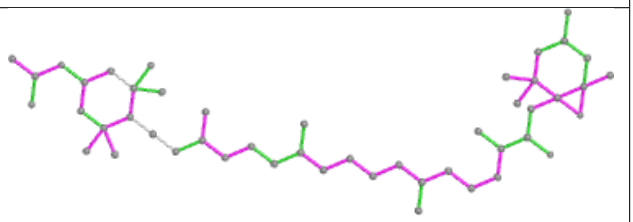

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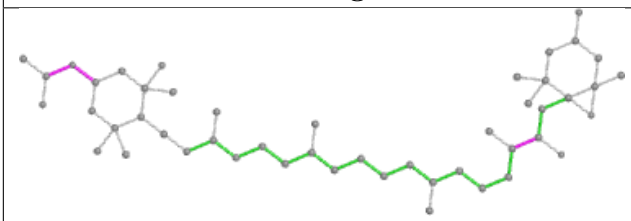

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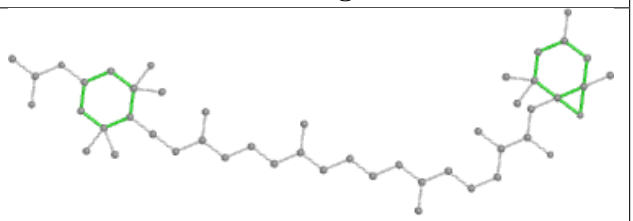
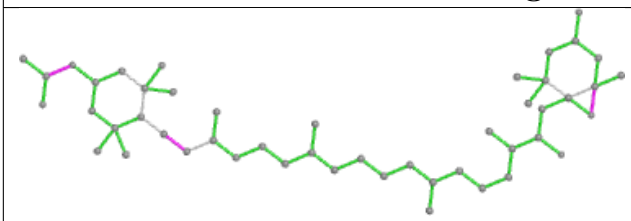


Rings

Ligand A86 11 320



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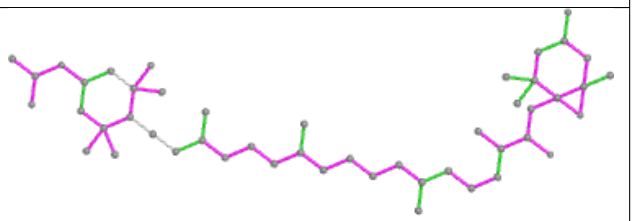

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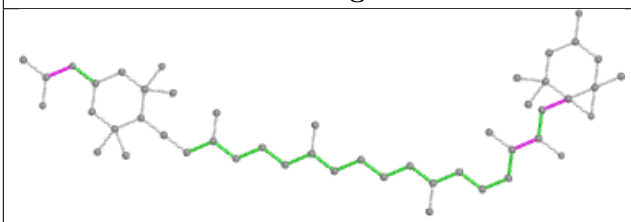

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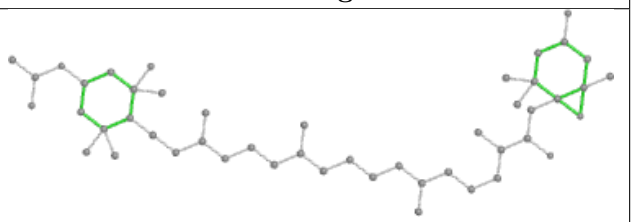

Rings

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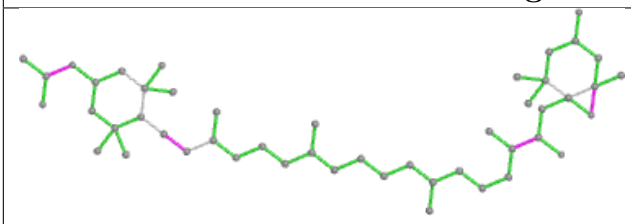

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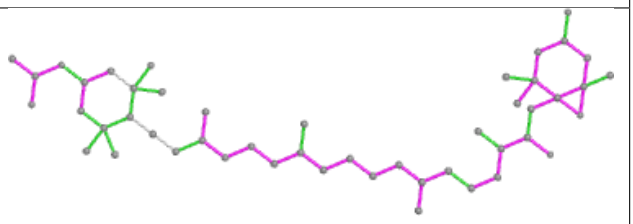

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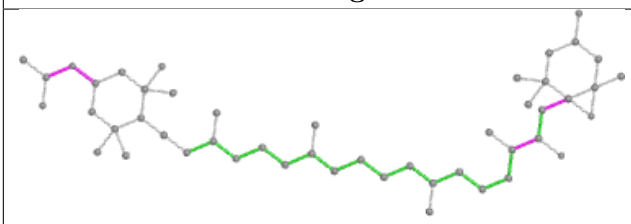

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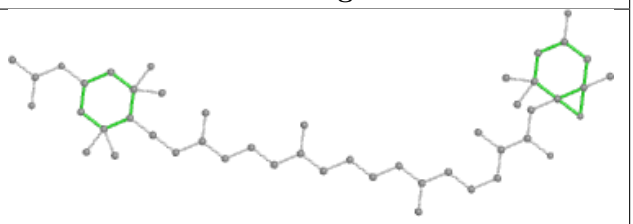

Rings

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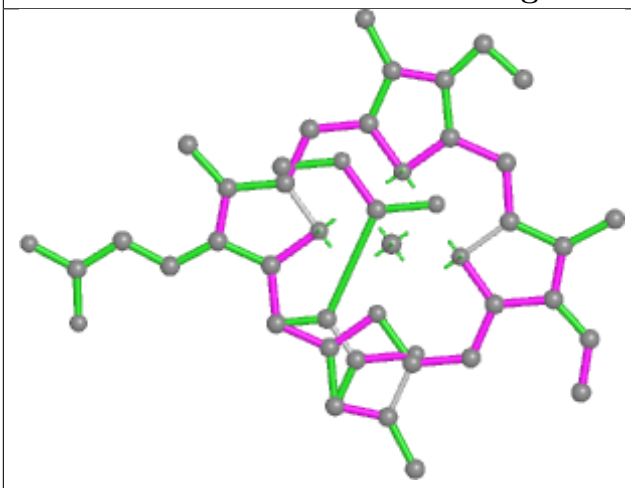

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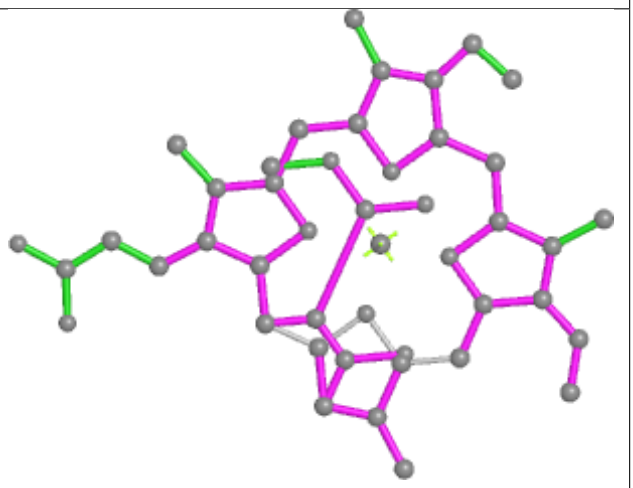

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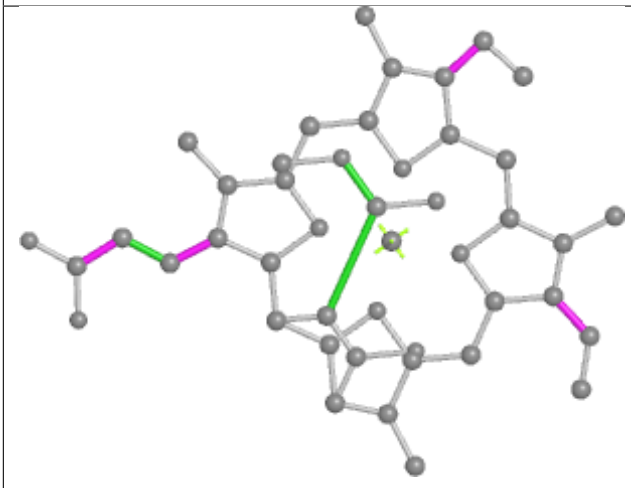

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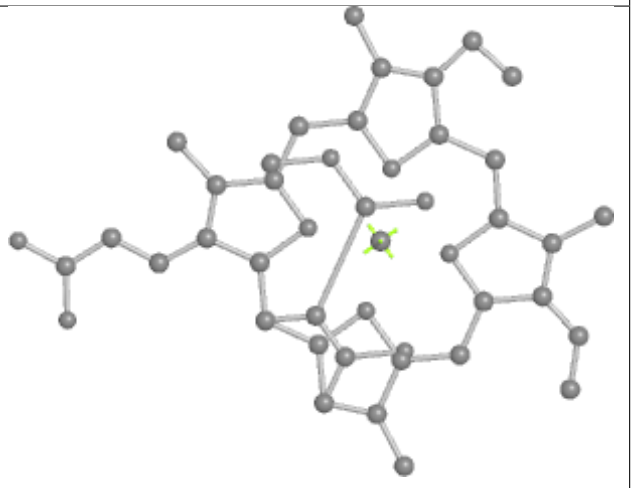
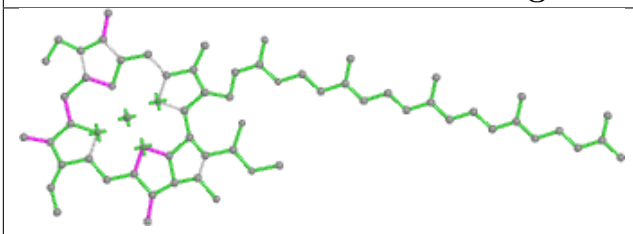


Rings

Ligand CLA 9 308



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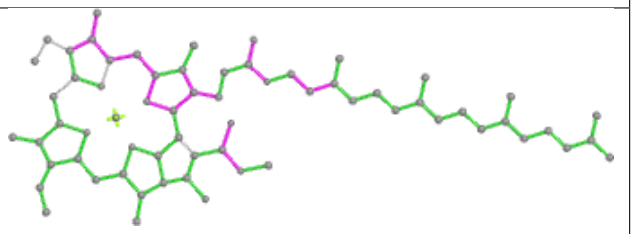

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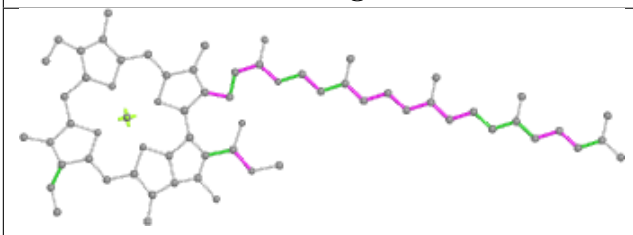

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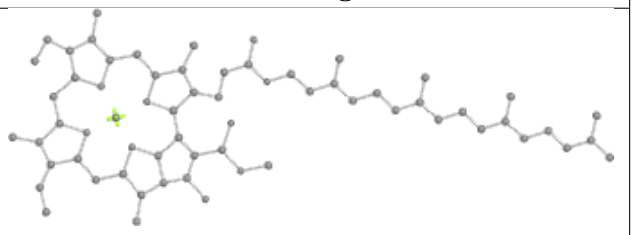
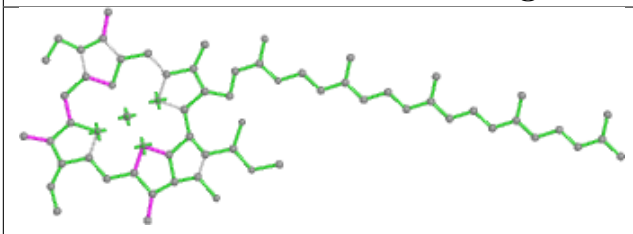


Rings

Ligand CLA 14 309



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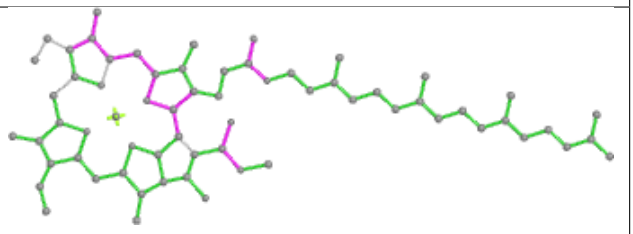

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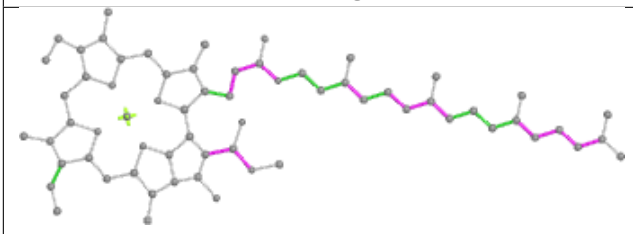

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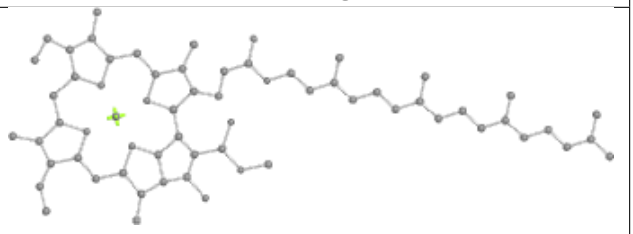

Rings

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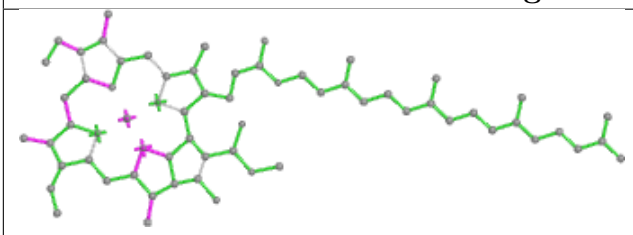

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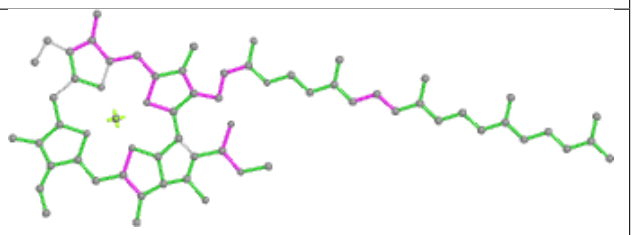

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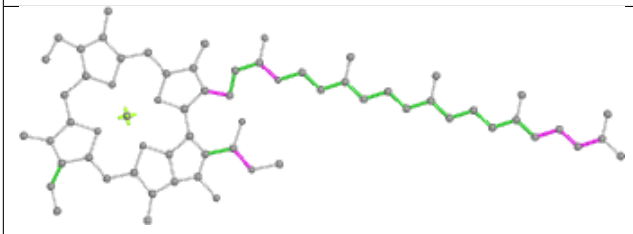

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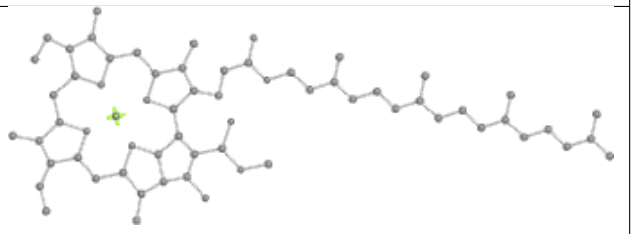
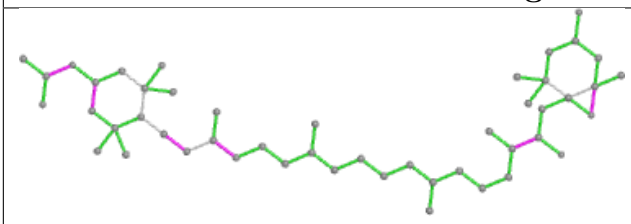


Rings

Ligand A86 16 303



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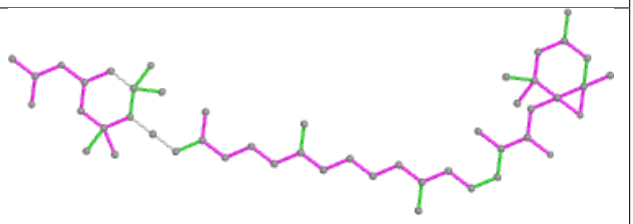

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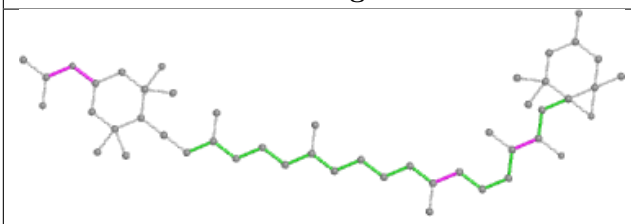

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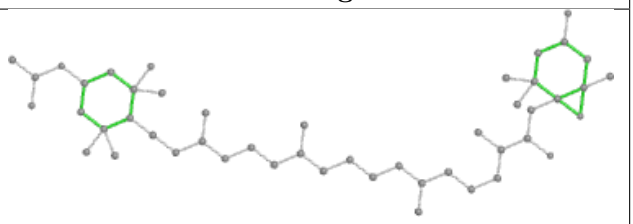
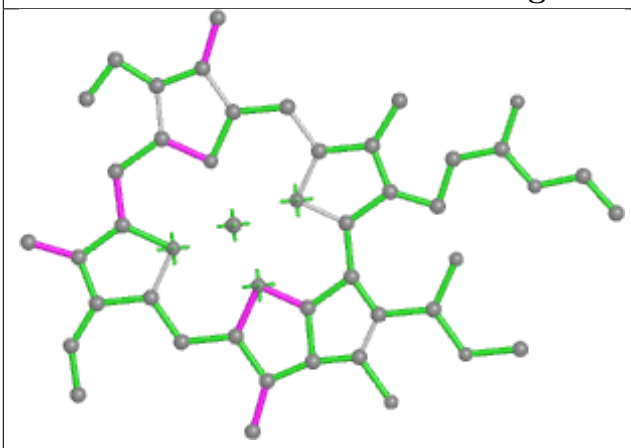


Rings

Ligand CLA 7 312



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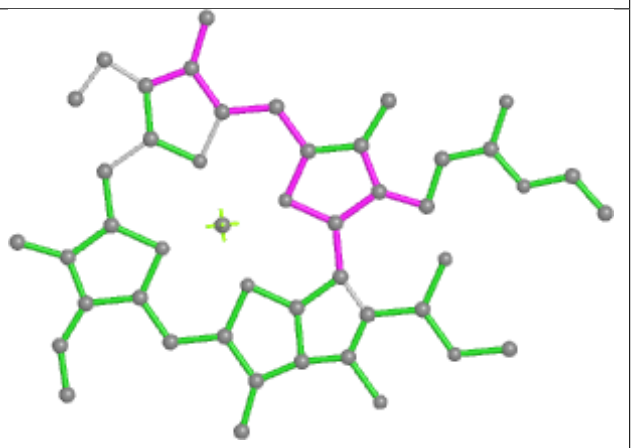

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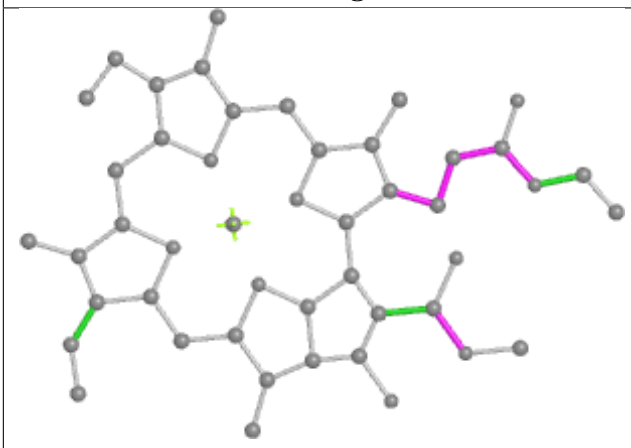

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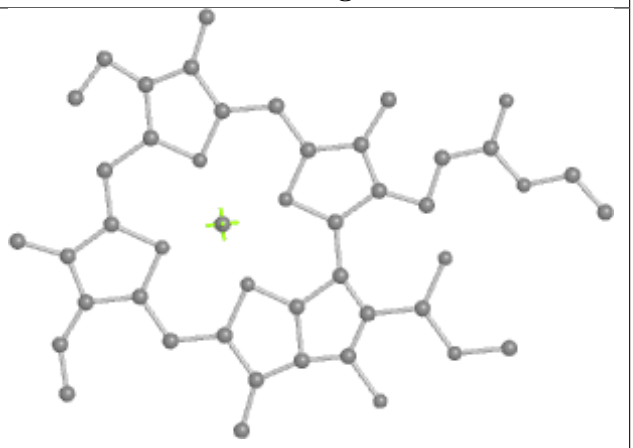
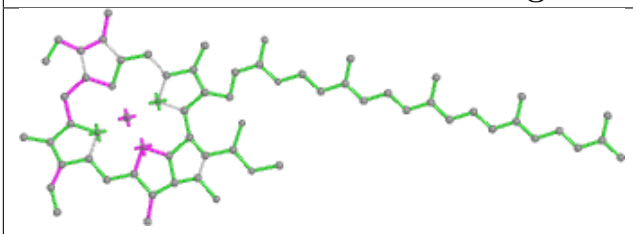


Rings

Ligand CLA d 401



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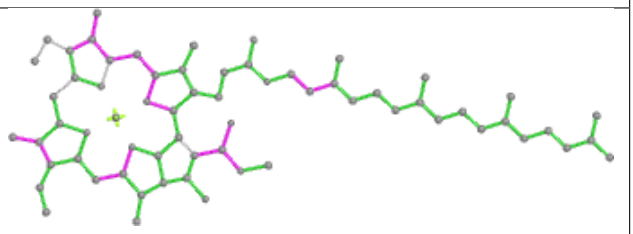

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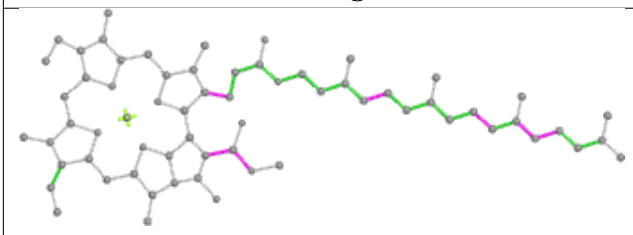

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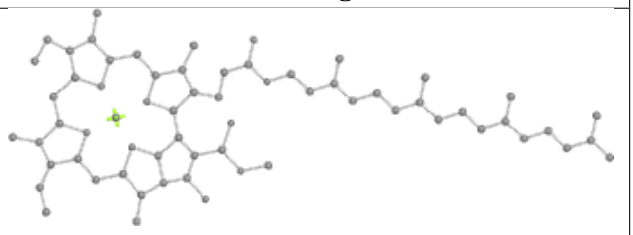
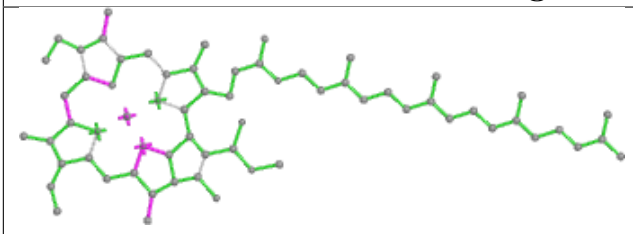


Rings

Ligand CLA 9 312



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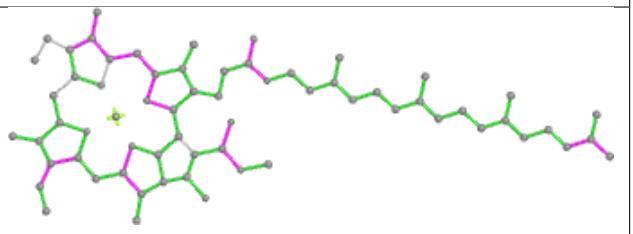
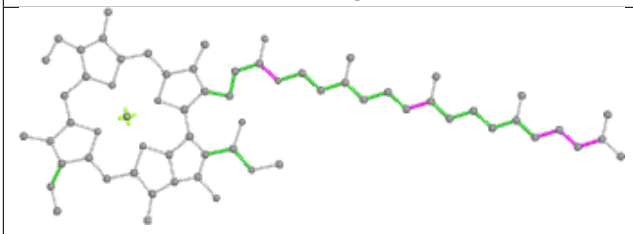


Bond angles



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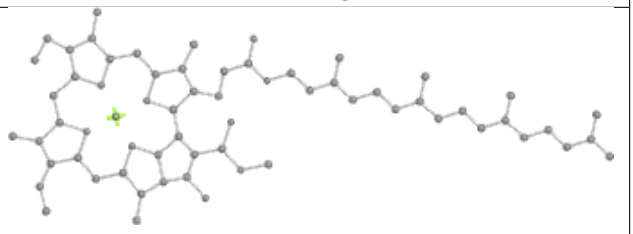
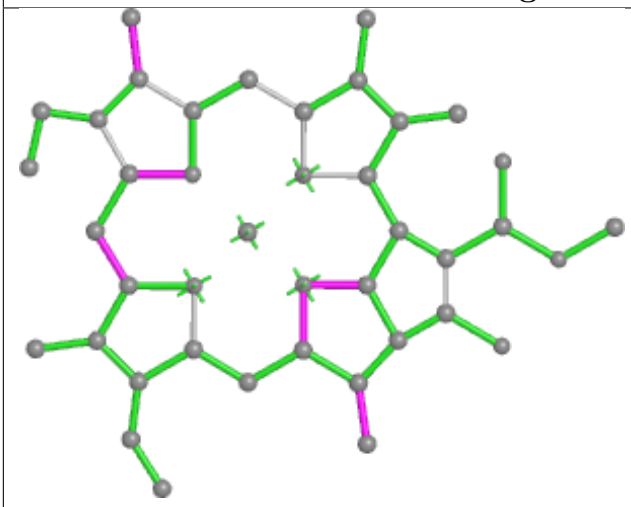


Rings

Ligand CLA 17 315



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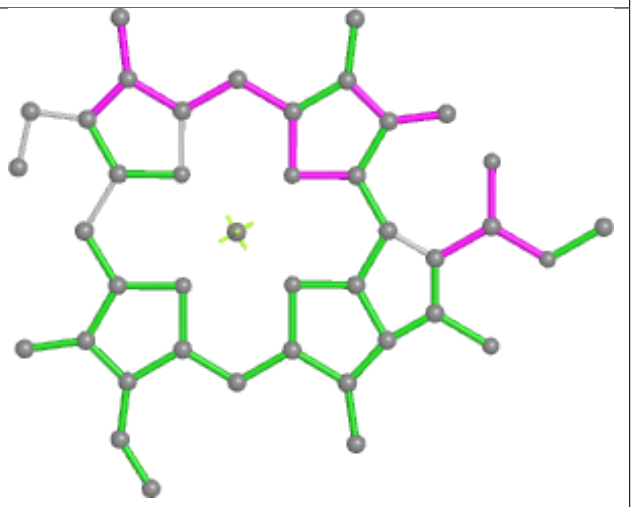

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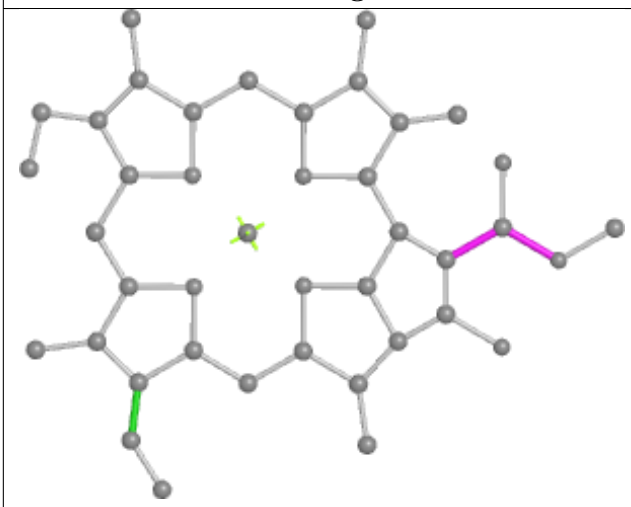
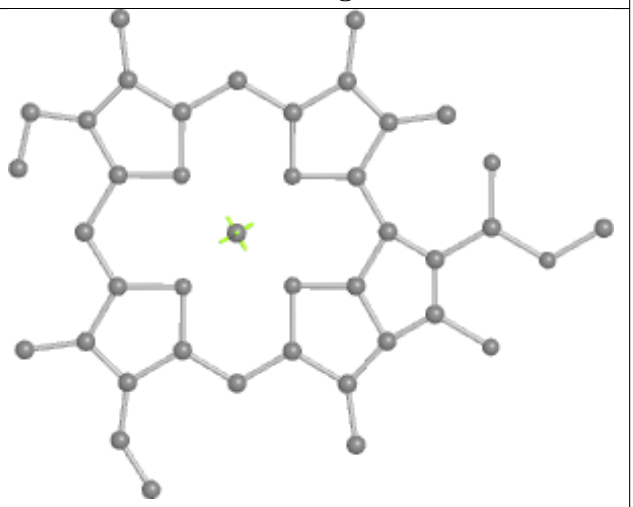
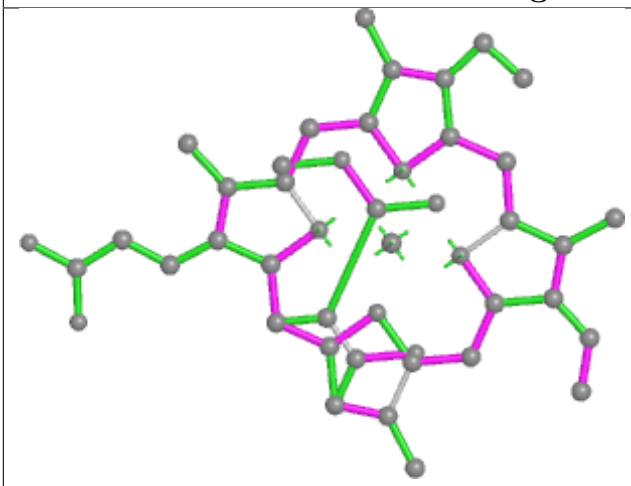


Torsions



Rings

Ligand KC2 4 310



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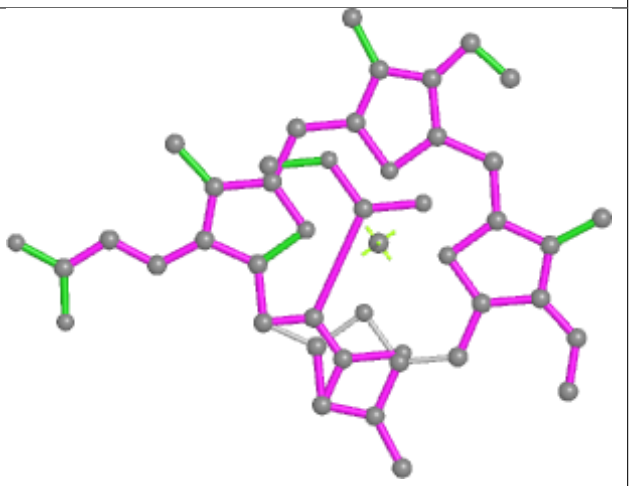

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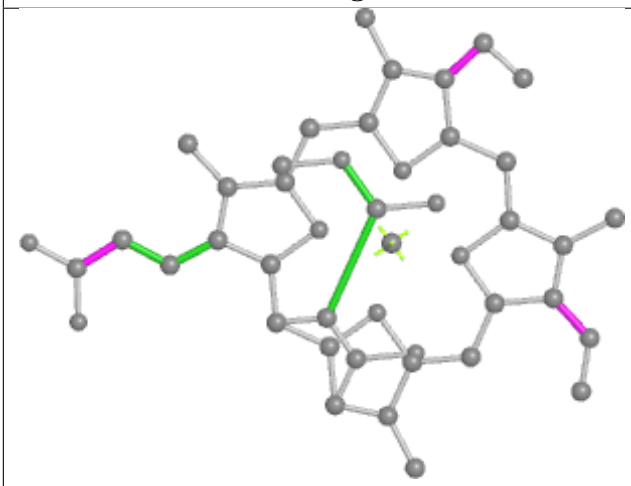

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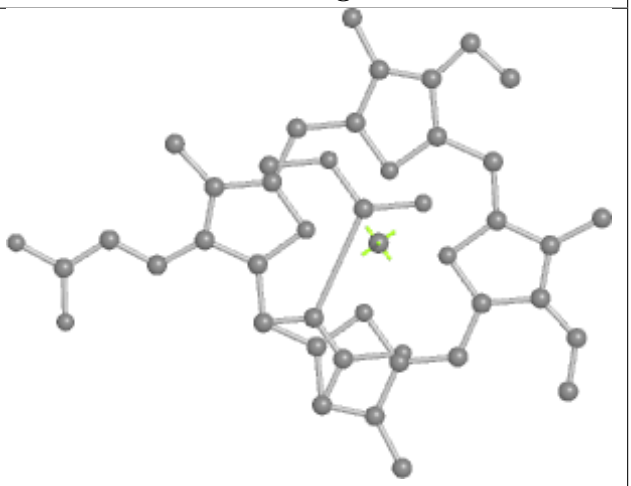
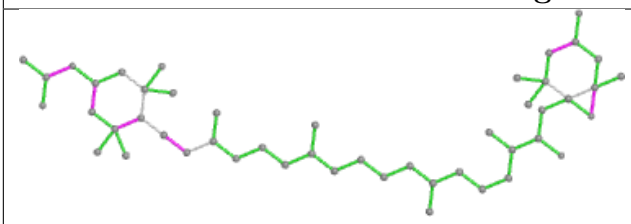


Rings

Ligand A86 8 305



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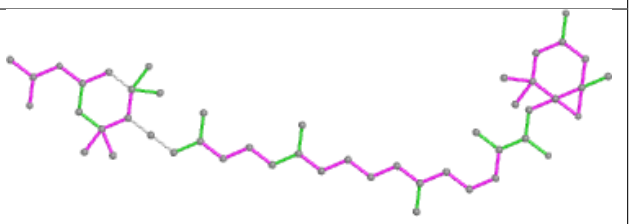

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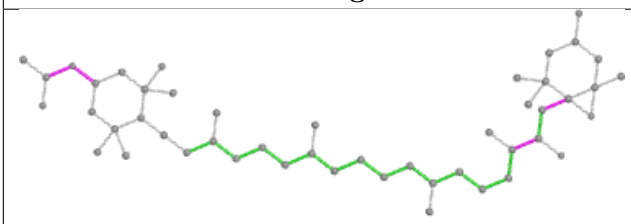

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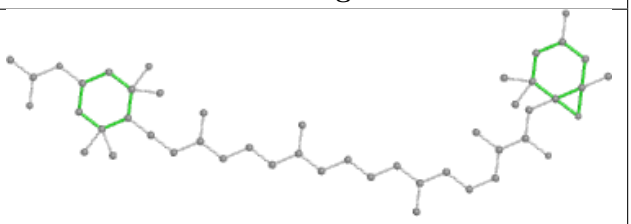
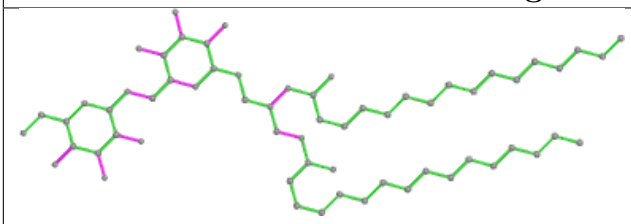


Rings

Ligand DGD c 520



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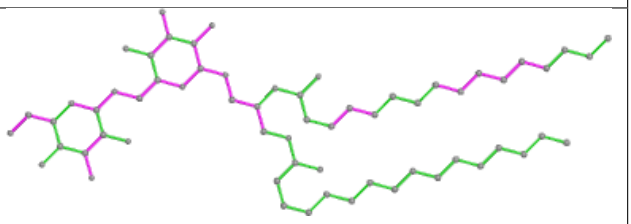

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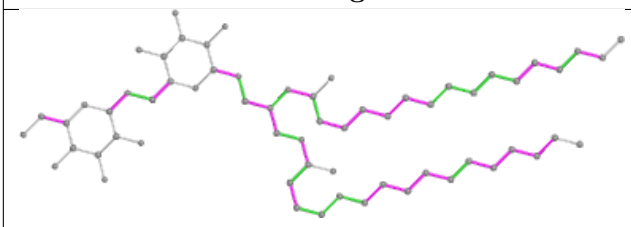

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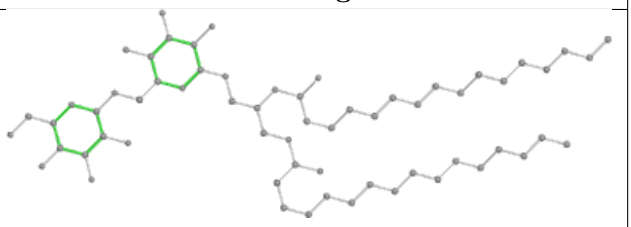
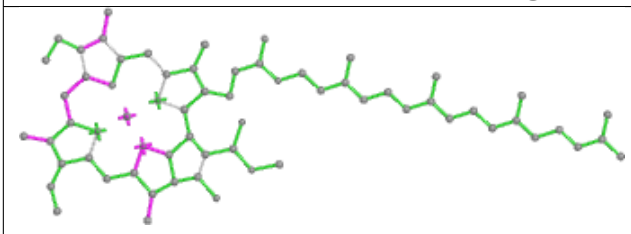


Rings

Ligand CLA B 616



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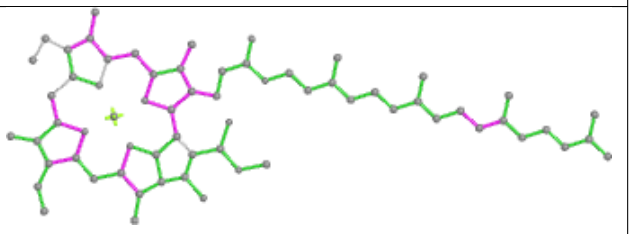

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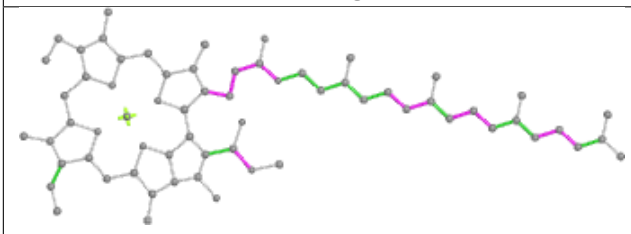

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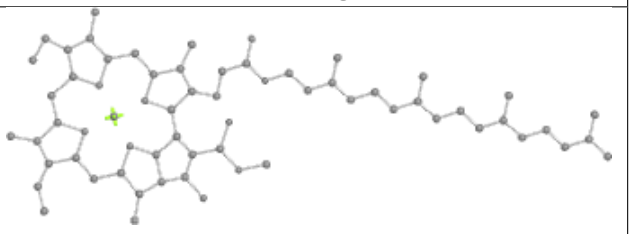

Rings

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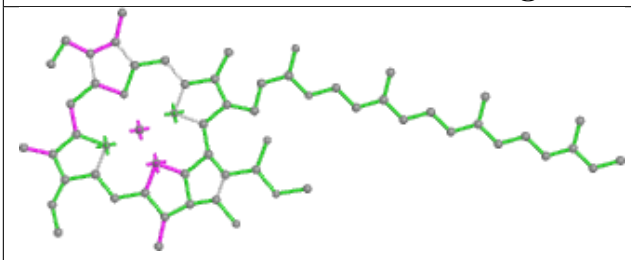

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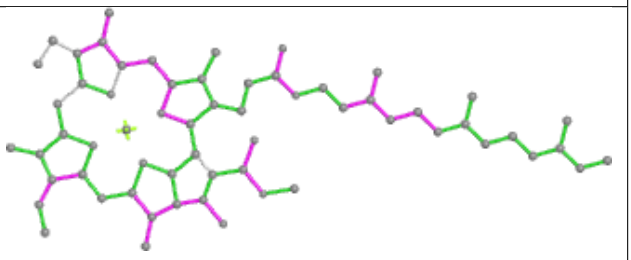

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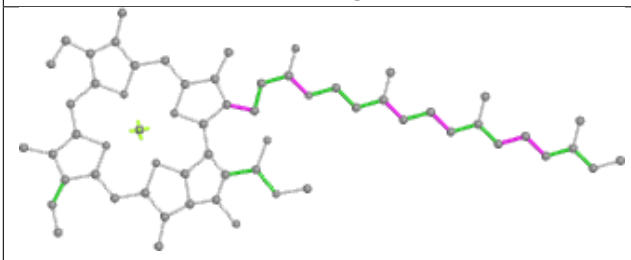

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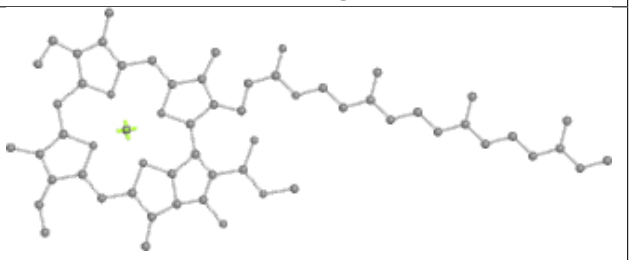
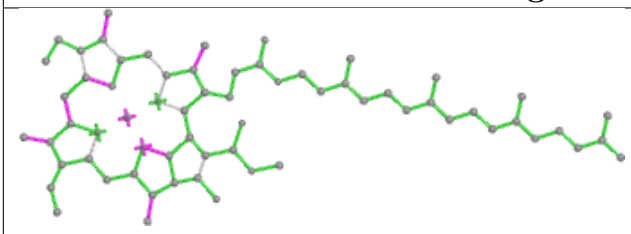


Rings

Ligand CLA b 613



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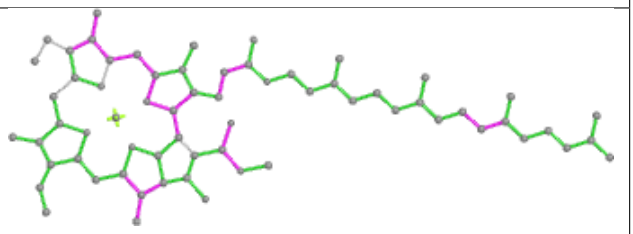

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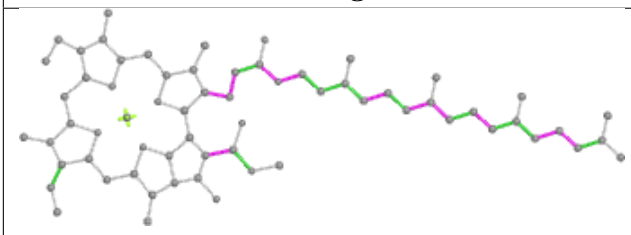

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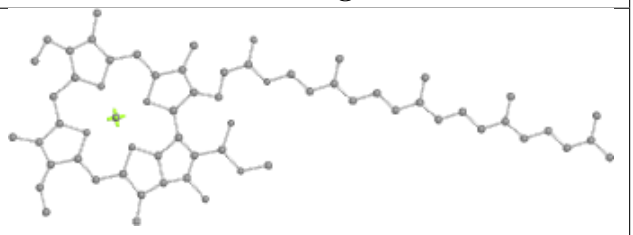

Rings

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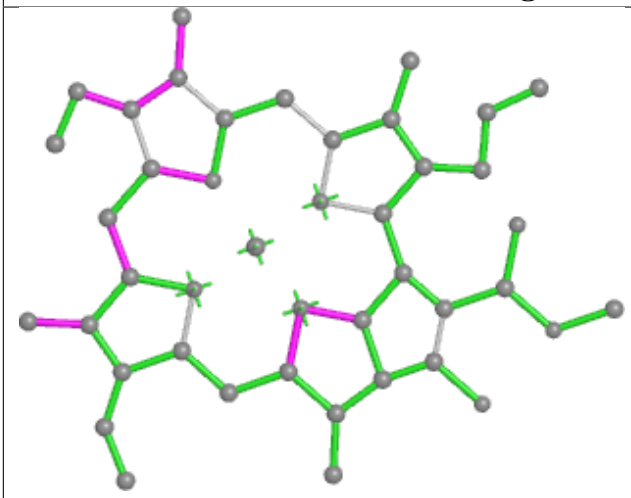

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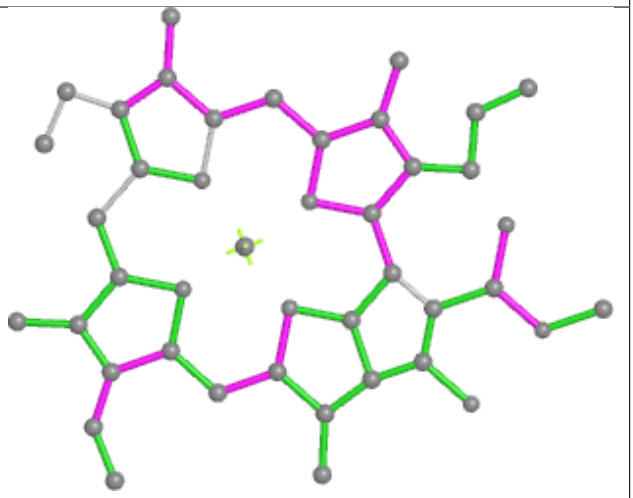

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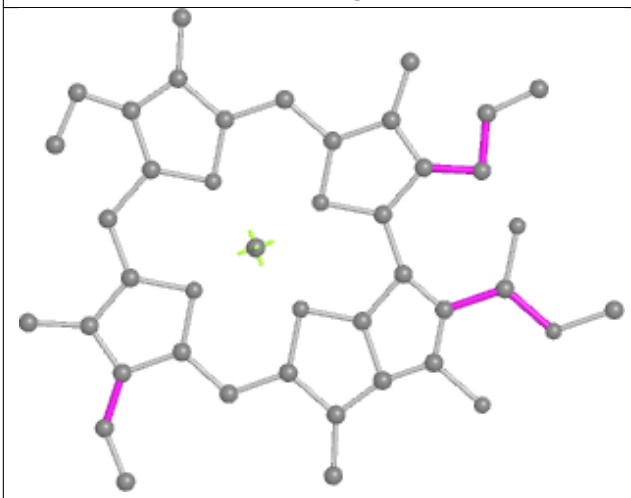

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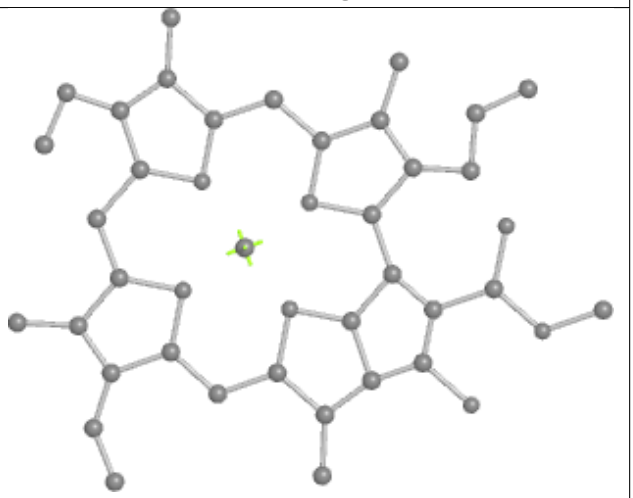
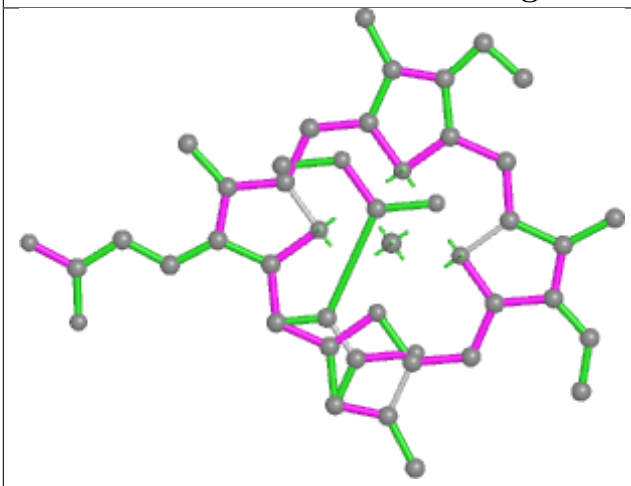


Rings

Ligand KC1 11 314



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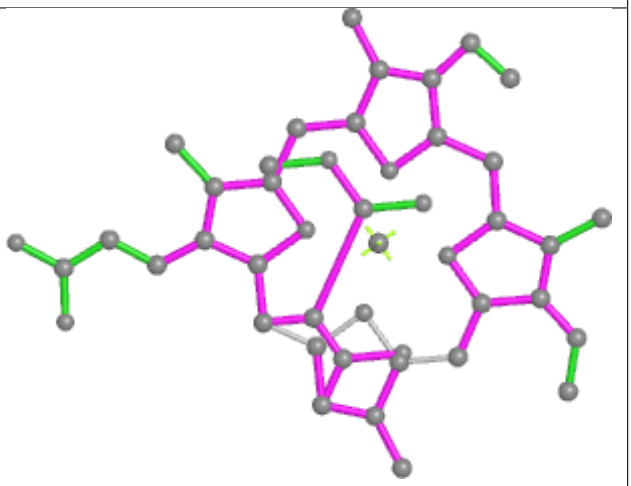

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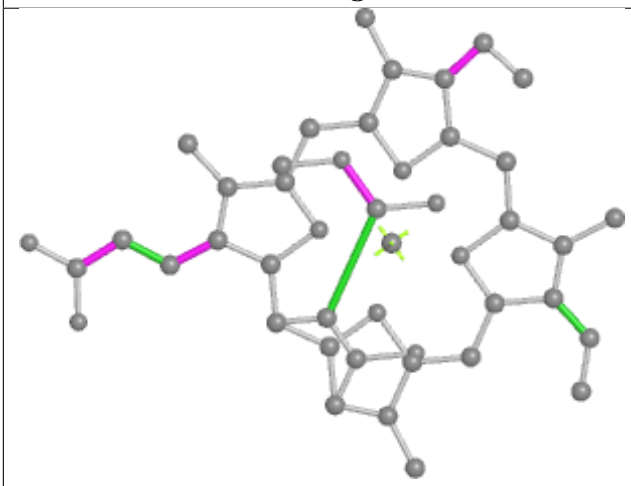

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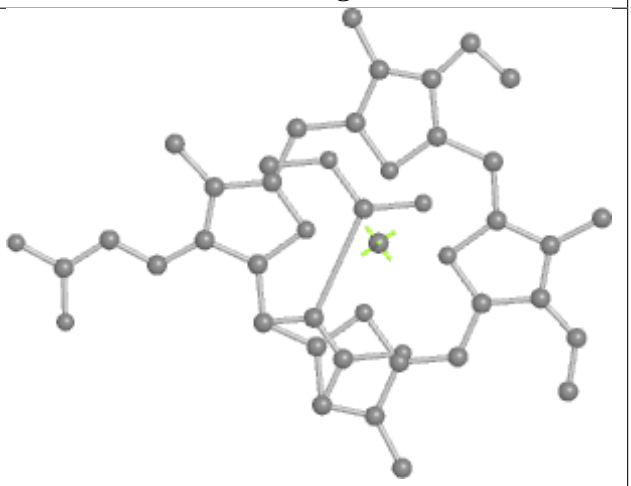
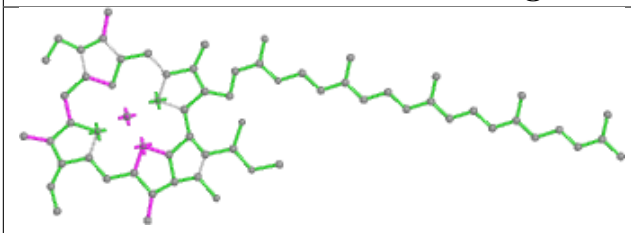


Rings

Ligand CLA C 513



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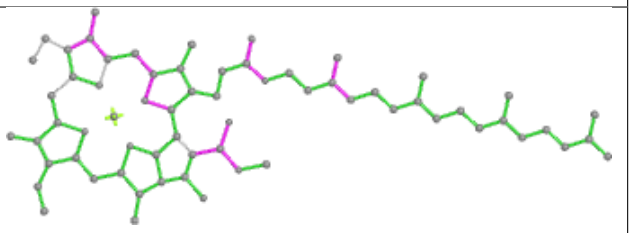

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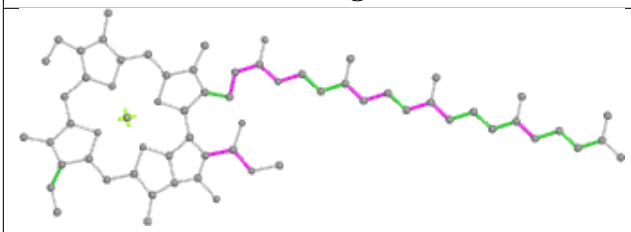

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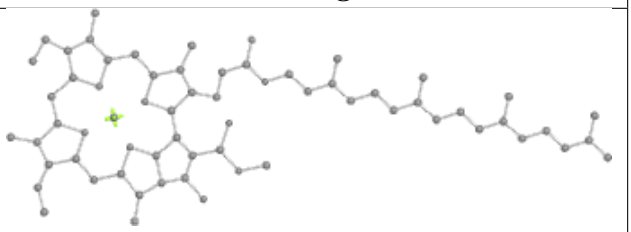
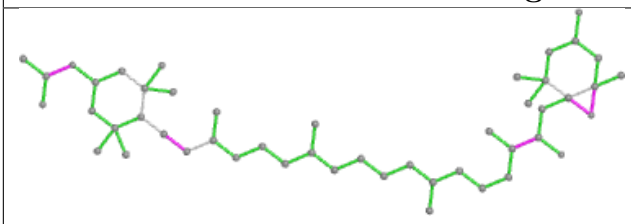


Rings

Ligand A86 18 301



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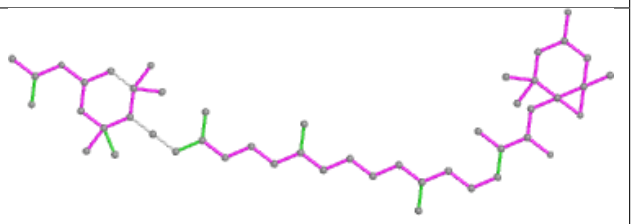

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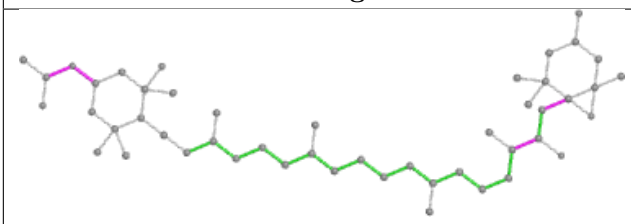

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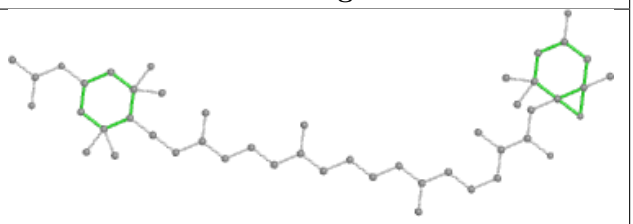
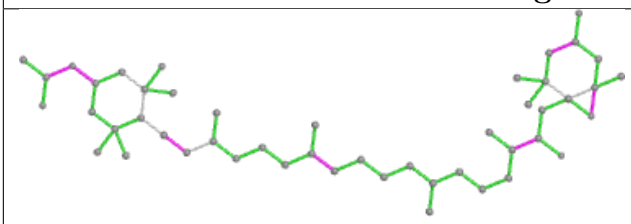


Rings

Ligand A86 1 303



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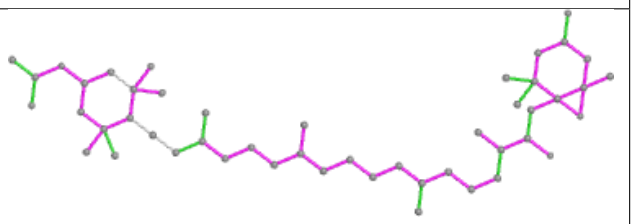

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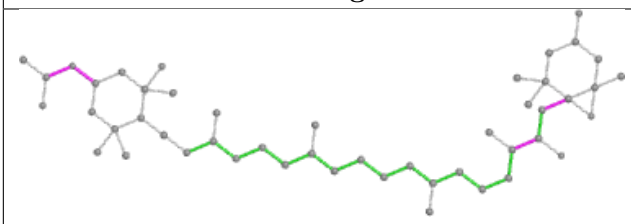

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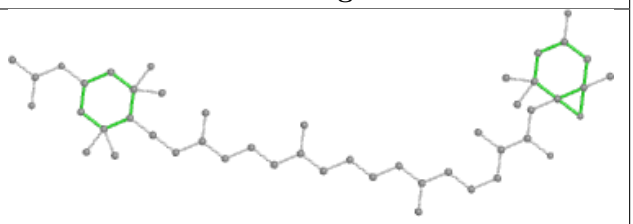
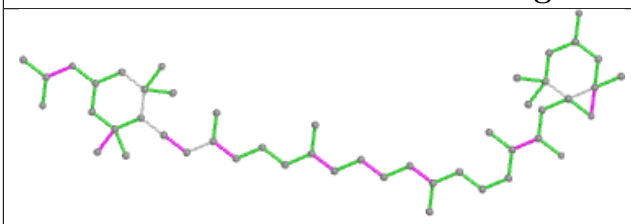


Rings

Ligand A86 3 301



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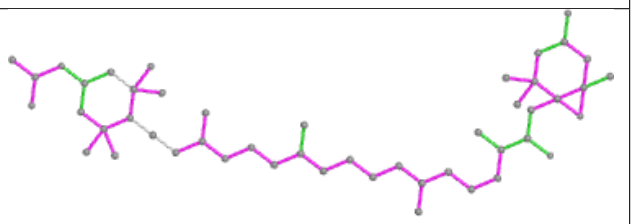
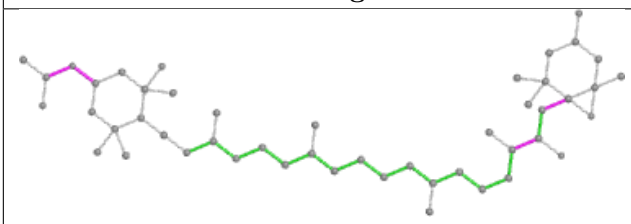


Bond angles



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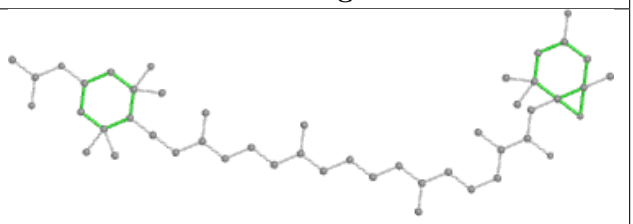
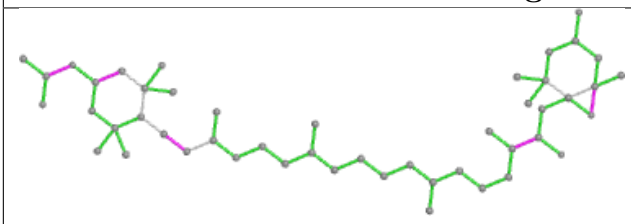


Rings

Ligand A86 15 304



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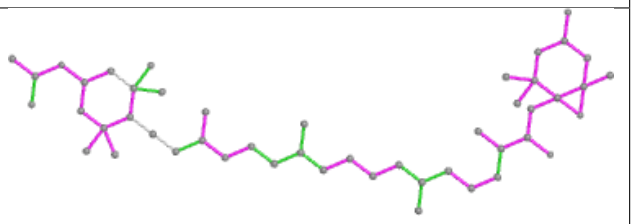

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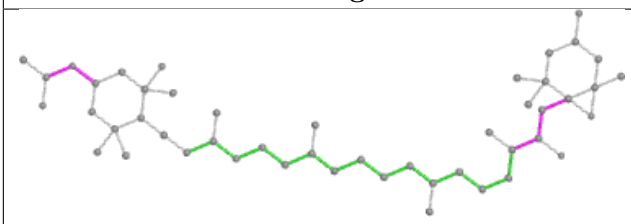

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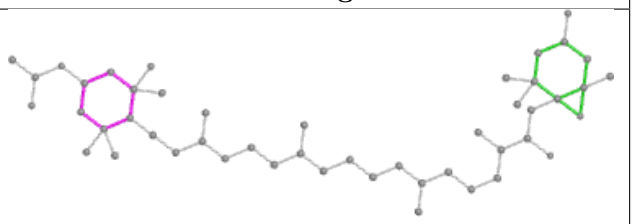
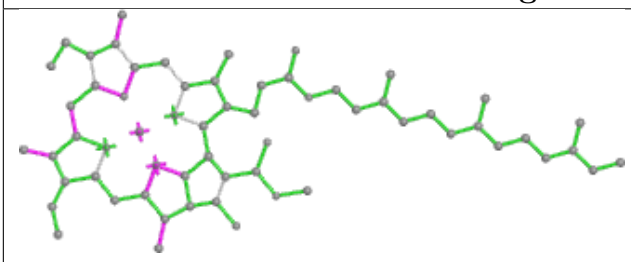


Rings

Ligand CLA 14 306



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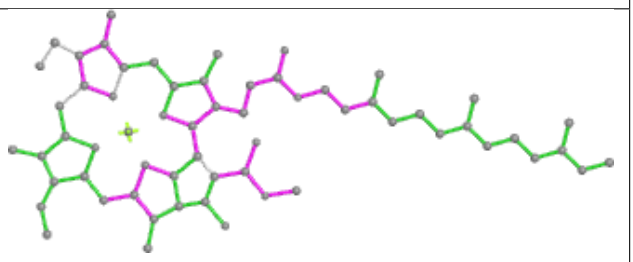

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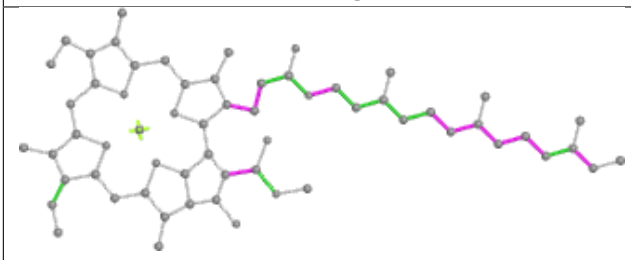
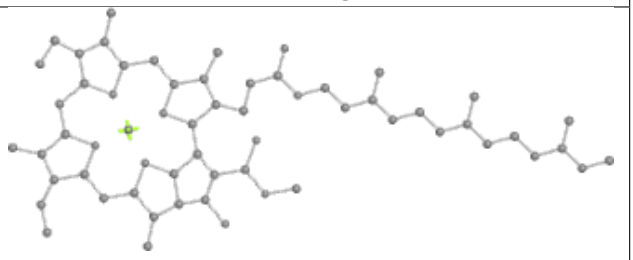
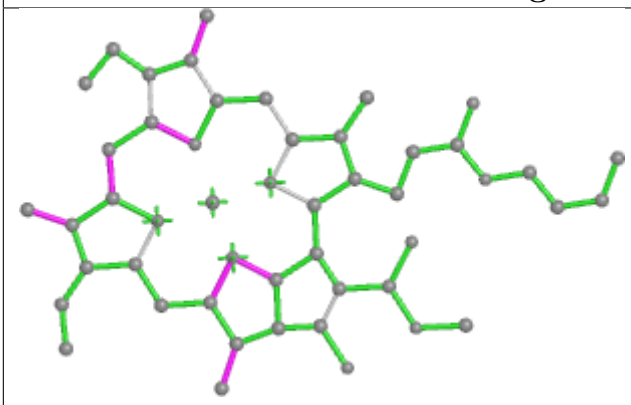


Torsions



Rings

Ligand CLA c 514



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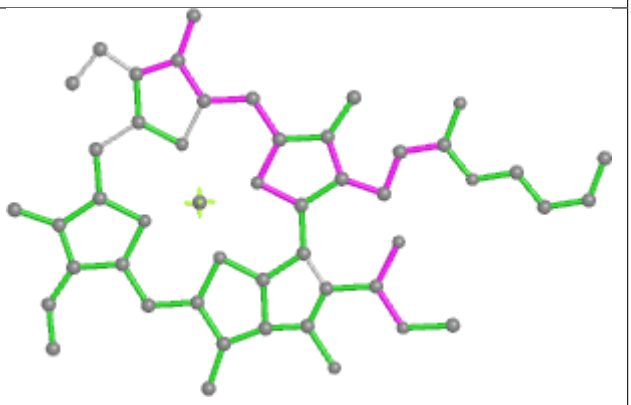

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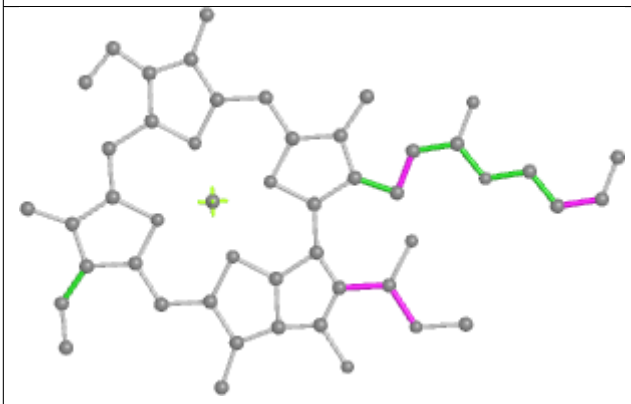

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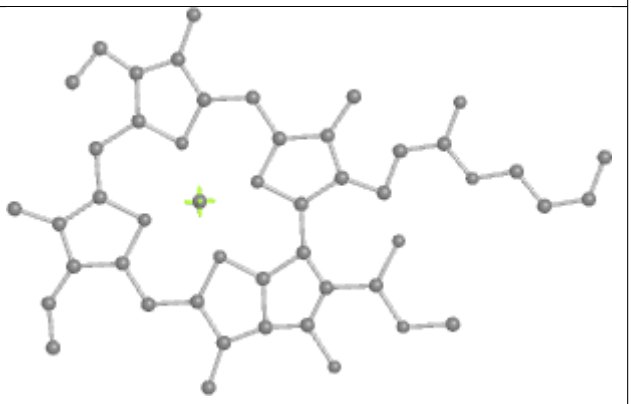
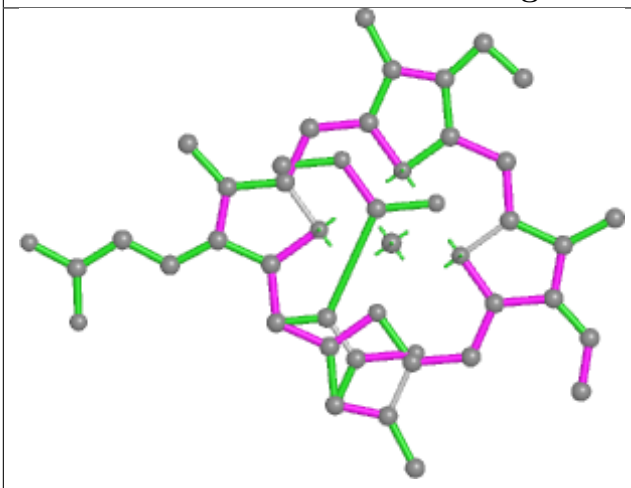


Rings

Ligand KC2 11 311



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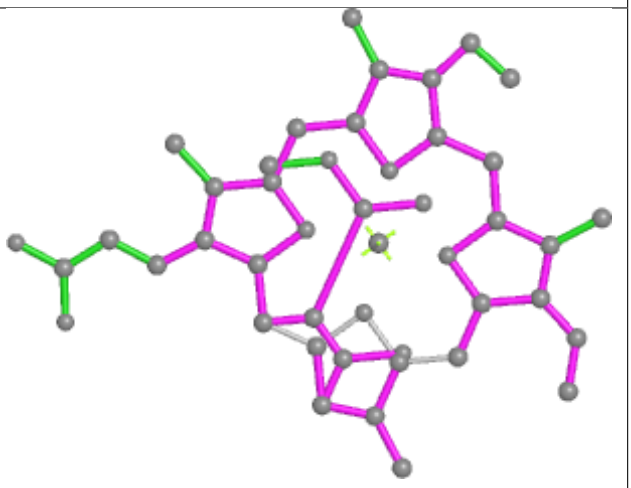

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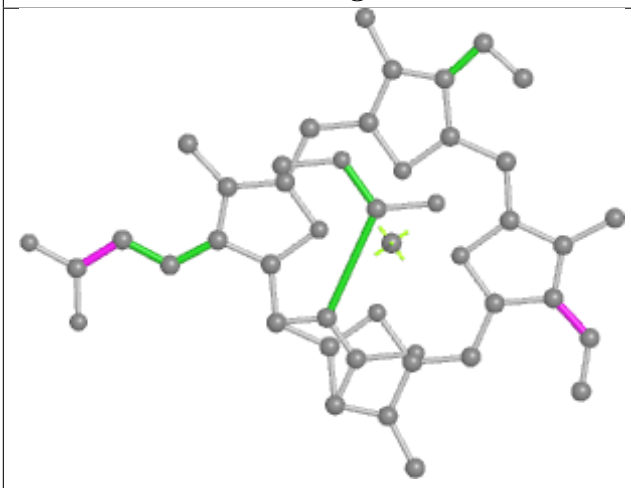

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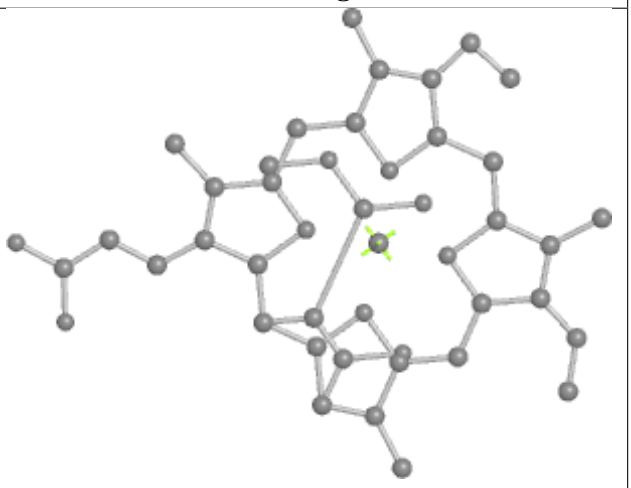
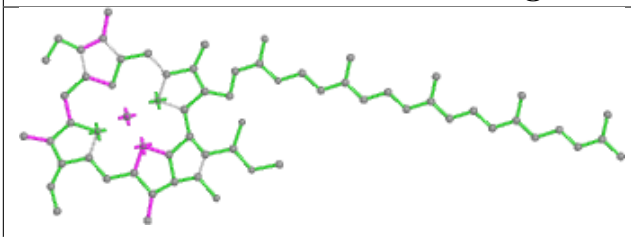


Rings

Ligand CLA w 203



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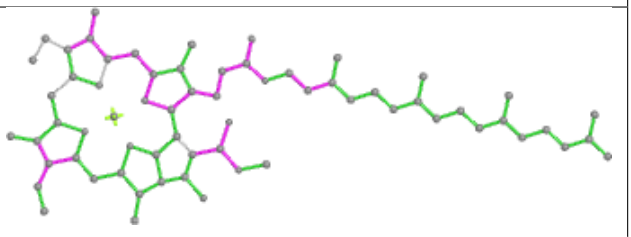

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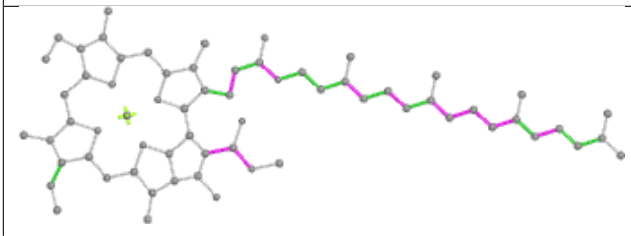

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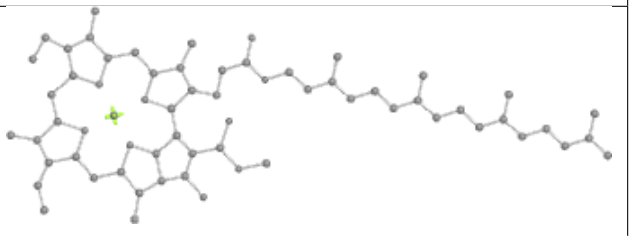
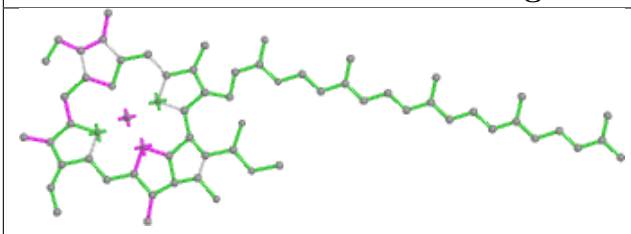


Rings

Ligand CLA C 508



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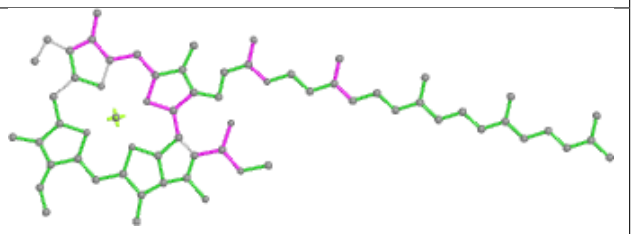

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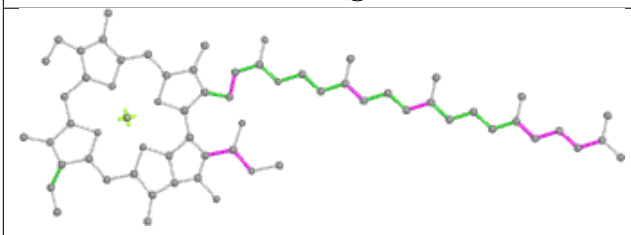

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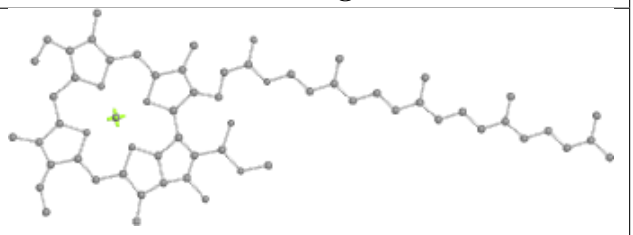
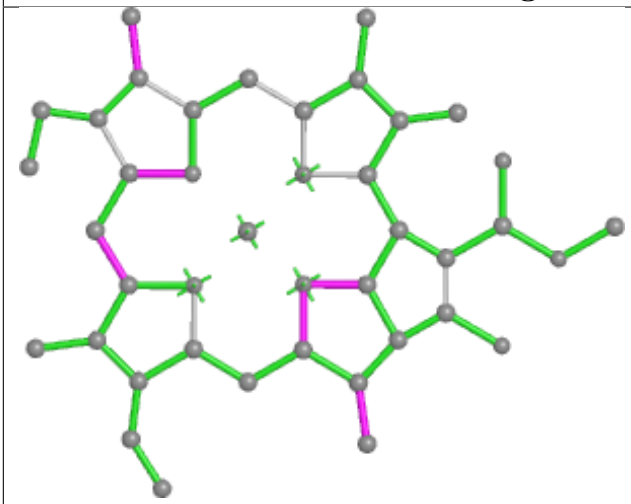


Rings

Ligand CLA 12 315



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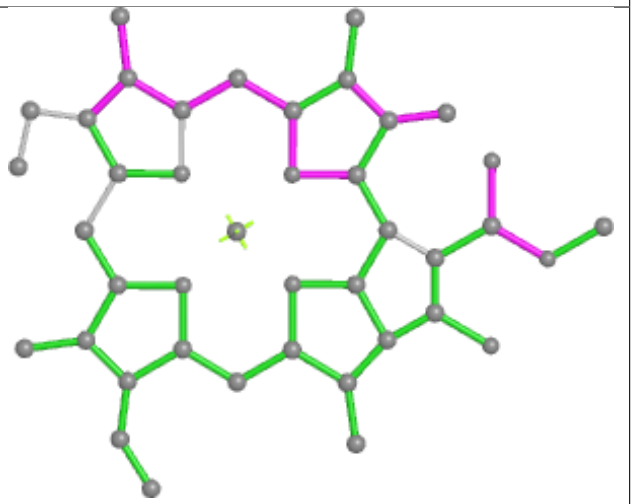

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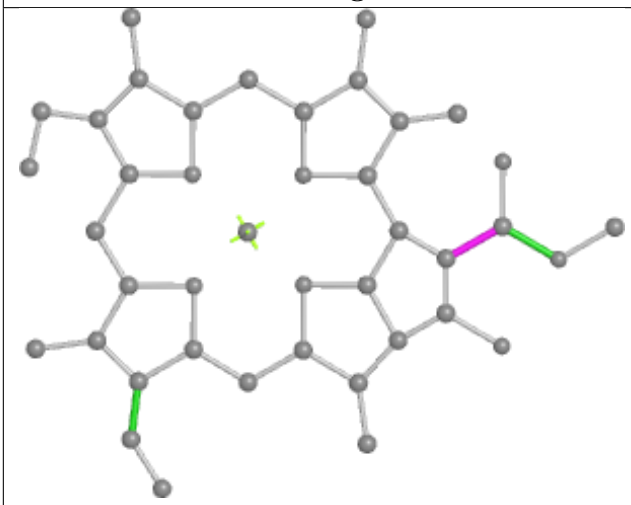

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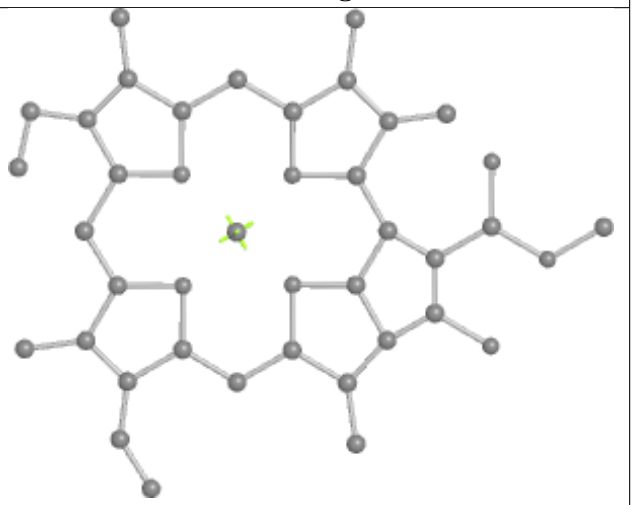
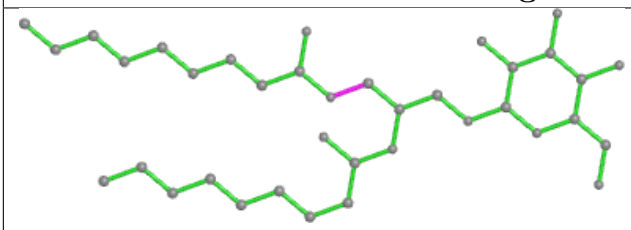


Rings

Ligand LMG D 408



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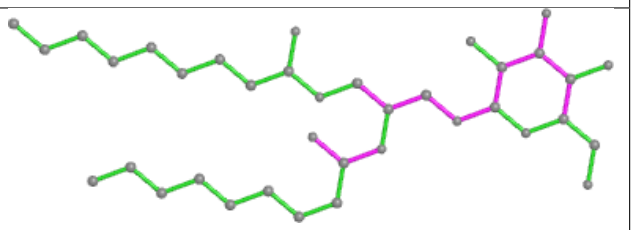

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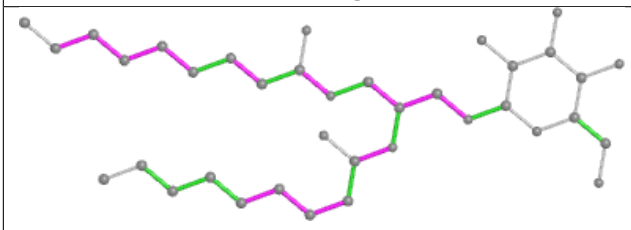

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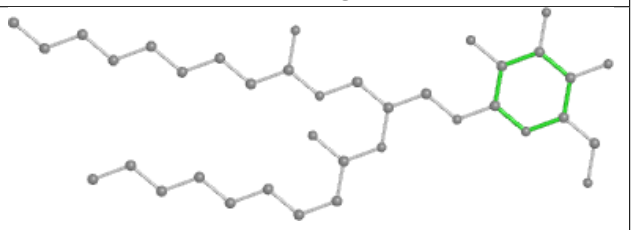
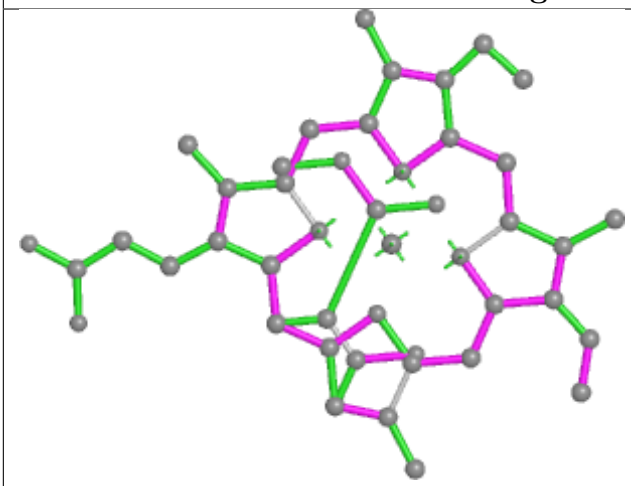


Rings

Ligand KC2 8 310



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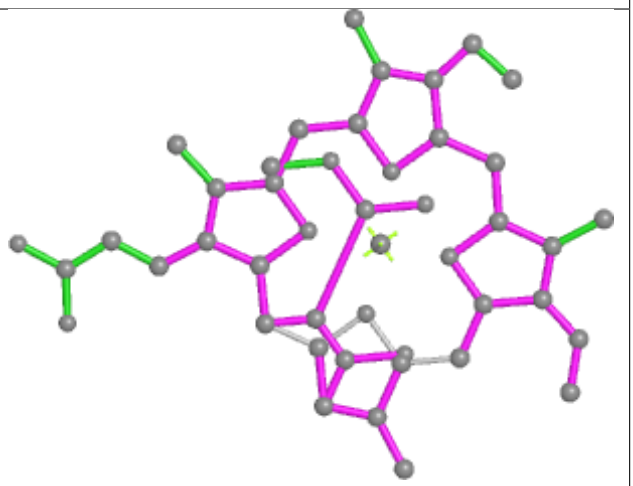

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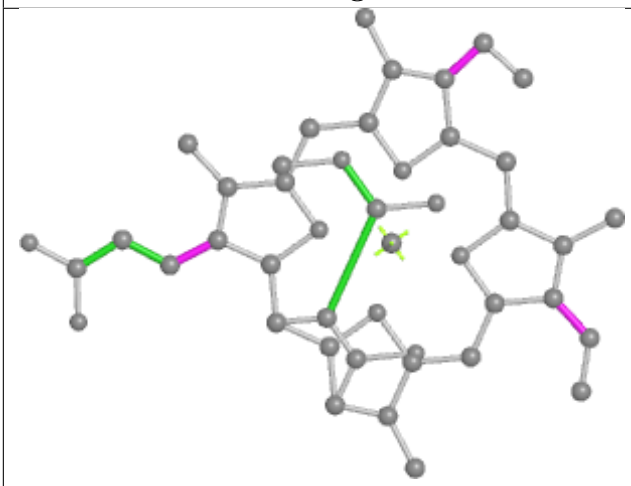

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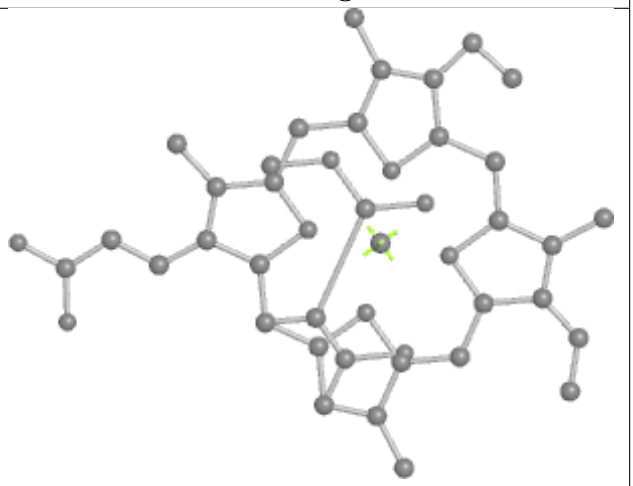
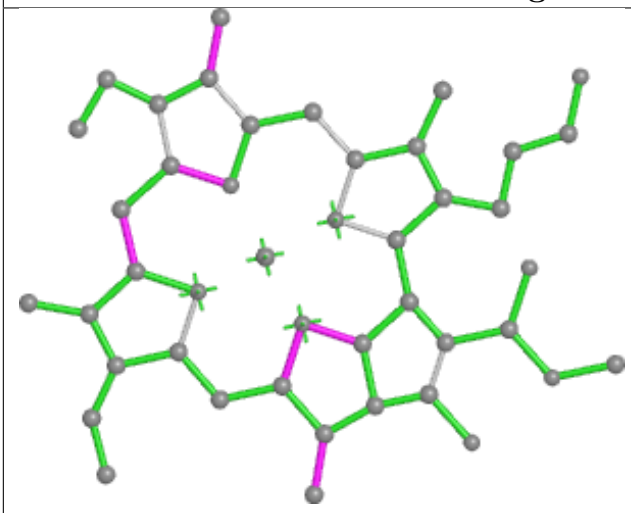


Rings

Ligand CLA 3 315



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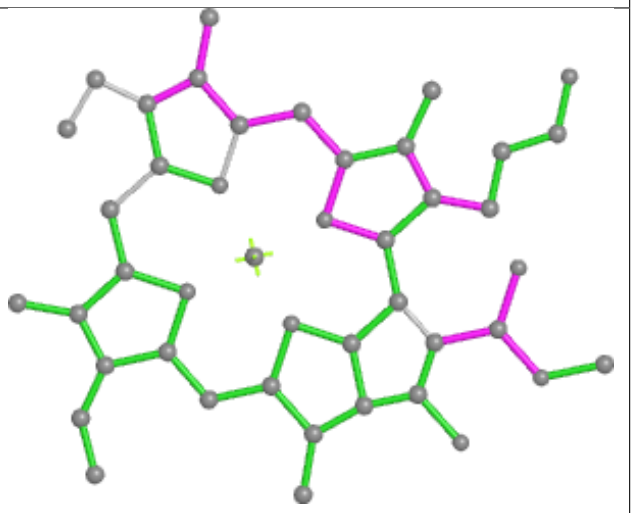

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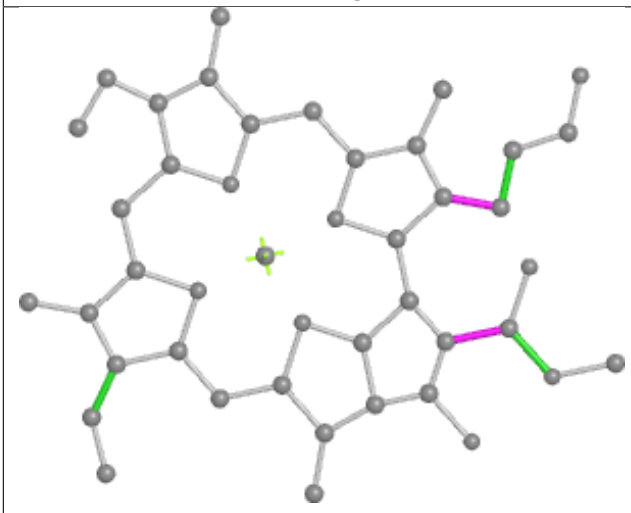

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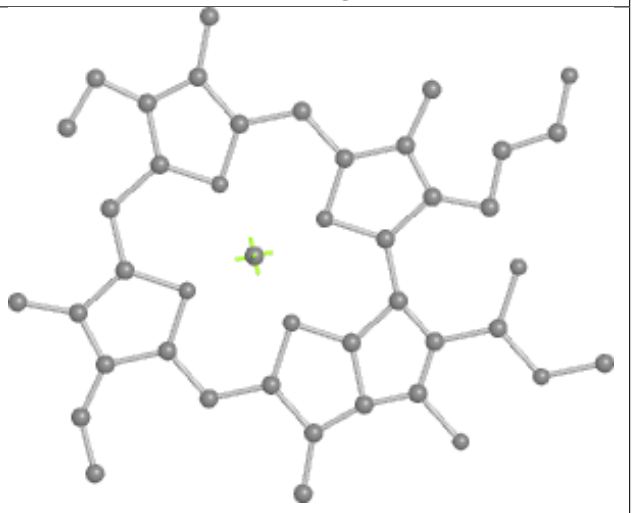
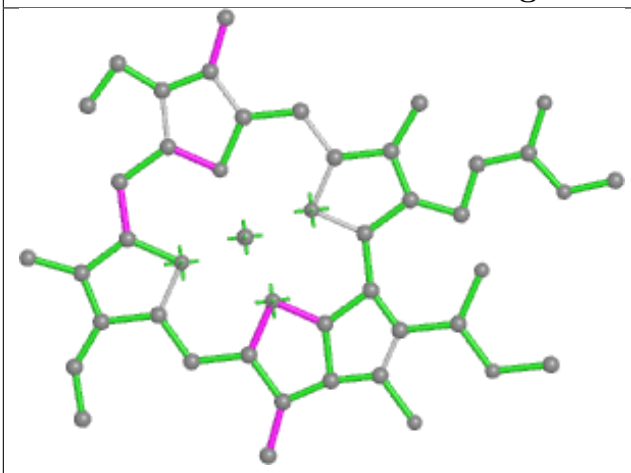


Rings

Ligand CLA 10 312



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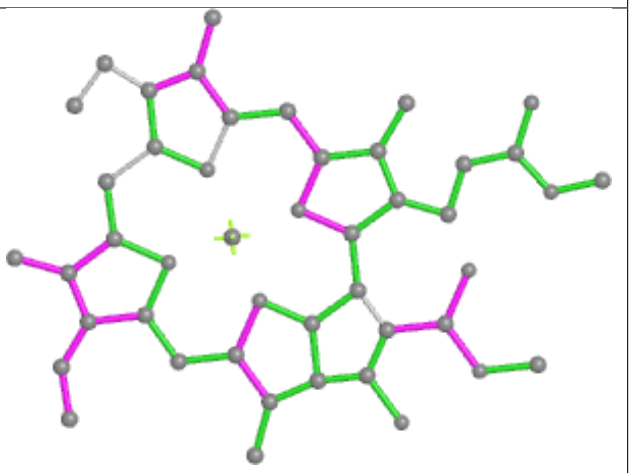

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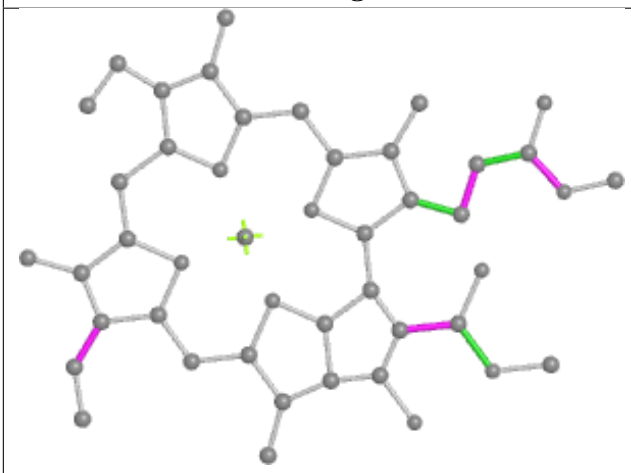

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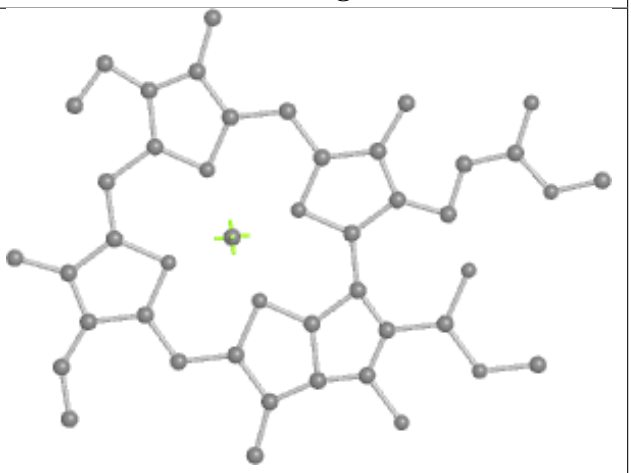
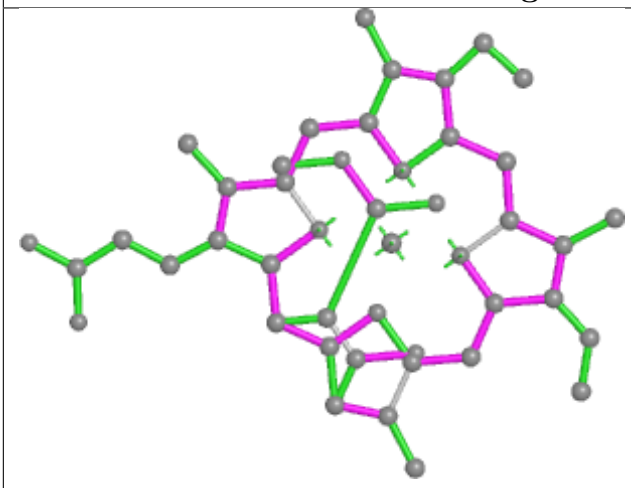


Rings

Ligand KC1 19 314



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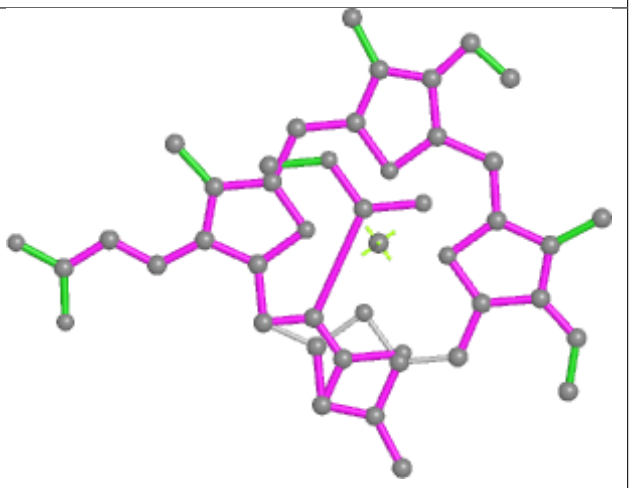

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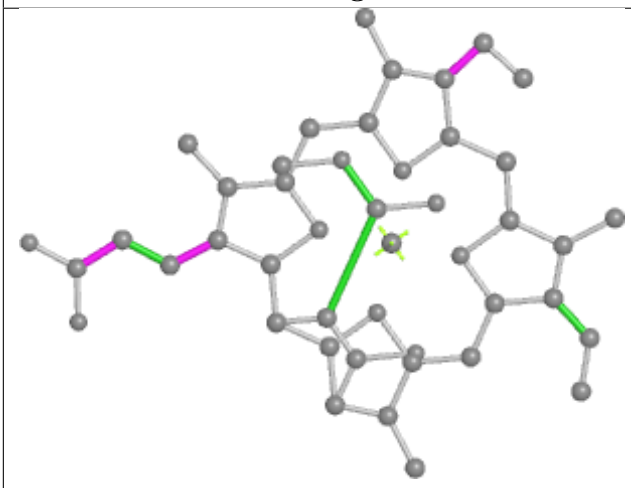

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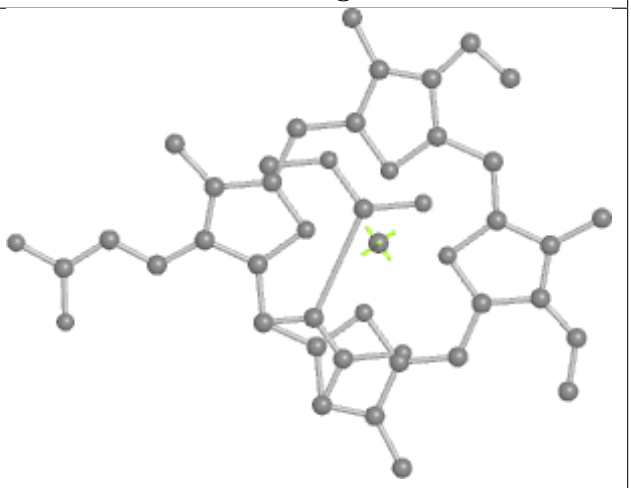
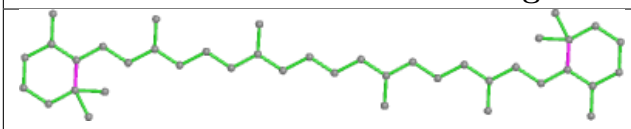


Rings

Ligand BCR B 617



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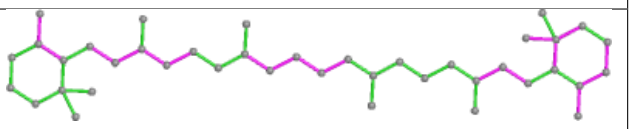

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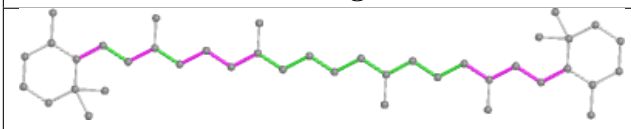
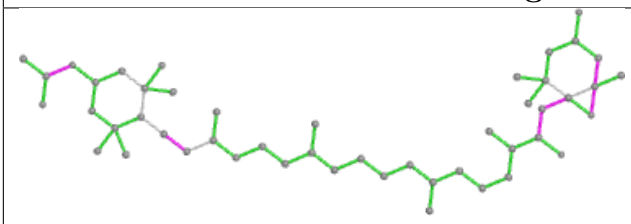


Torsions

Rings

Ligand A86 19 305



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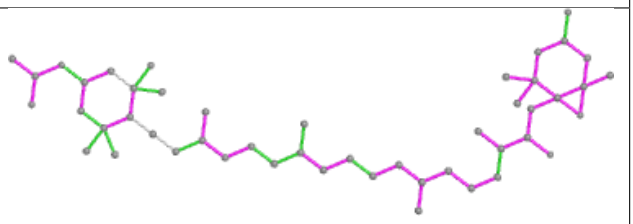
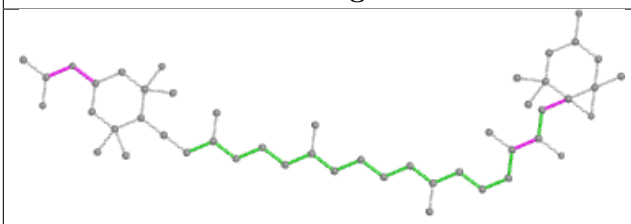


Bond angles



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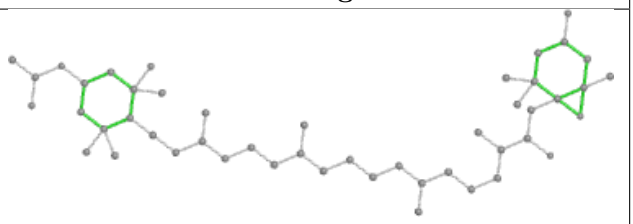
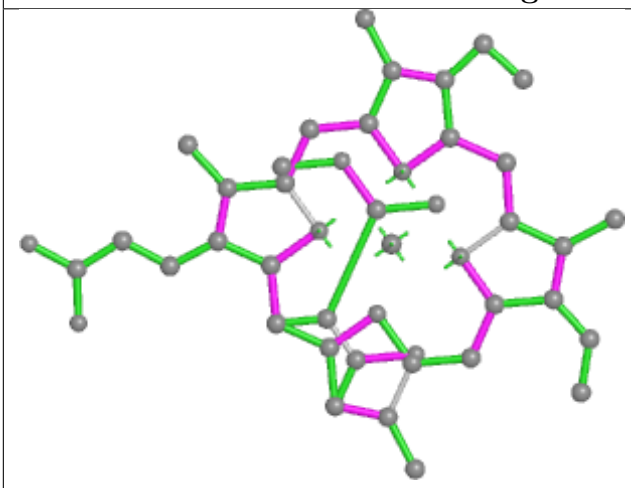


Rings

Ligand KC1 10 315



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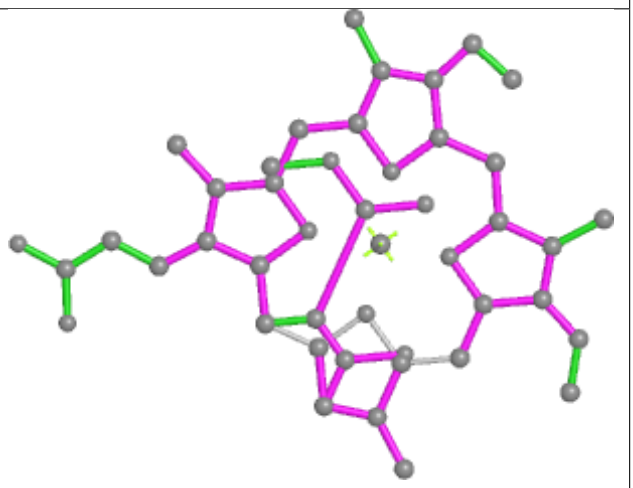
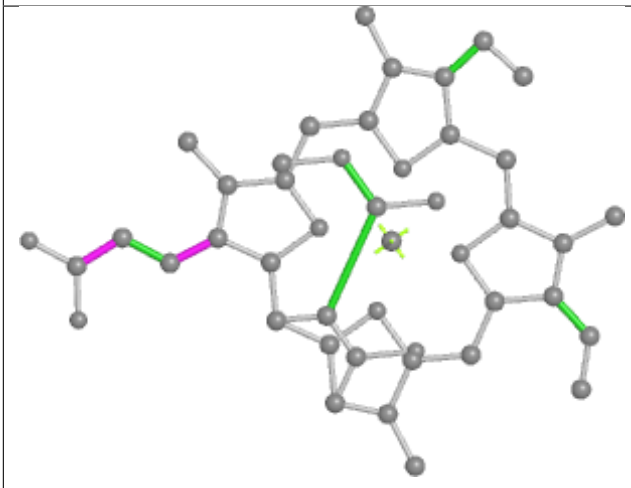


Bond angles



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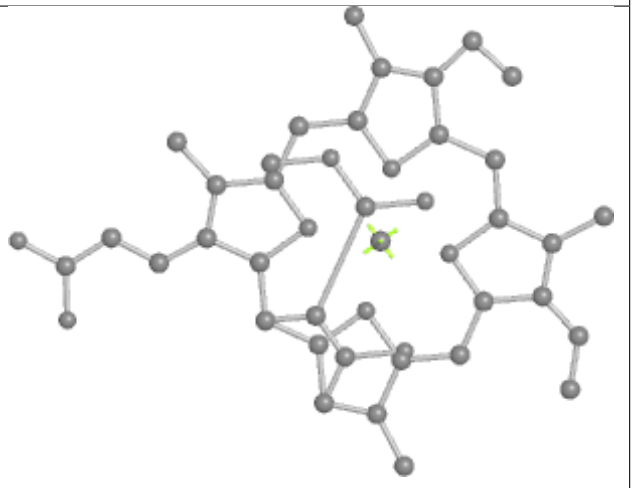
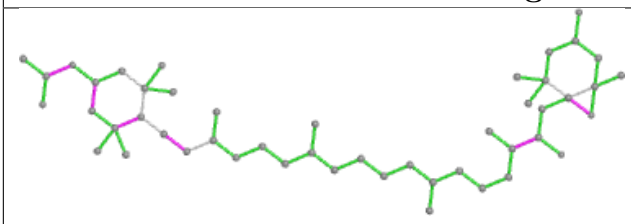


Rings

Ligand A86 18 304



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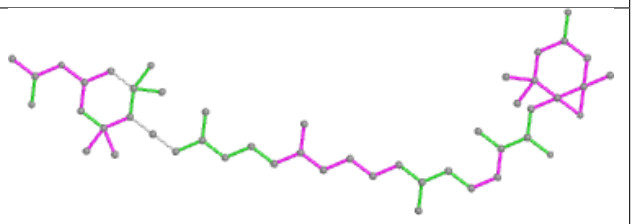

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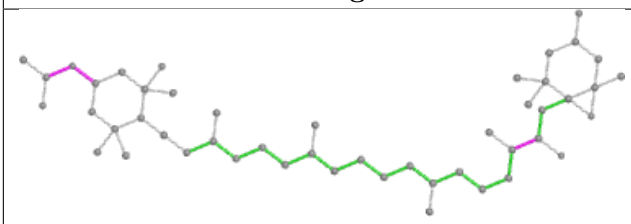

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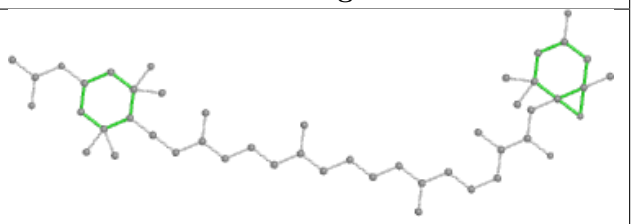
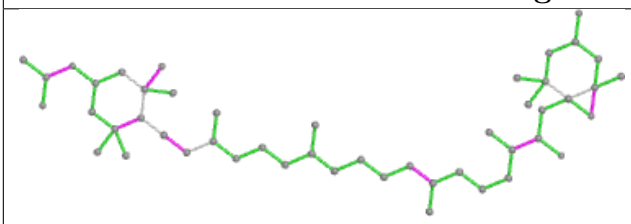


Rings

Ligand A86 3 304



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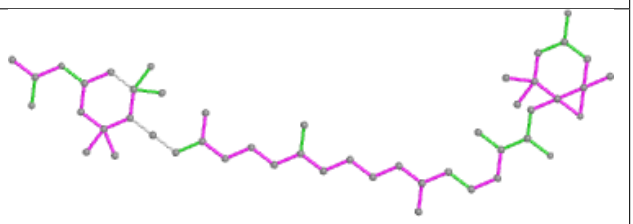

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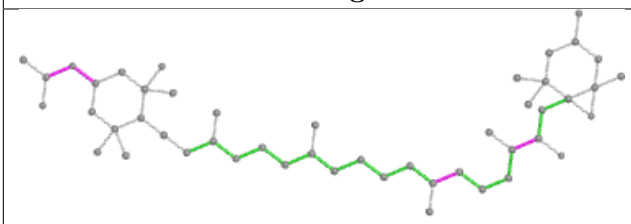

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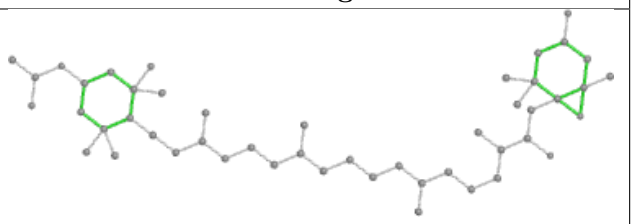
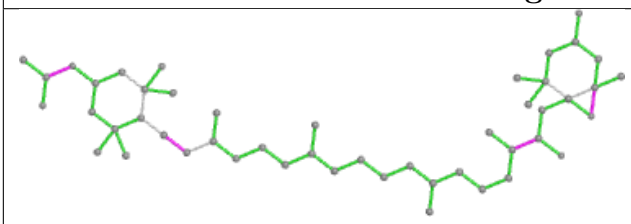


Rings

Ligand A86 17 304



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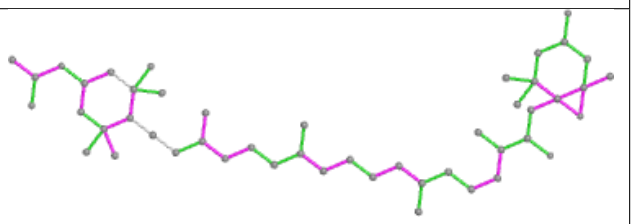

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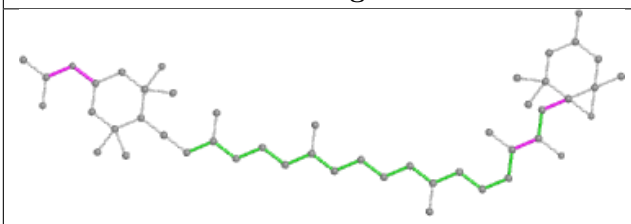

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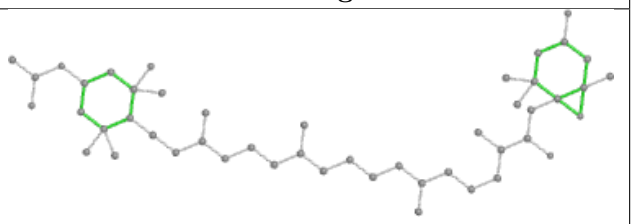

Rings

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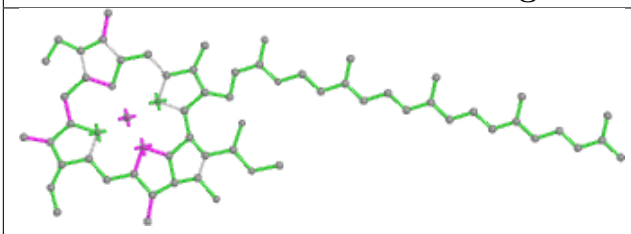

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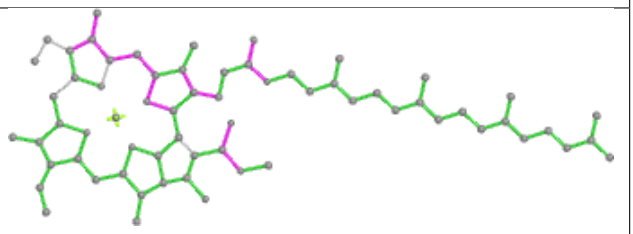

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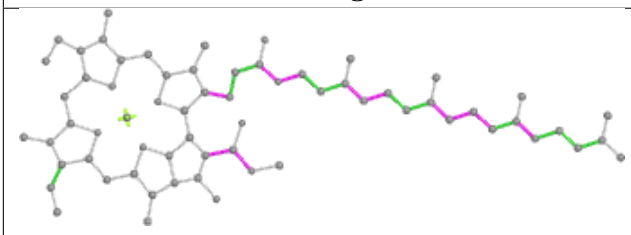

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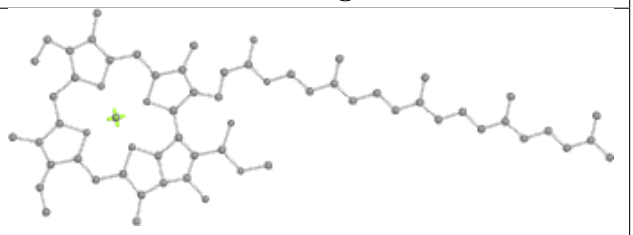

Rings

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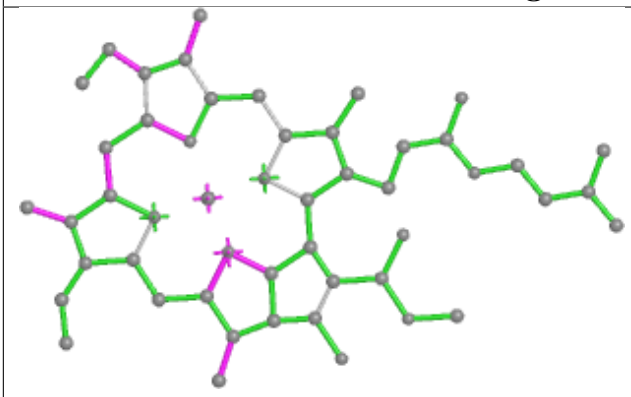

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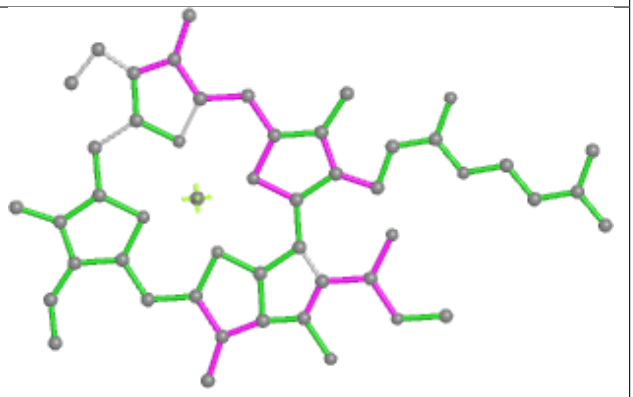

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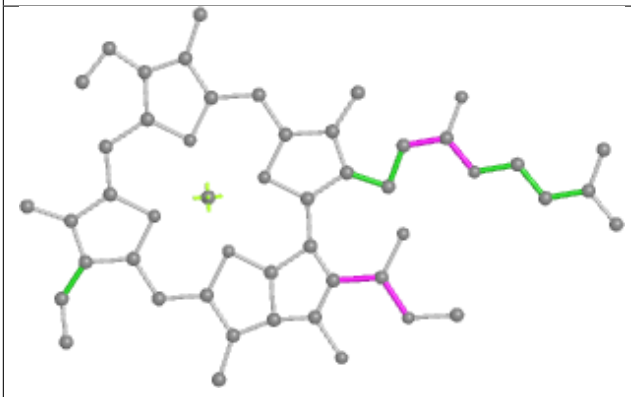

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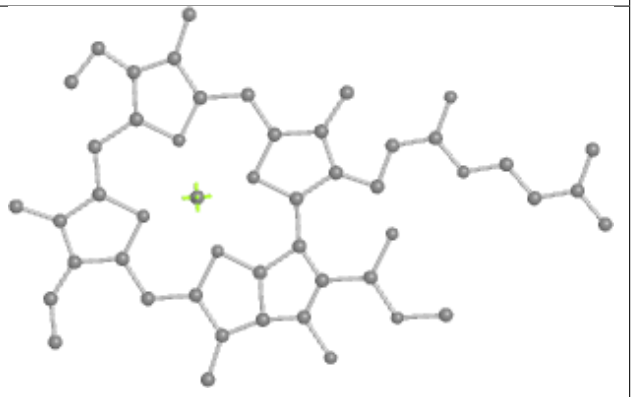

Rings

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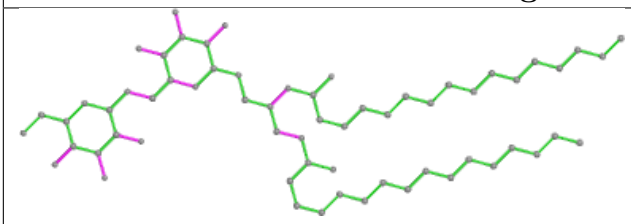

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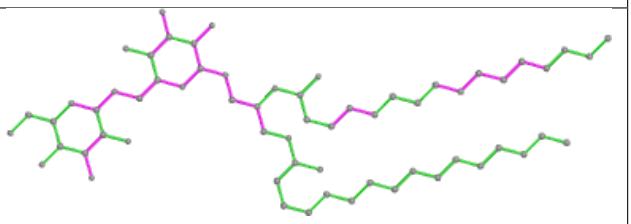

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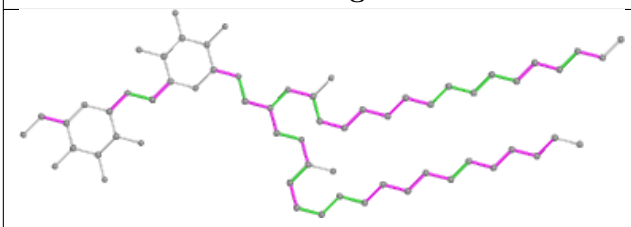

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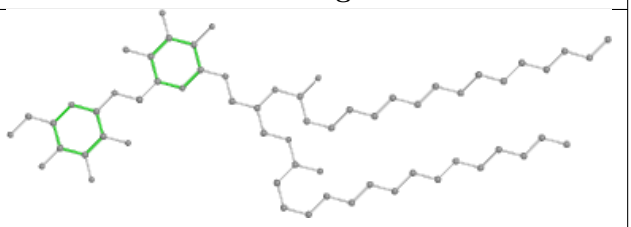

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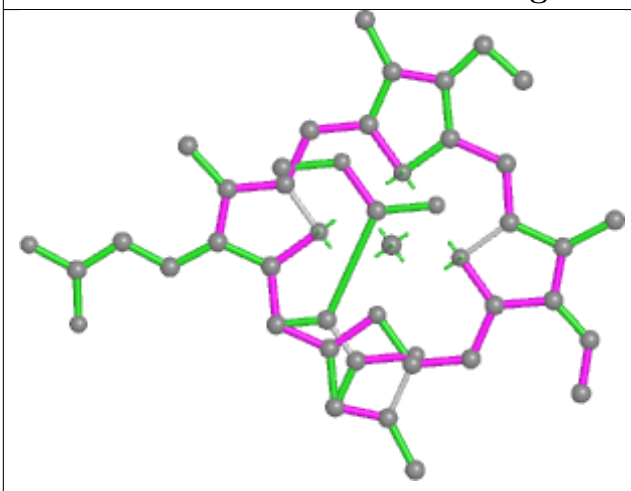

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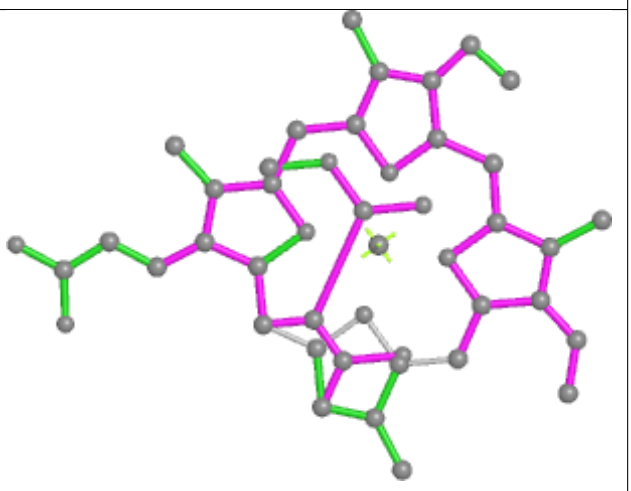

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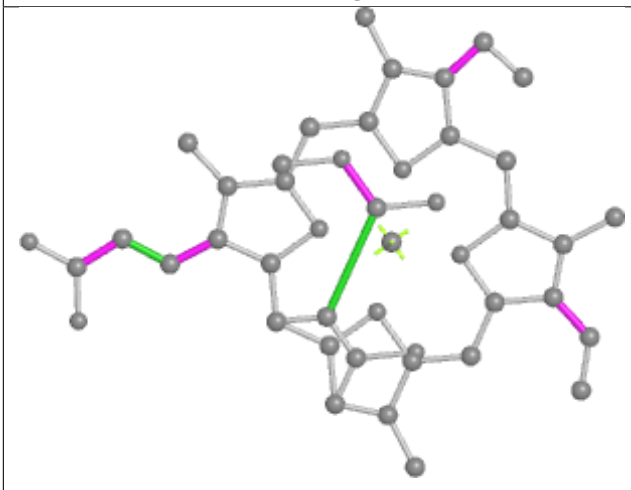

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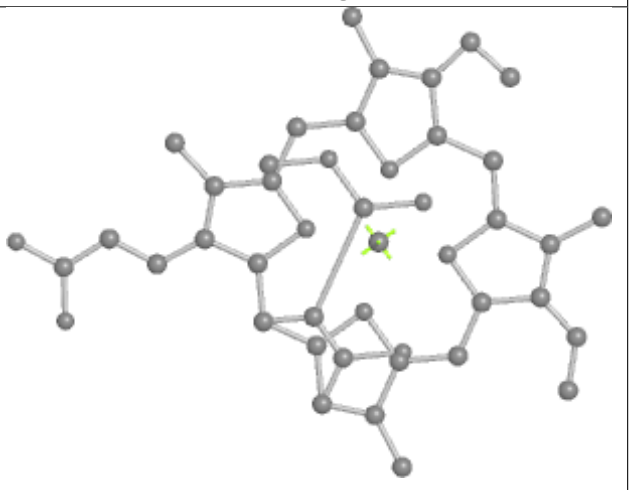

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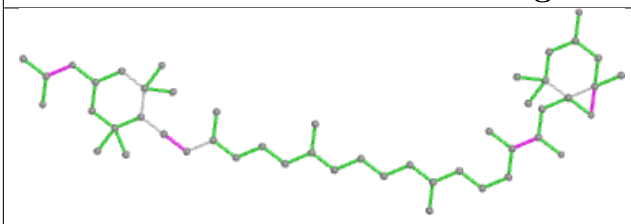

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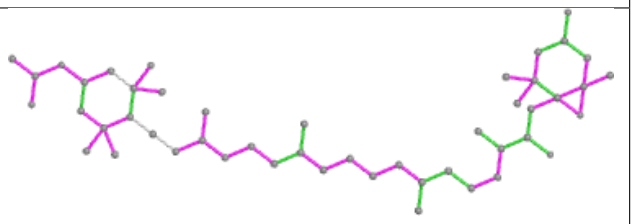

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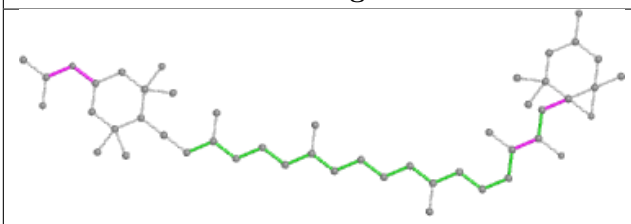

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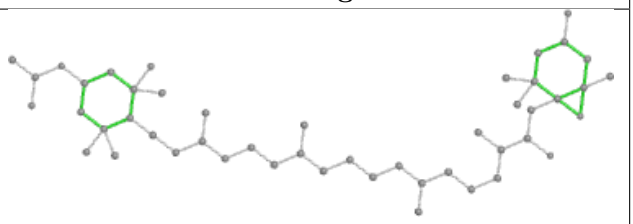

Rings

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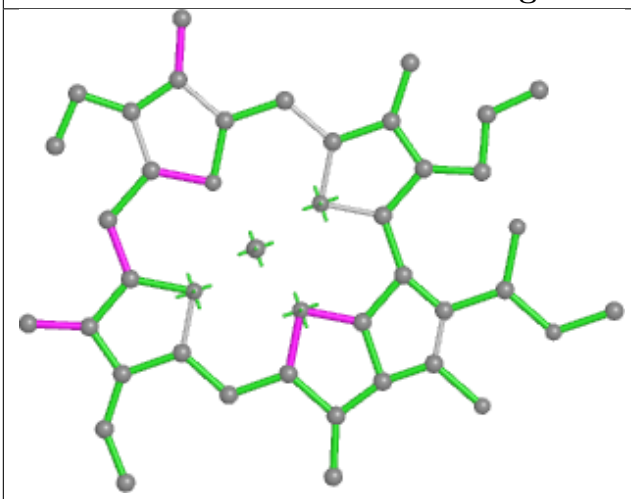

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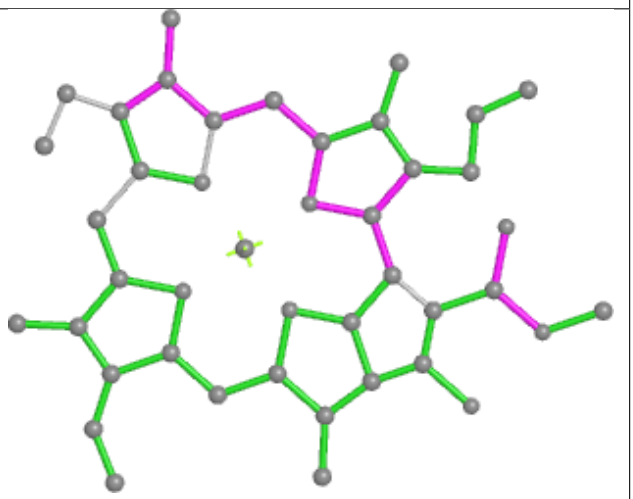

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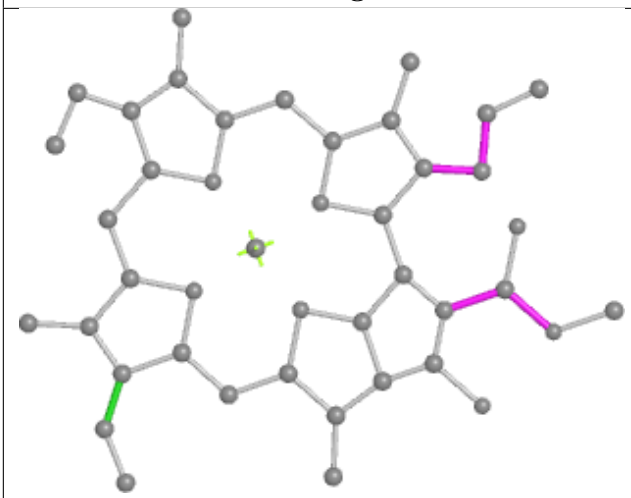

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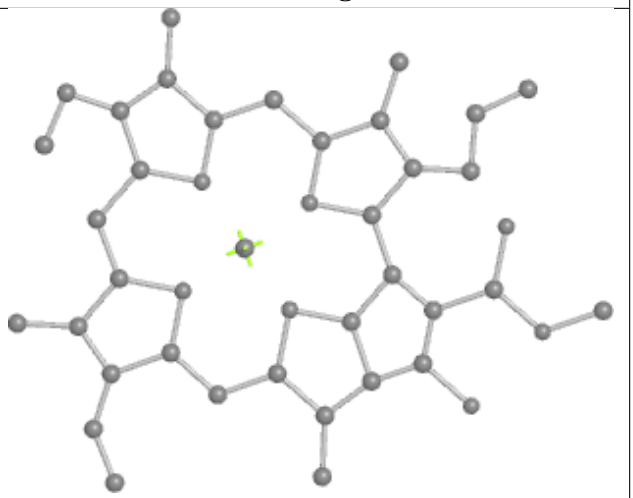

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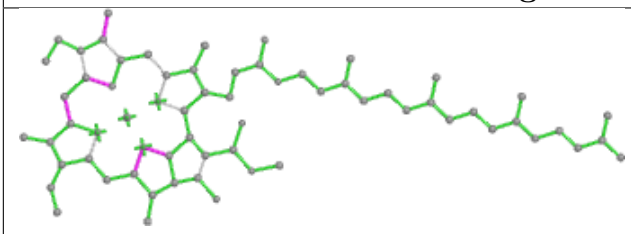

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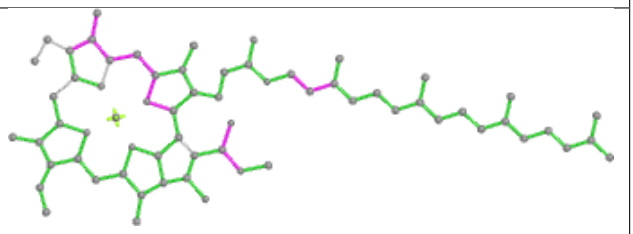

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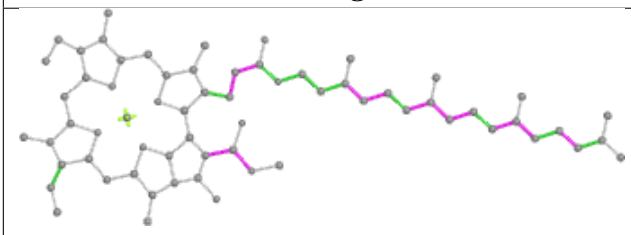

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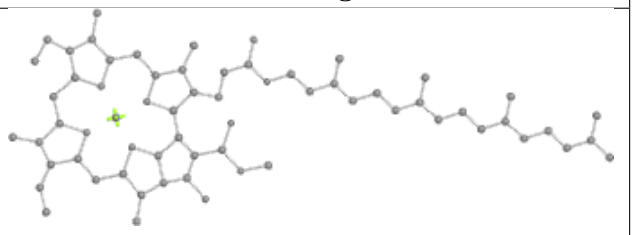

Rings

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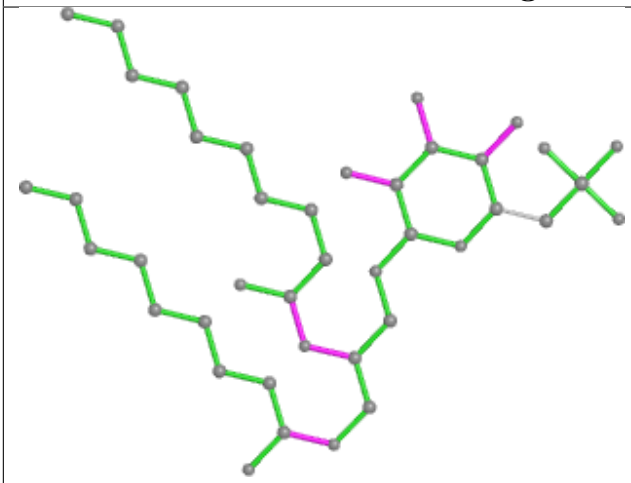

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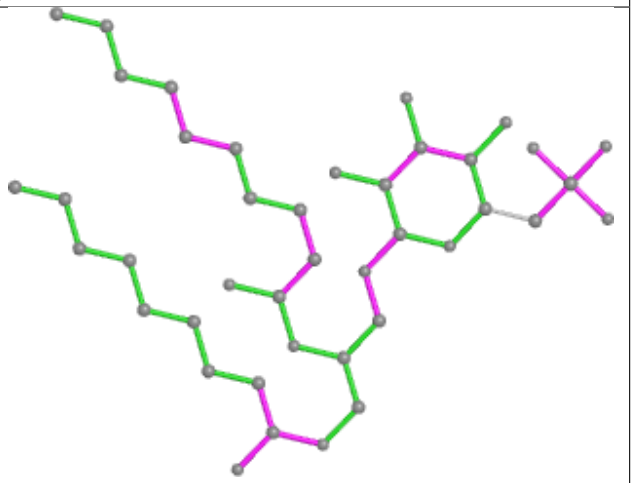

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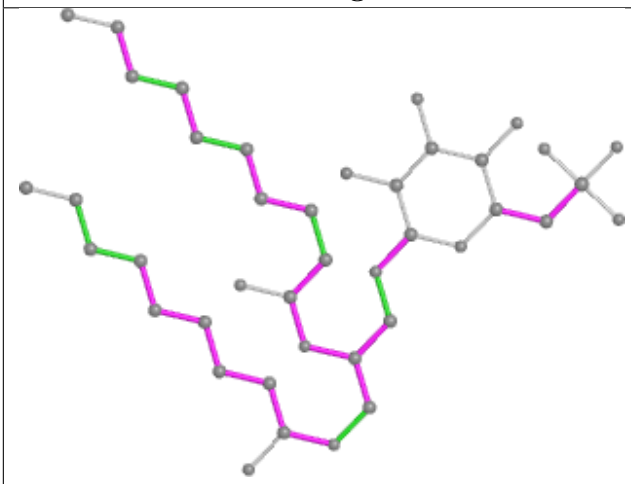

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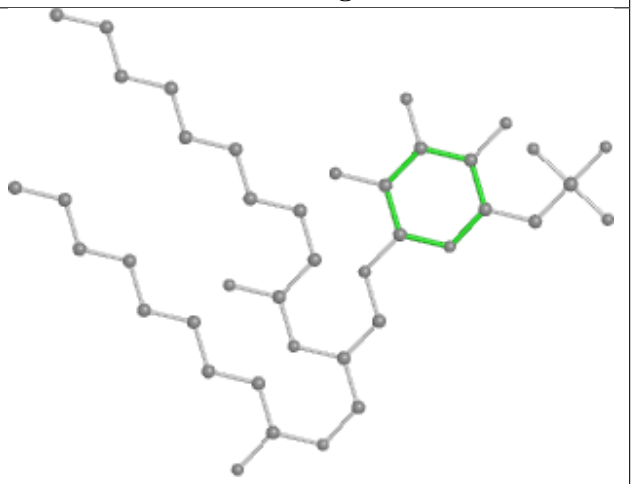

Rings

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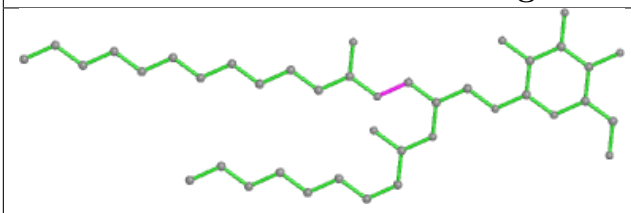

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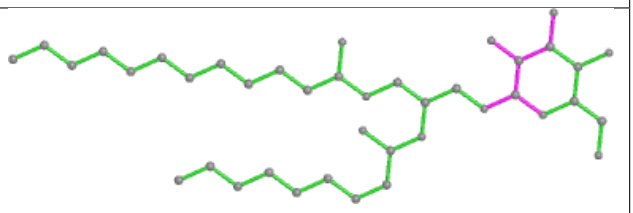

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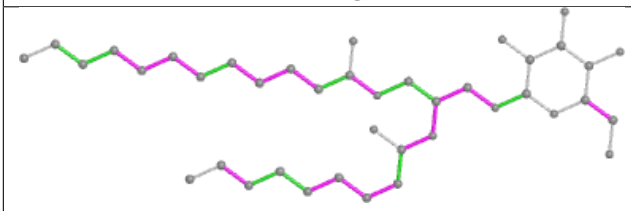

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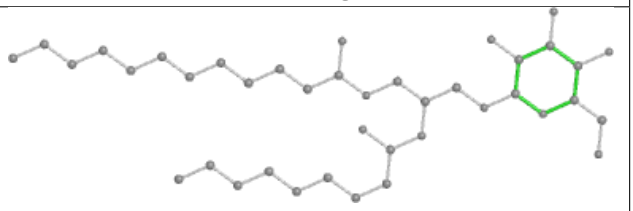

Rings

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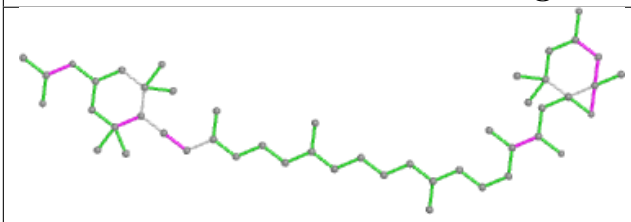

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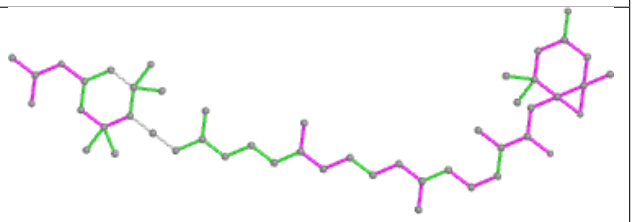

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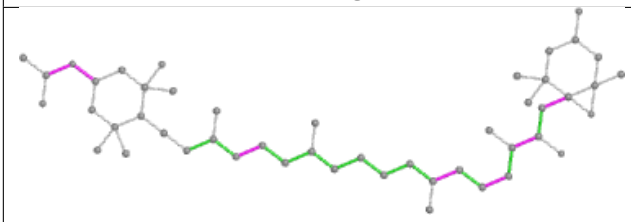

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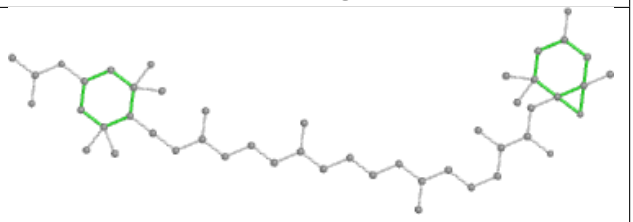

Rings

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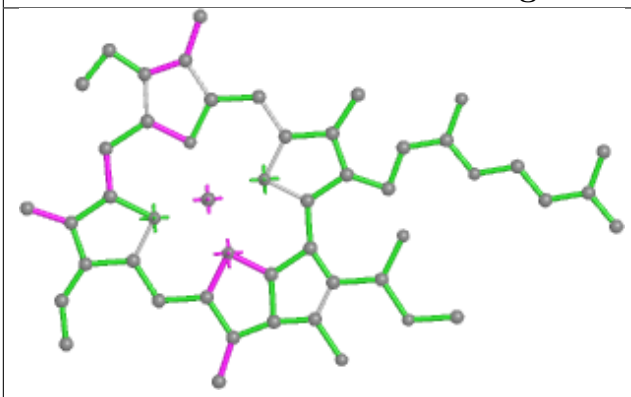

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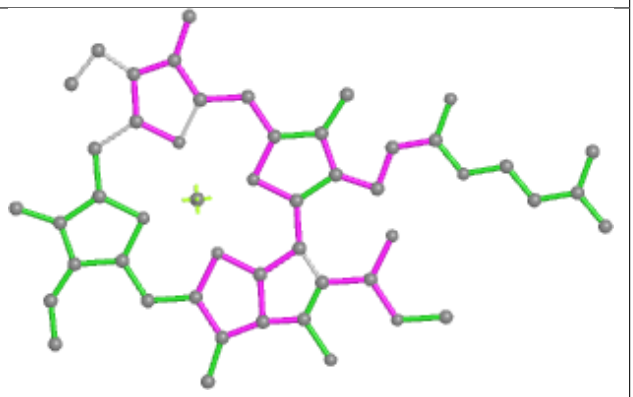

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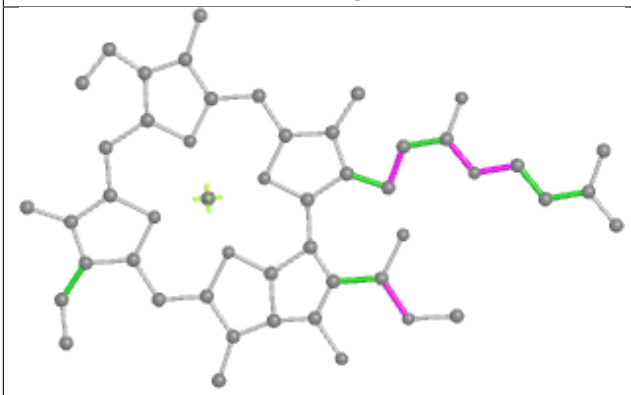

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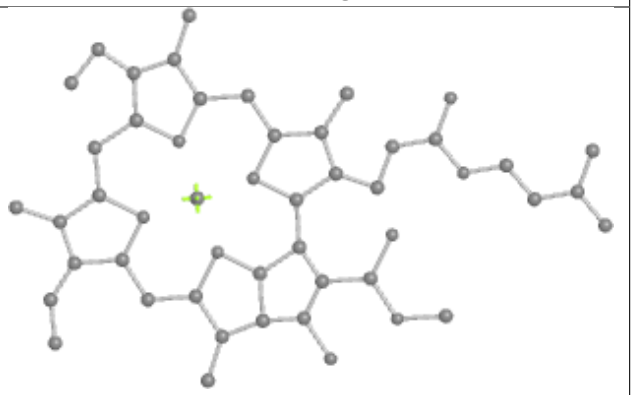
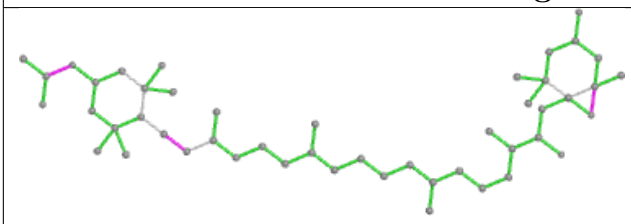


Rings

Ligand A86 1 302



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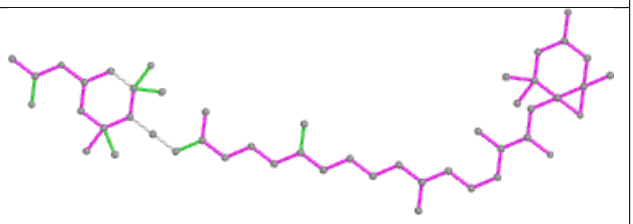

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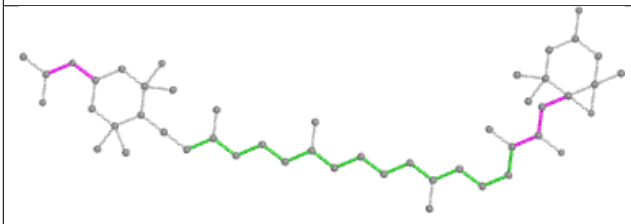
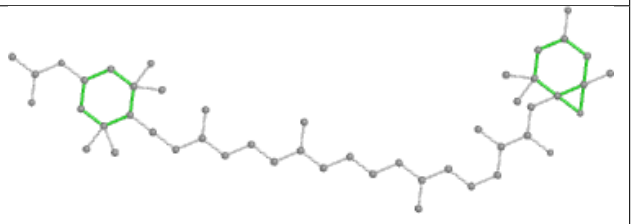
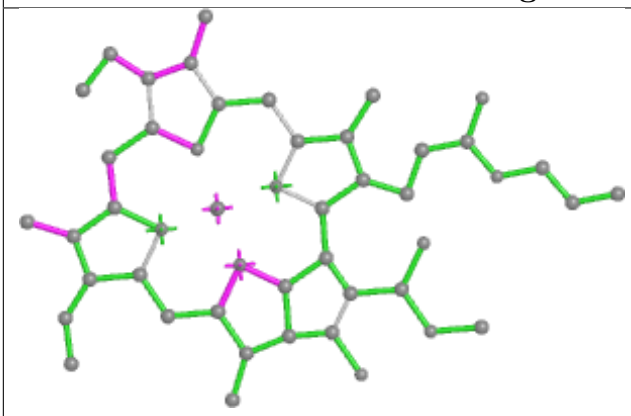


Torsions



Rings

Ligand CLA 10 307



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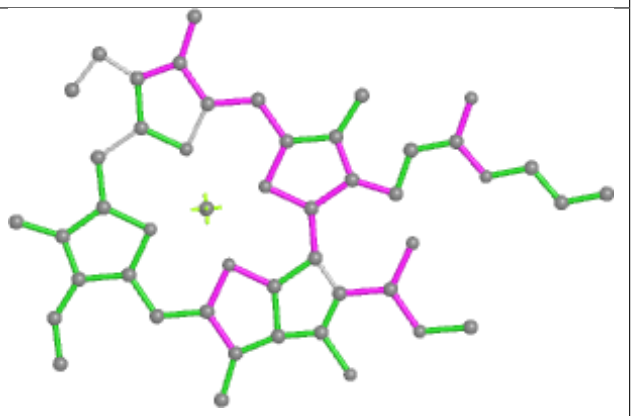

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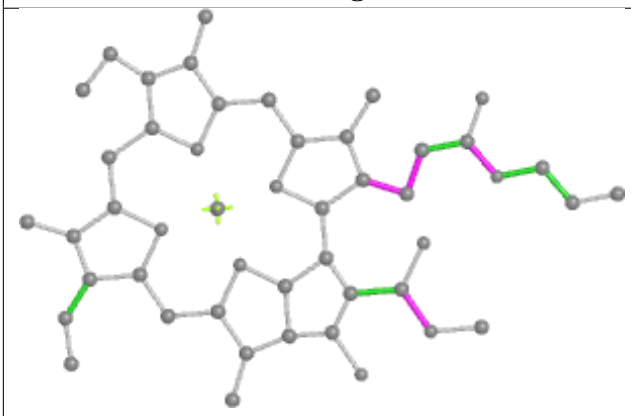

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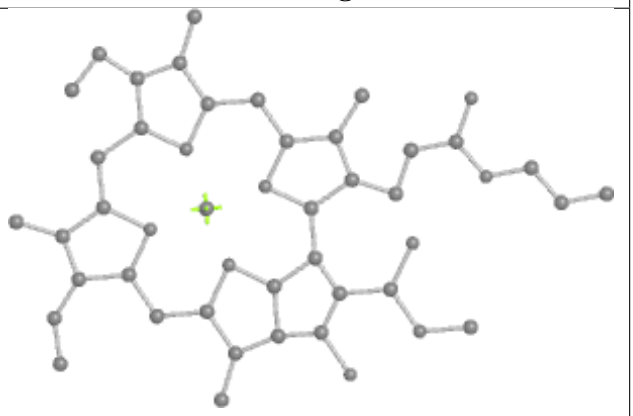
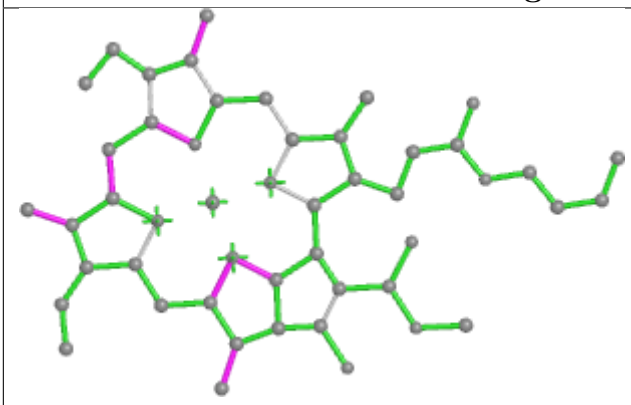


Rings

Ligand CLA C 514



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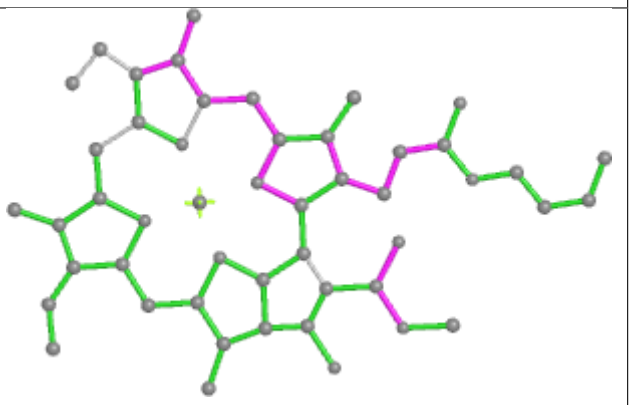

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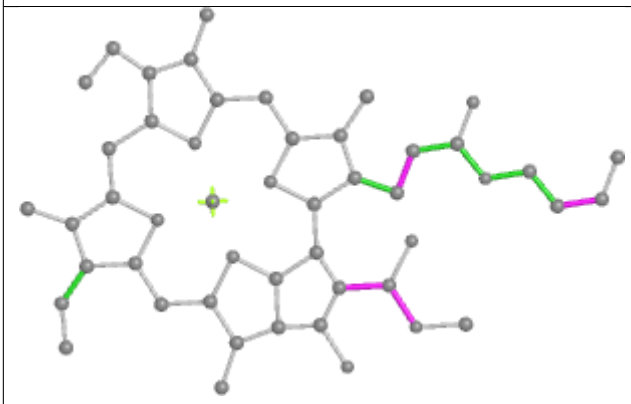

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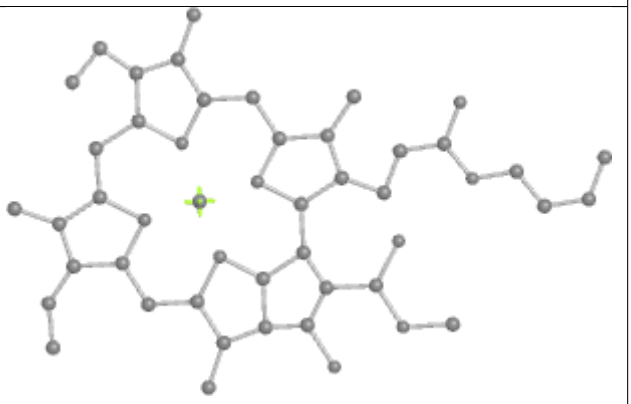
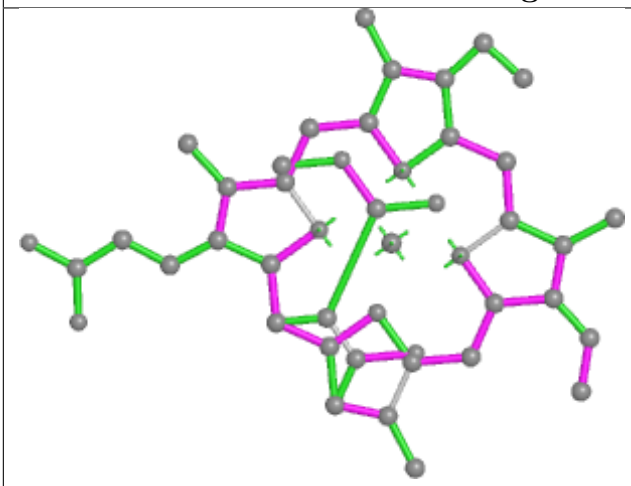


Rings

Ligand KC2 13 311



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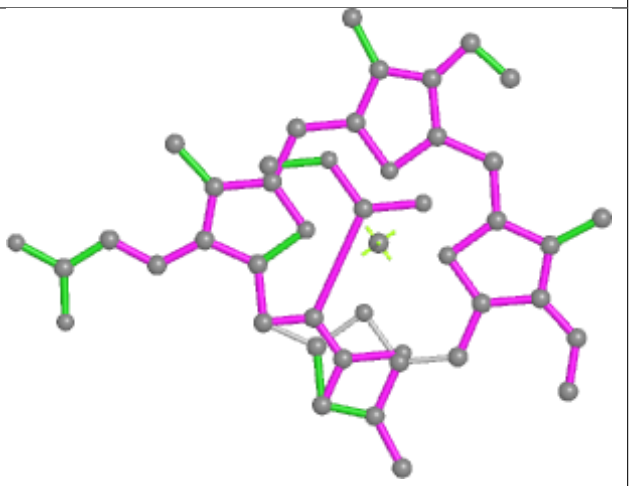

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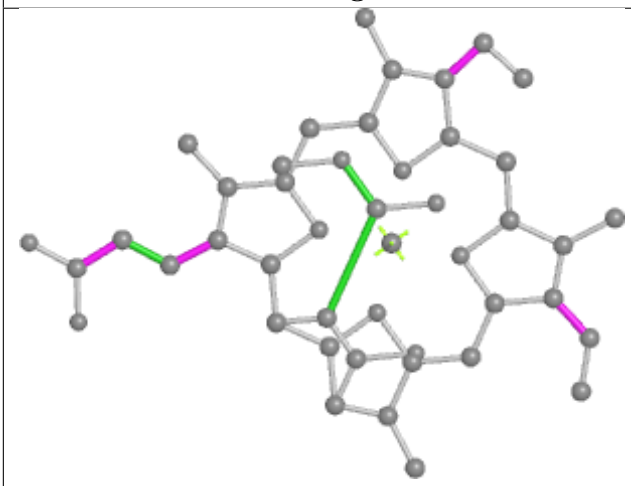

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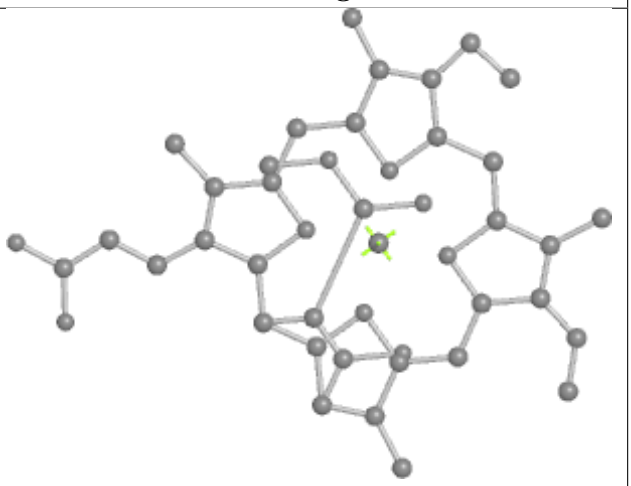
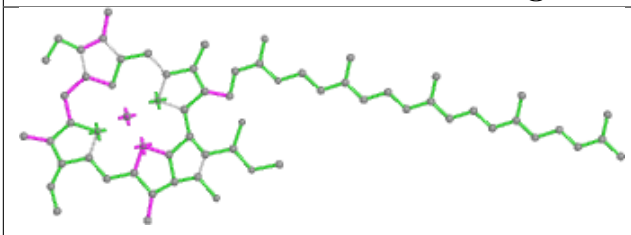


Rings

Ligand CLA b 603



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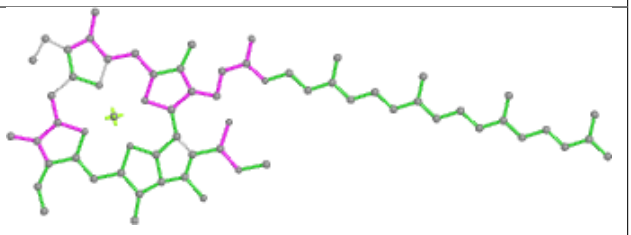

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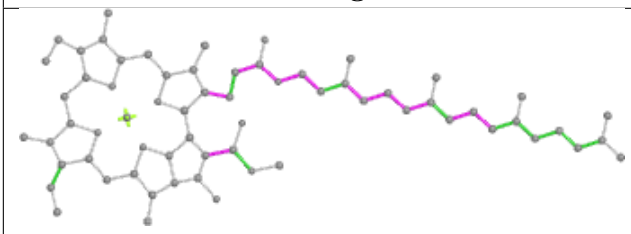

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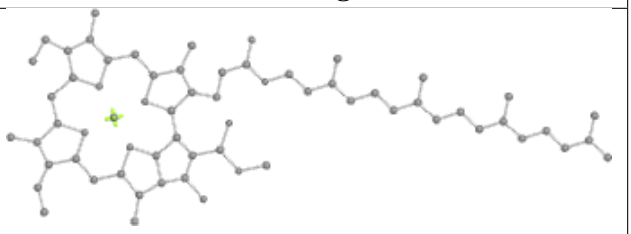
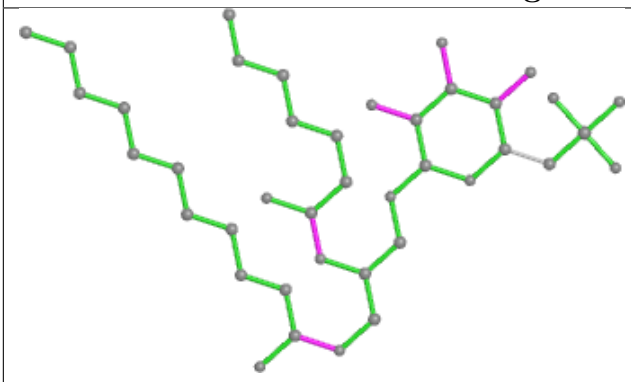


Rings

Ligand SQD A 411



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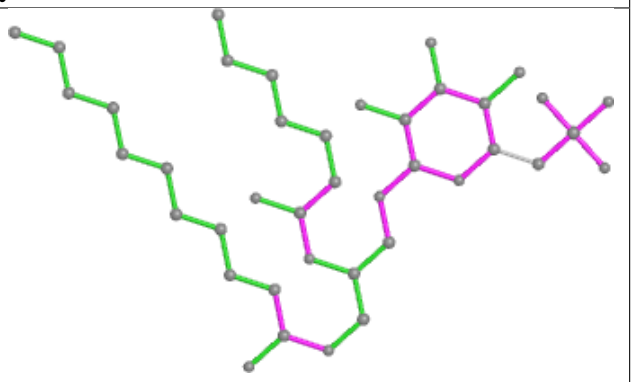

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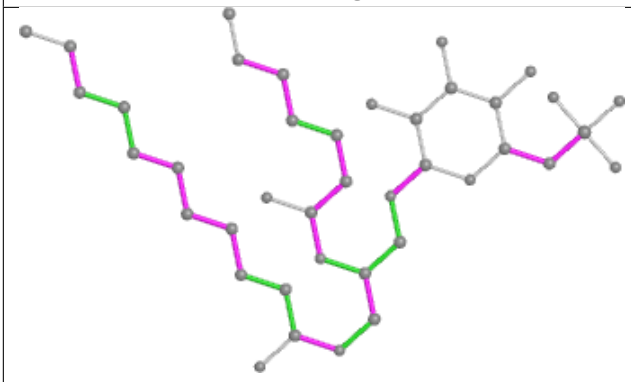

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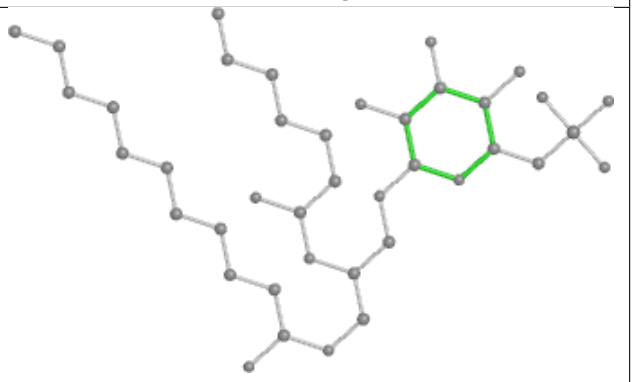
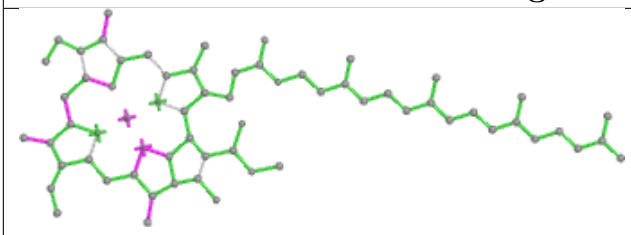


Rings

Ligand CLA 5 307



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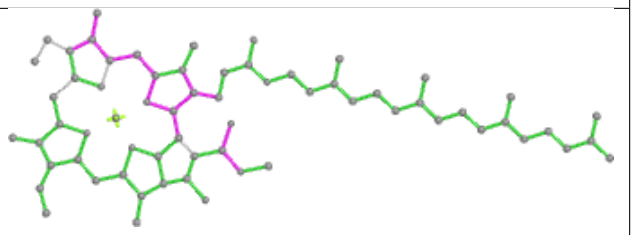

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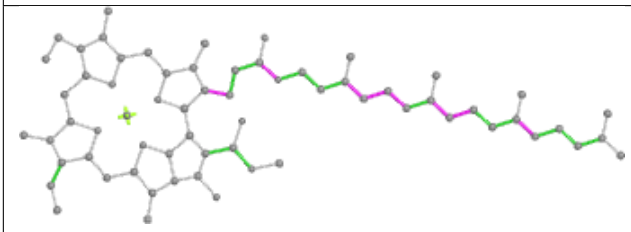

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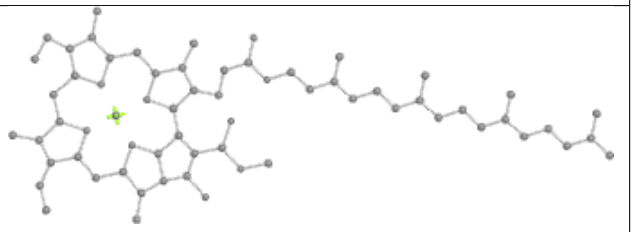
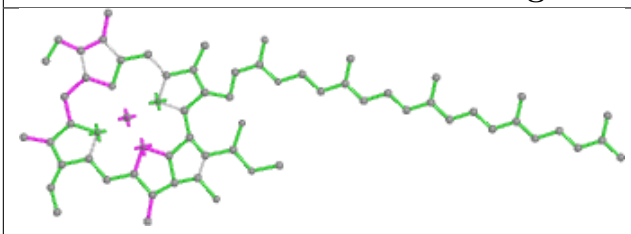


Rings

Ligand CLA b 608



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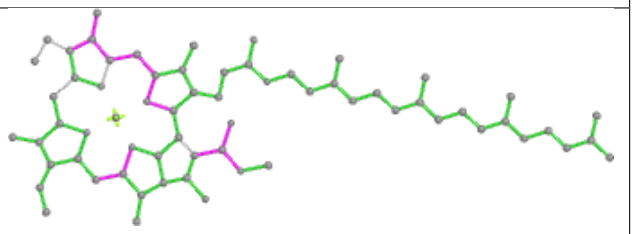

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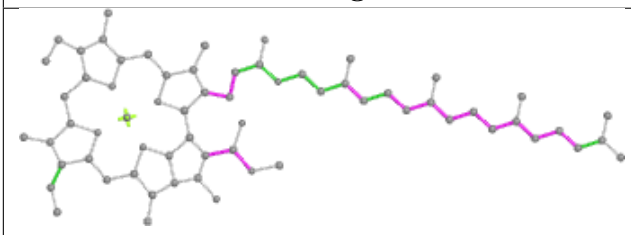

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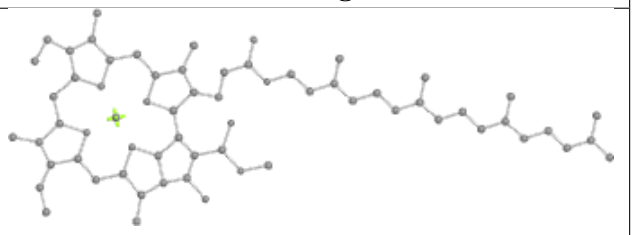
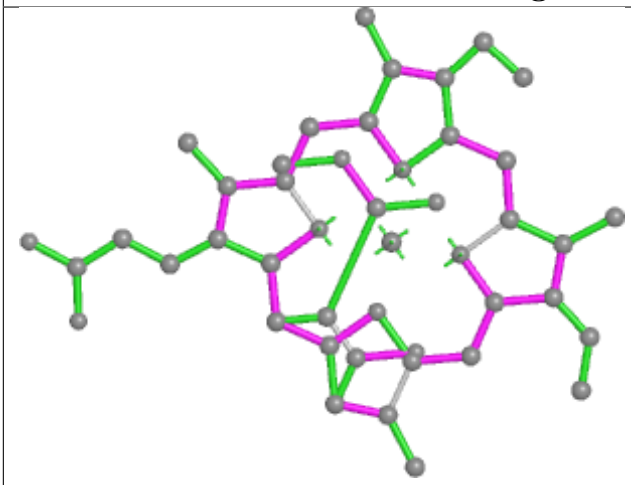


Rings

Ligand KC1 5 313



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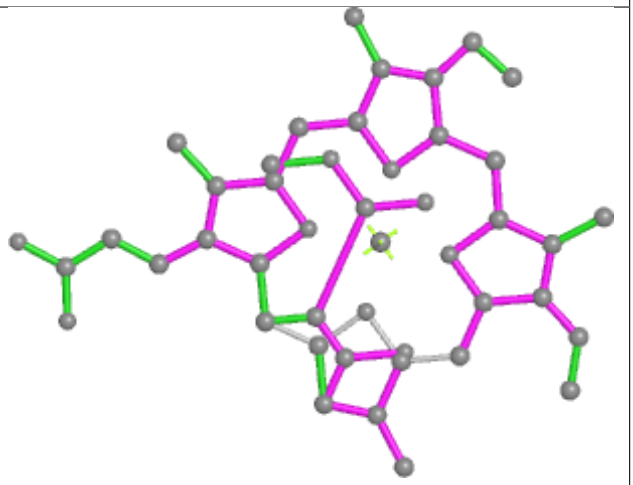

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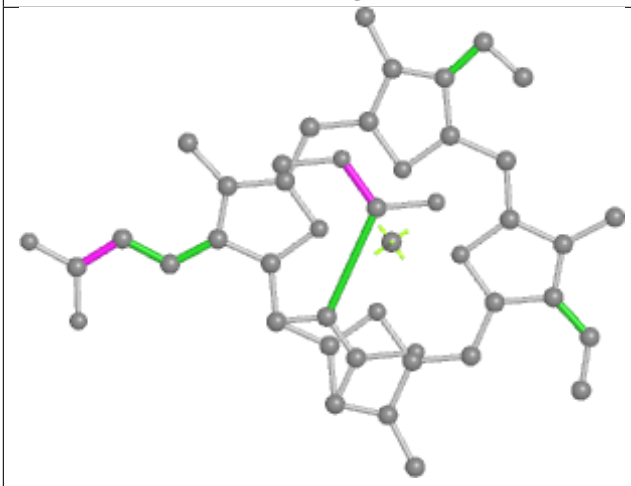

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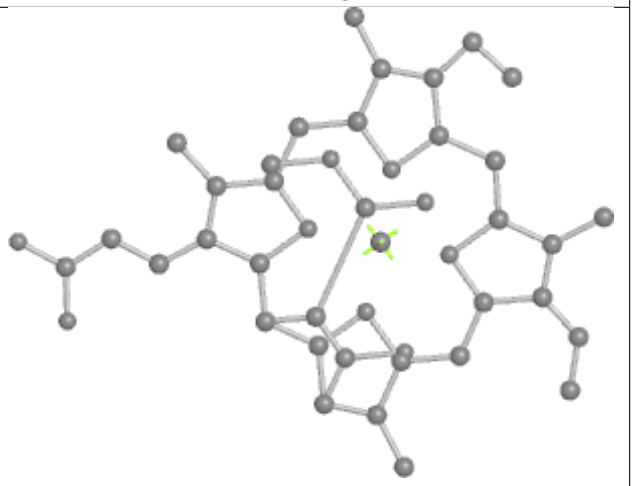
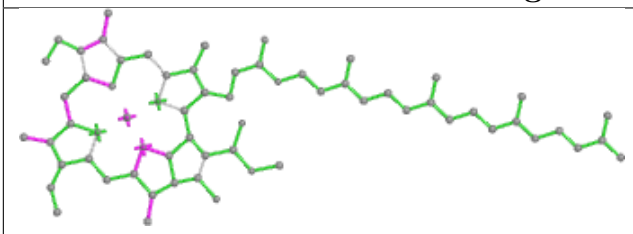


Rings

Ligand CLA B 608



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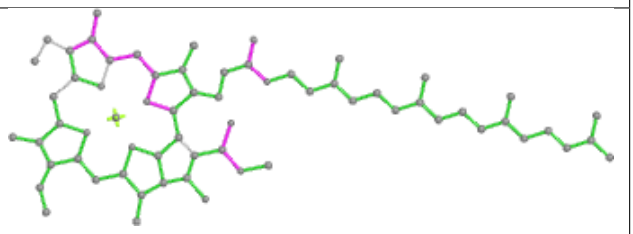

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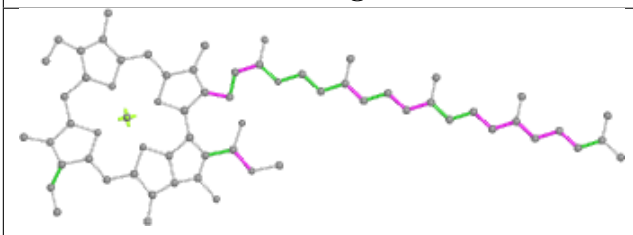

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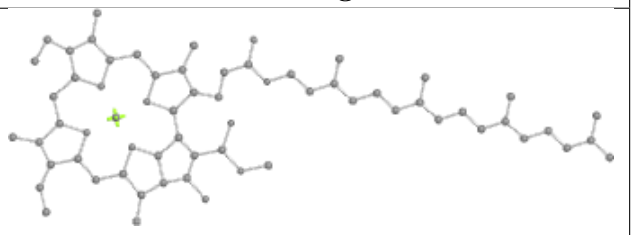
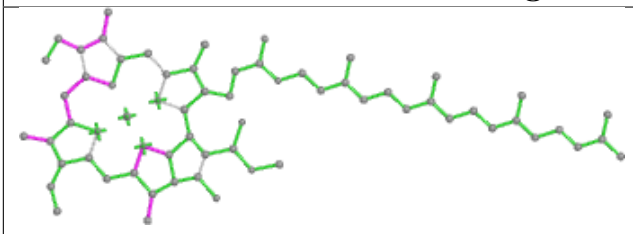


Rings

Ligand CLA B 615



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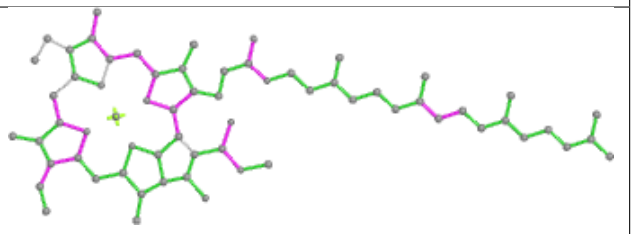

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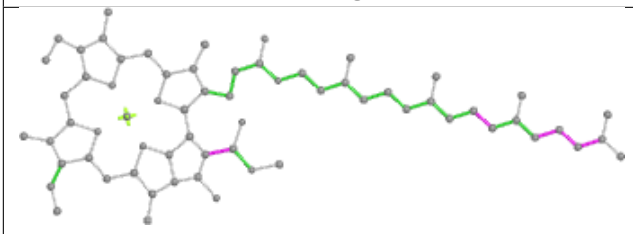

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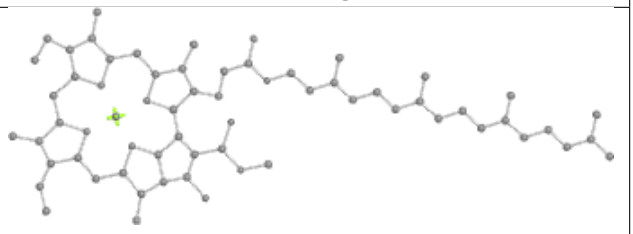
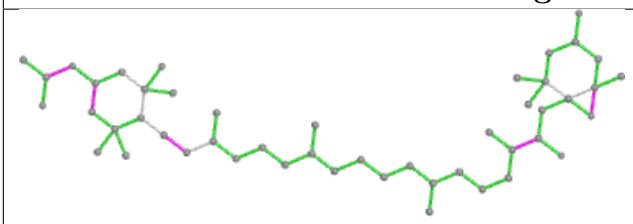


Rings

Ligand A86 5 301



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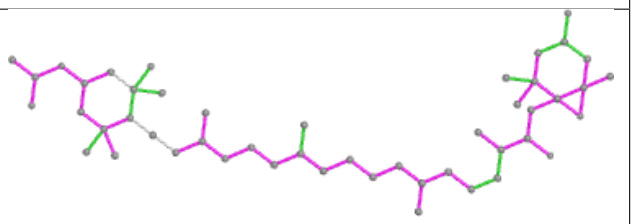
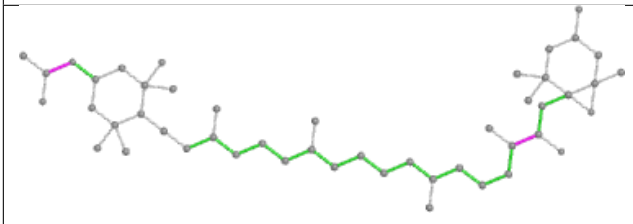


Bond angles



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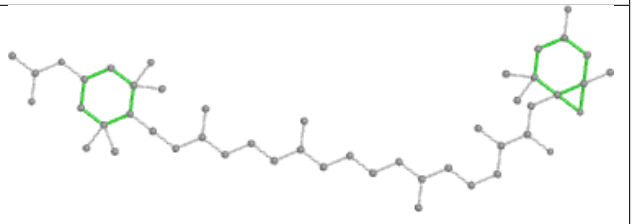
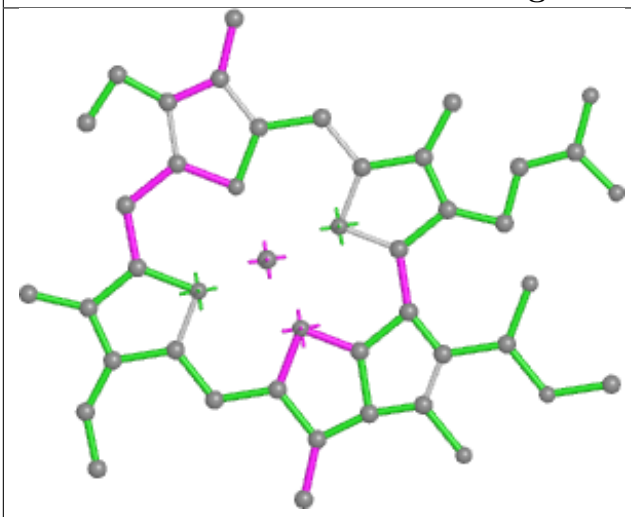


Rings

Ligand CLA 5 311



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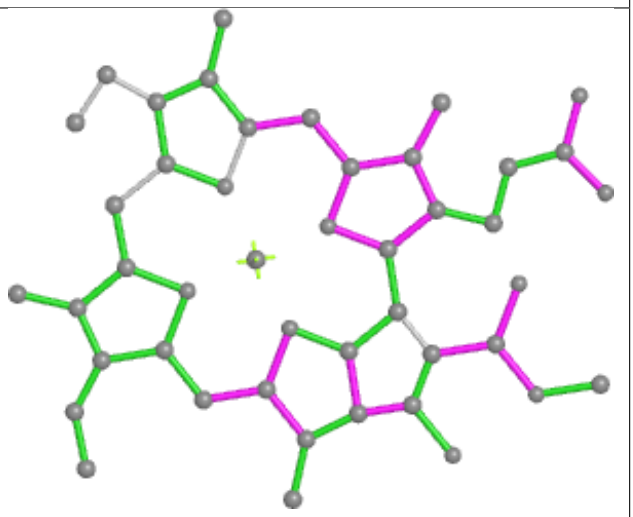
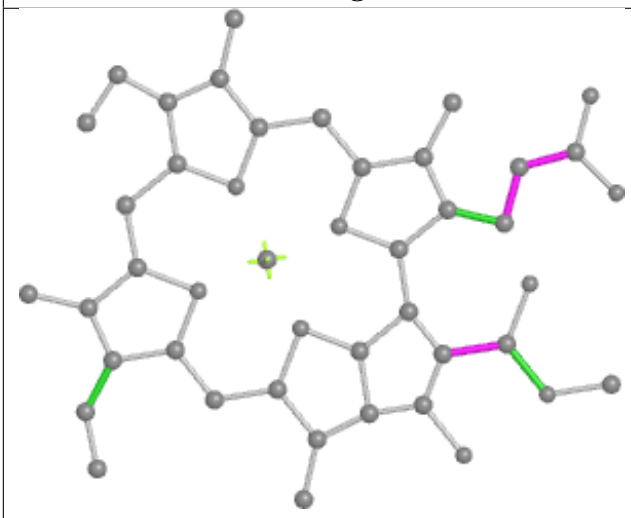


Bond angles



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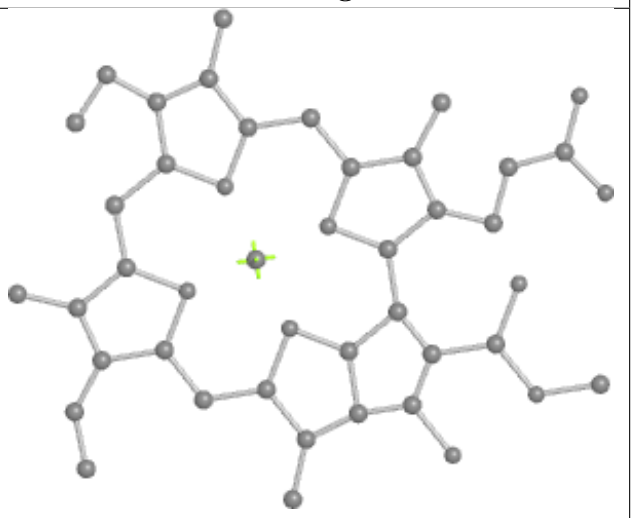
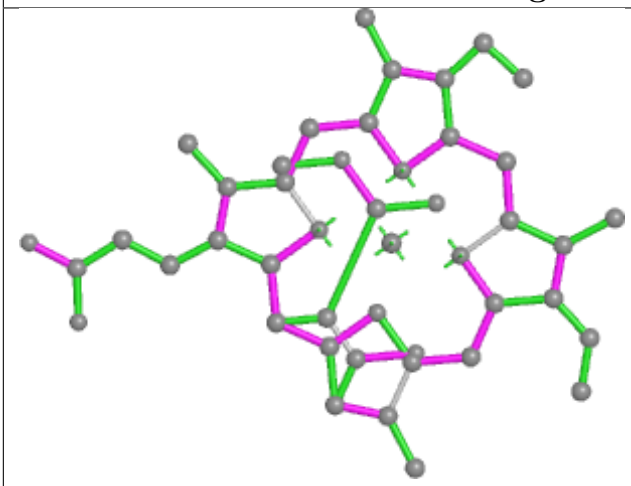


Rings

Ligand KC1 p 609



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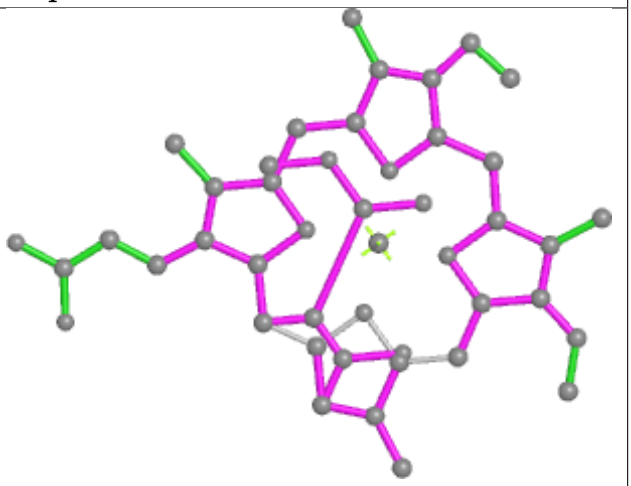
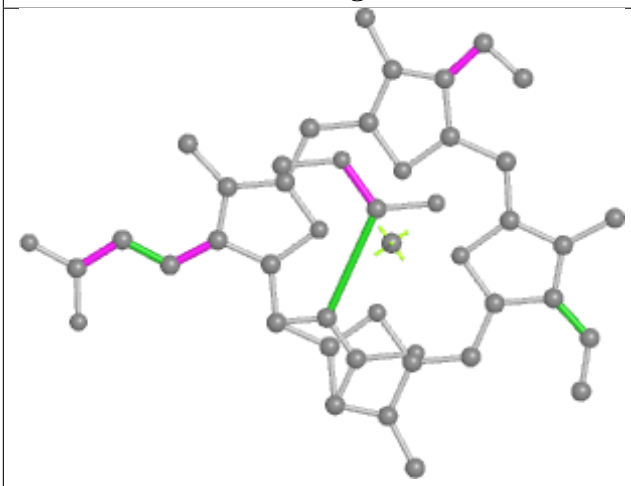


Bond angles



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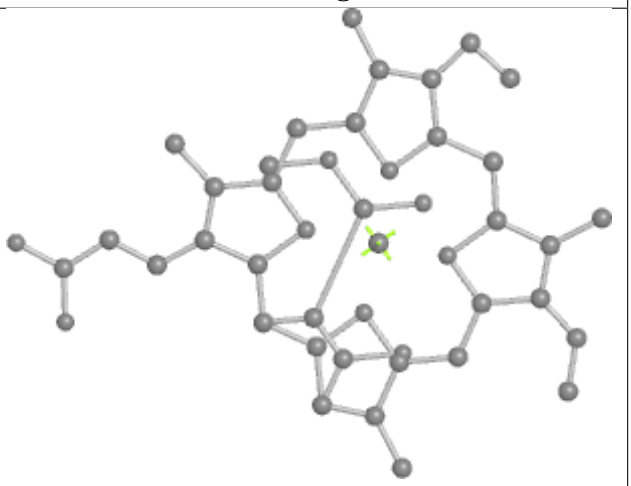
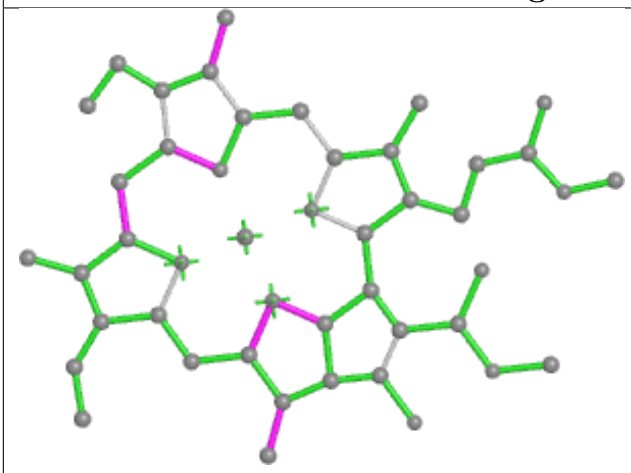
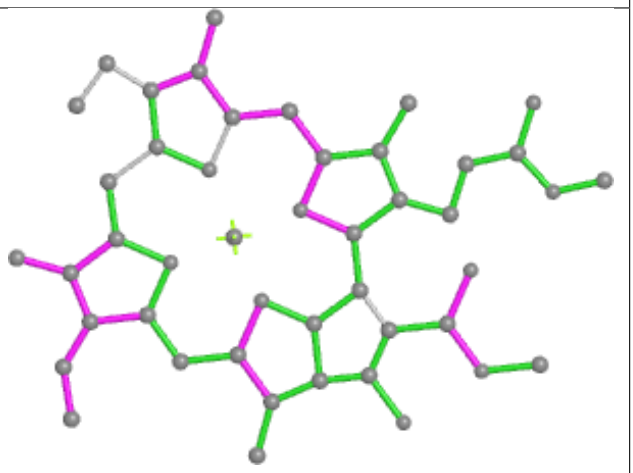


Rings

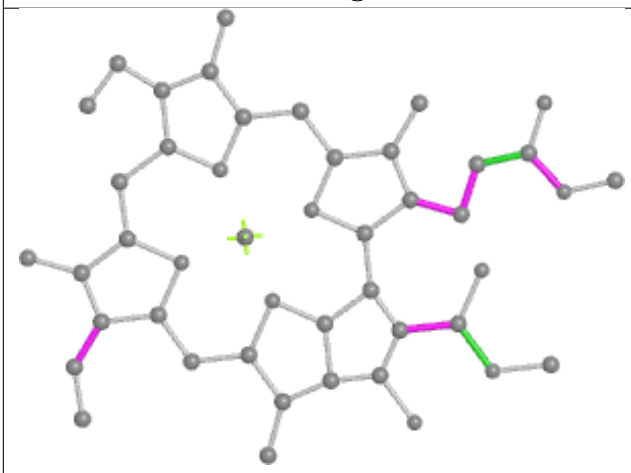
Ligand CLA 0 312



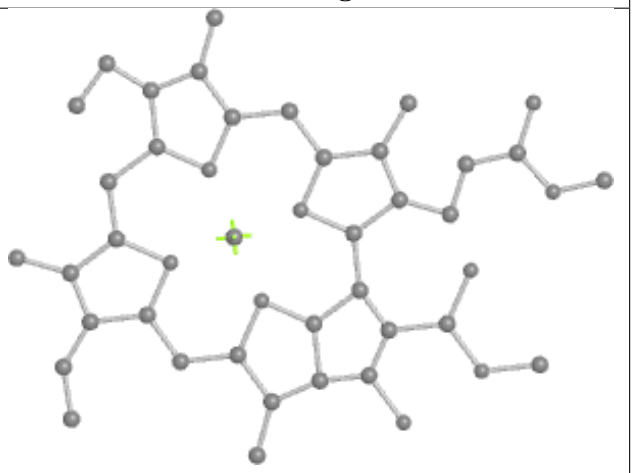
Bond lengths



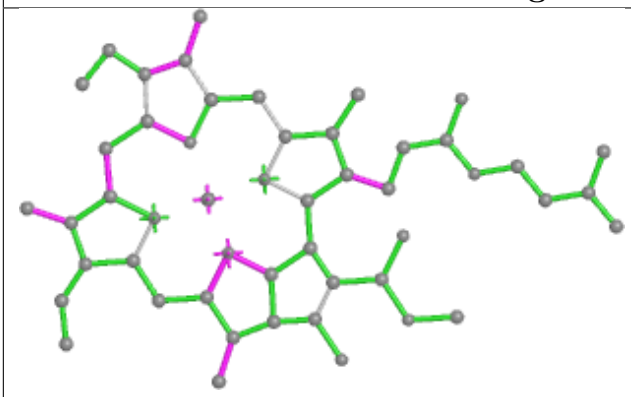
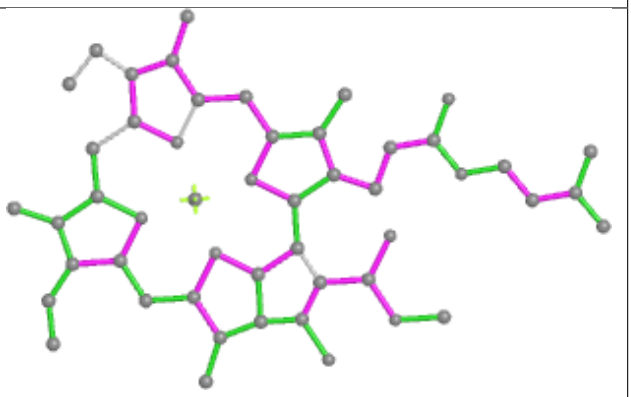
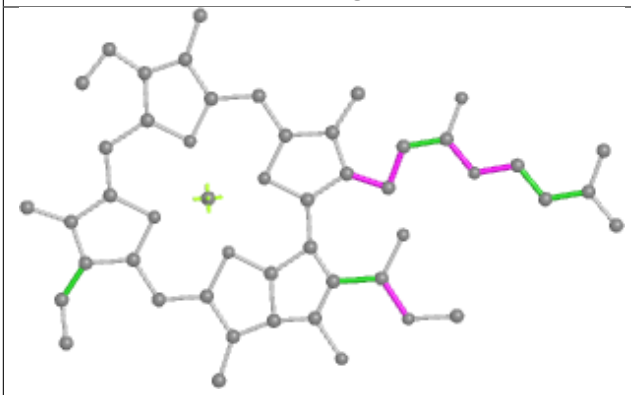
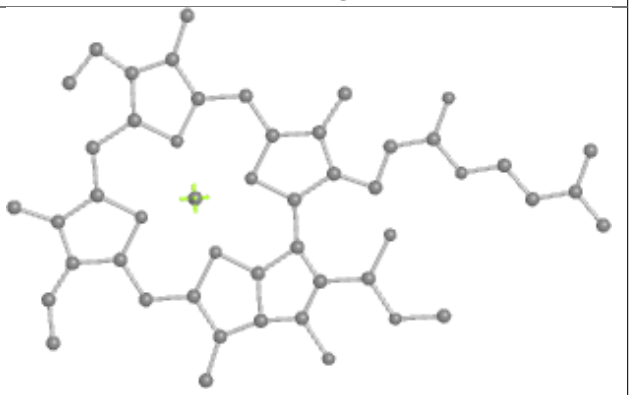
Bond angles

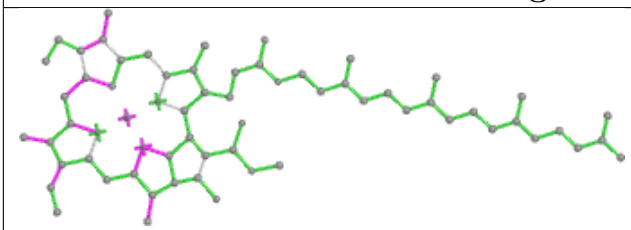
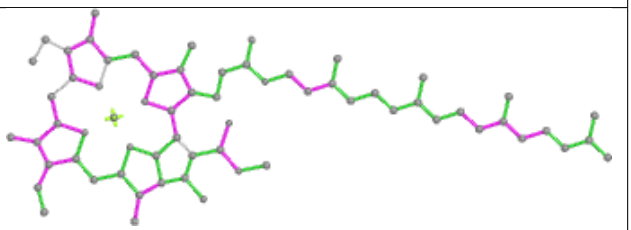
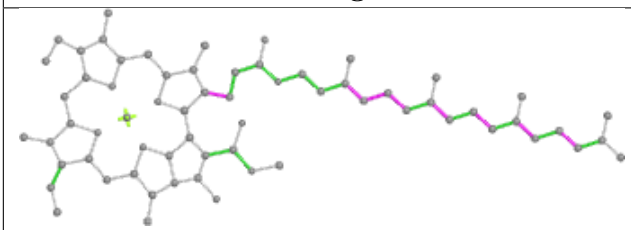
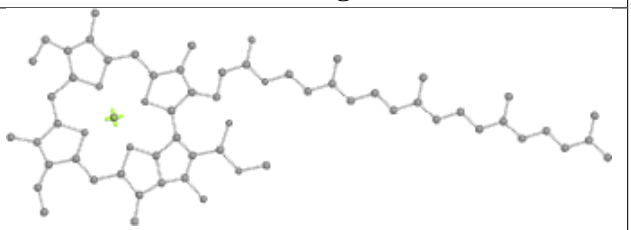


Torsions

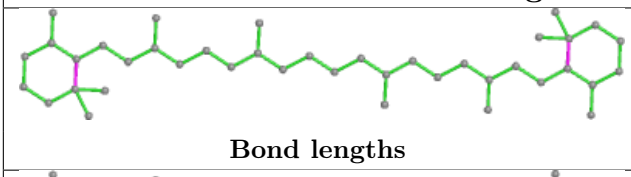


Rings

Ligand CLA 7 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 619



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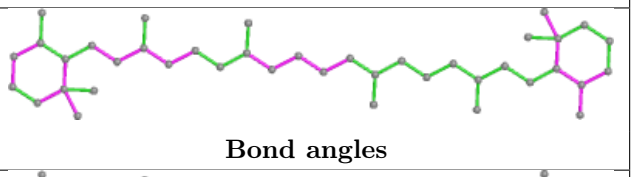

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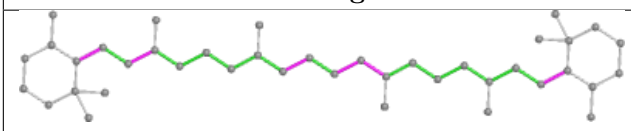

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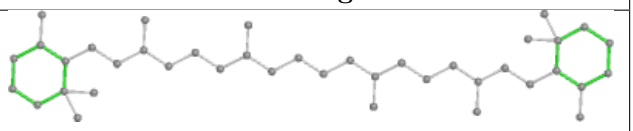
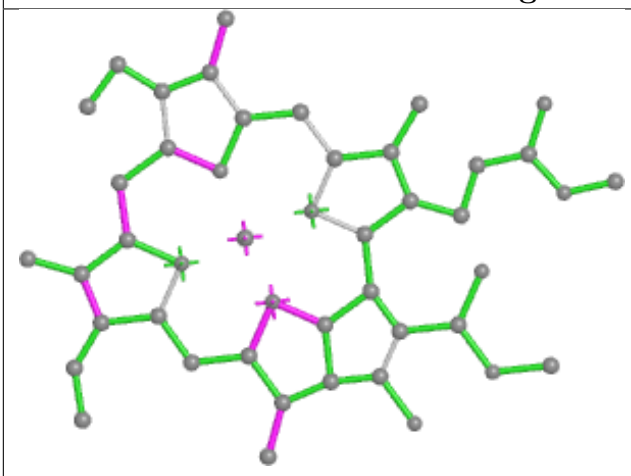


Rings

Ligand CLA 14 311



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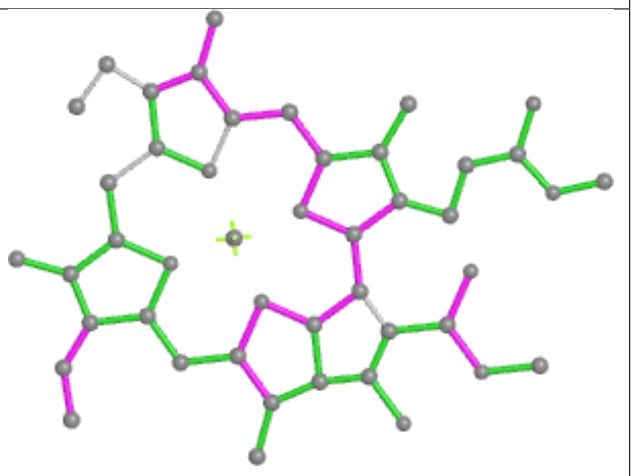

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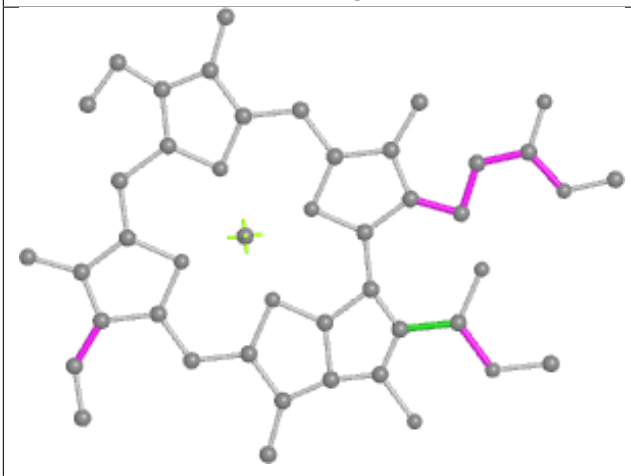

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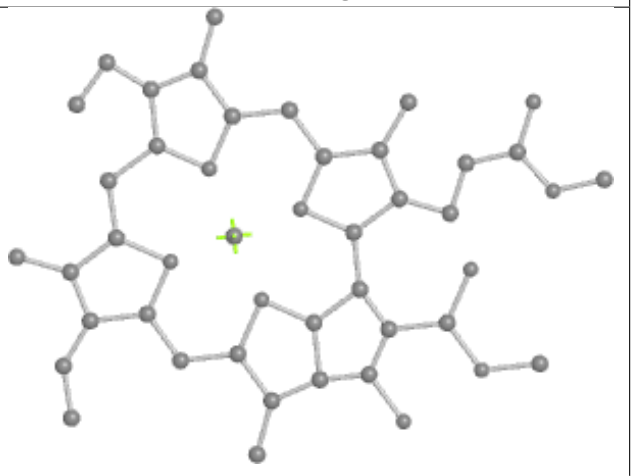
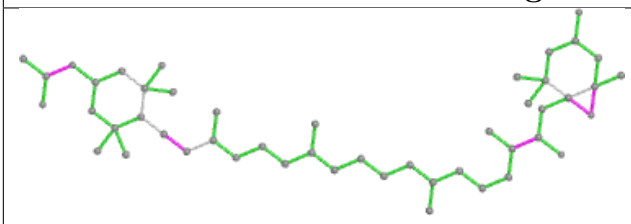


Rings

Ligand A86 16 304



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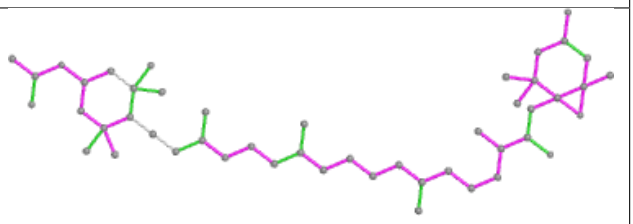

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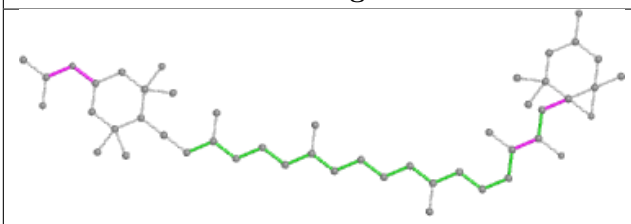

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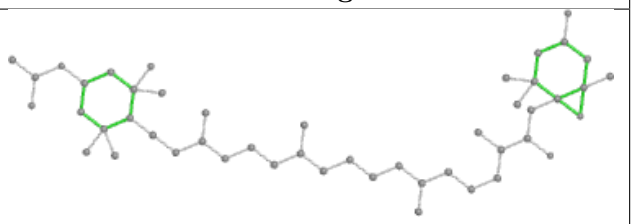
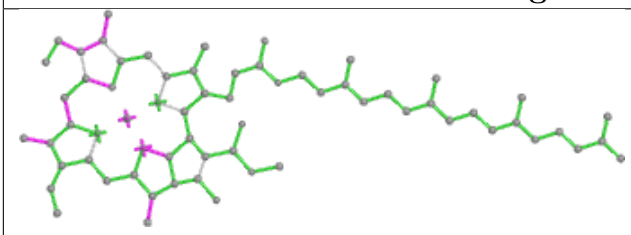


Rings

Ligand CLA c 512



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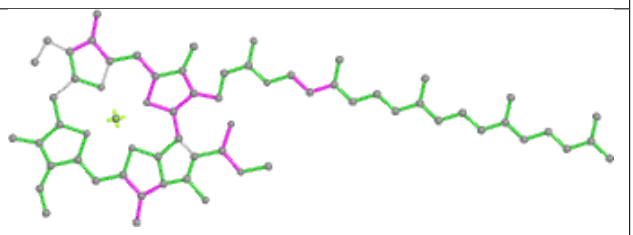

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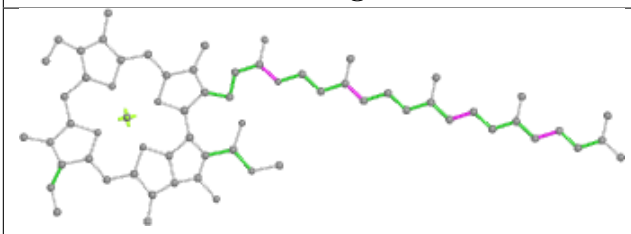

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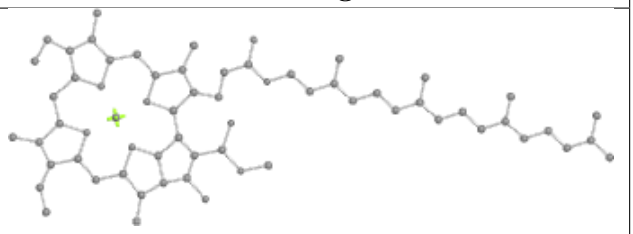
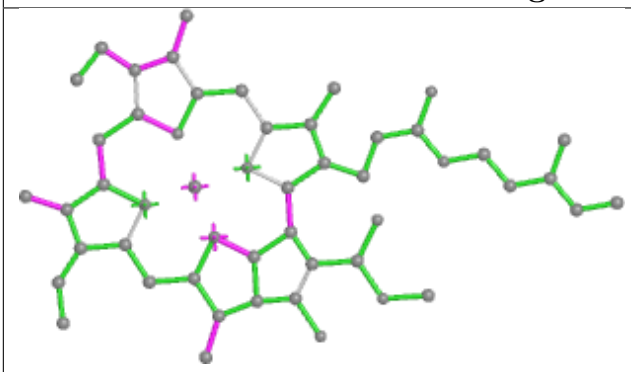


Rings

Ligand CLA 4 312



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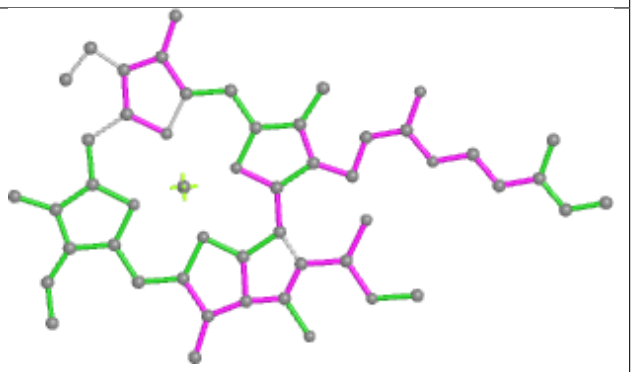

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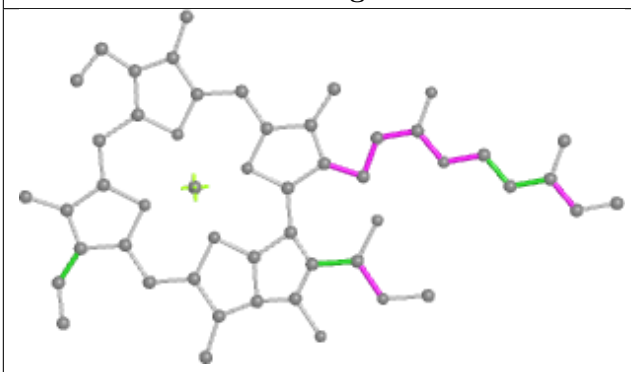

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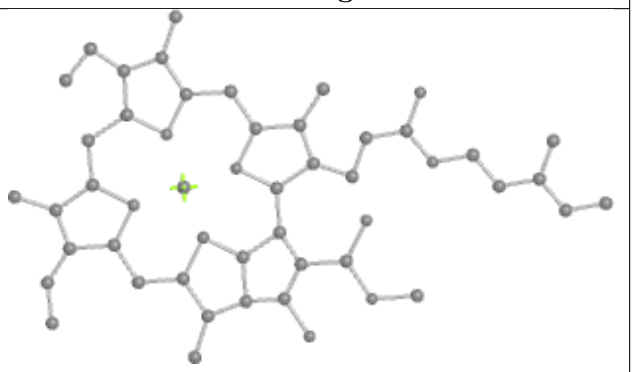
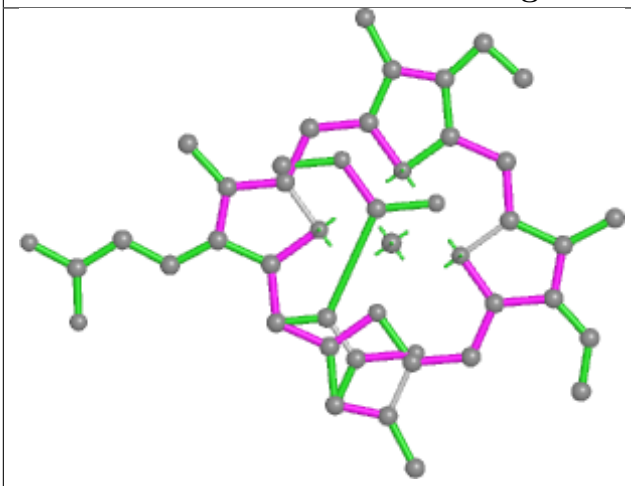


Rings

Ligand KC1 16 315



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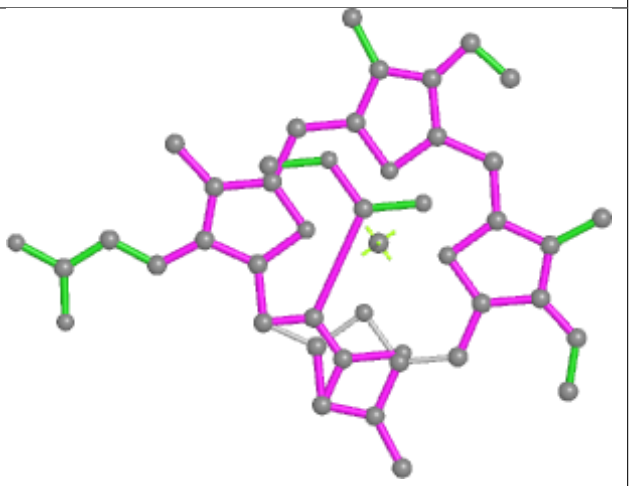

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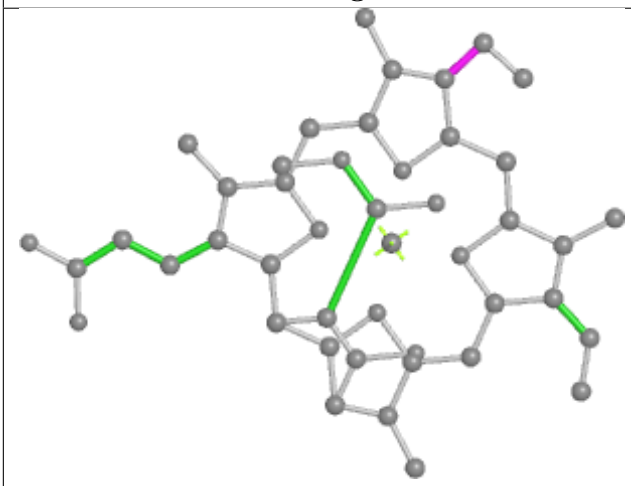

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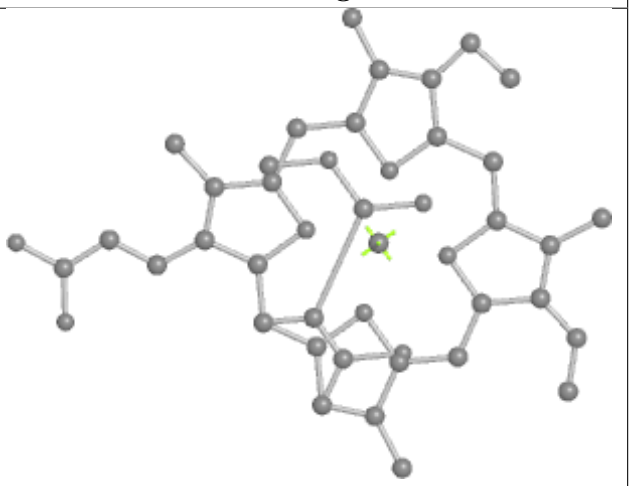
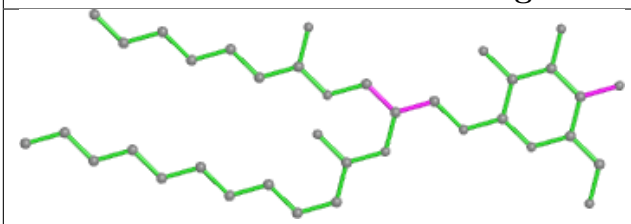


Rings

Ligand LMG 15 314



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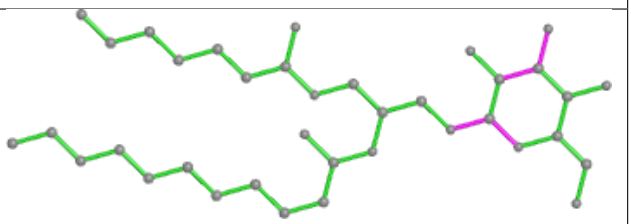

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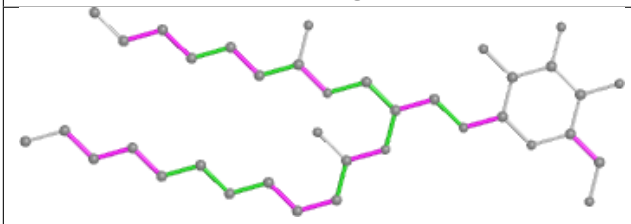

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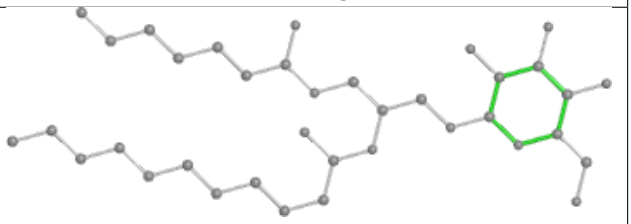
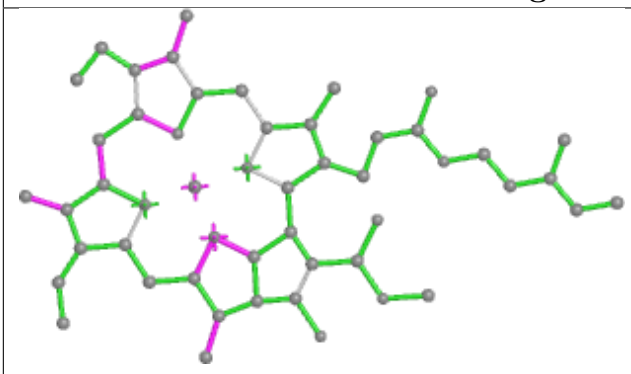


Rings

Ligand CLA z 101



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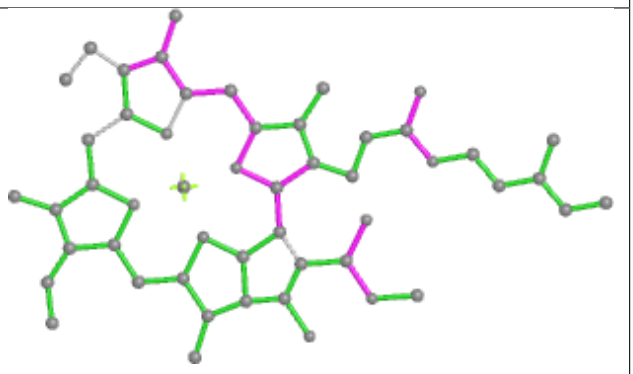

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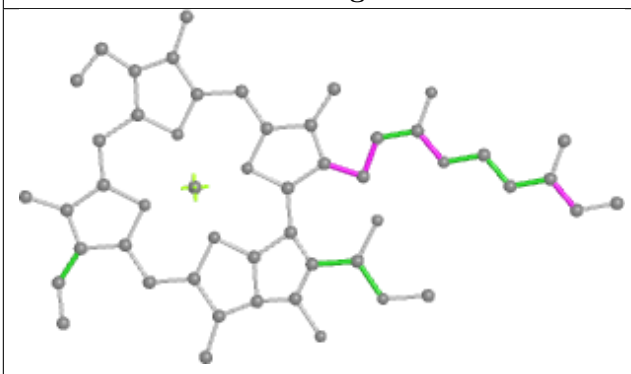

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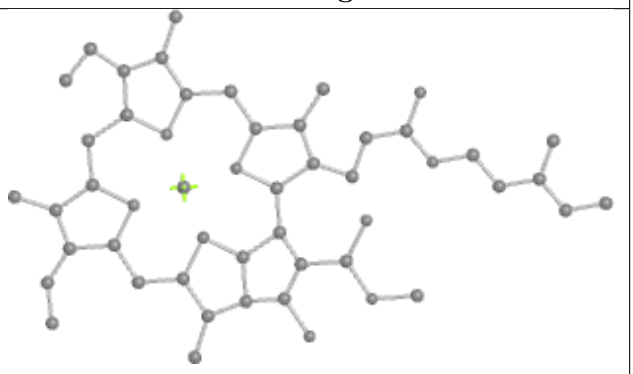
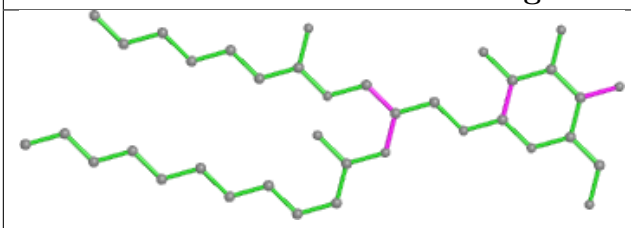


Rings

Ligand LMG 5 315



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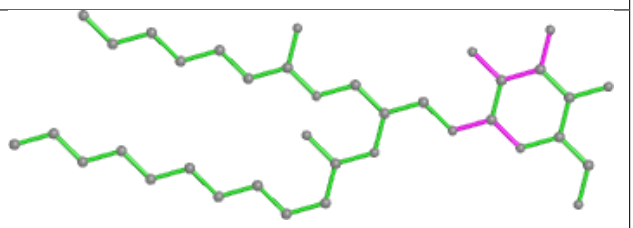

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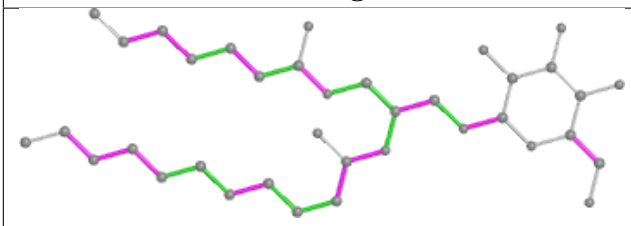

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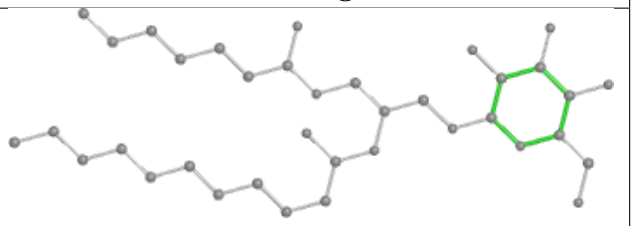
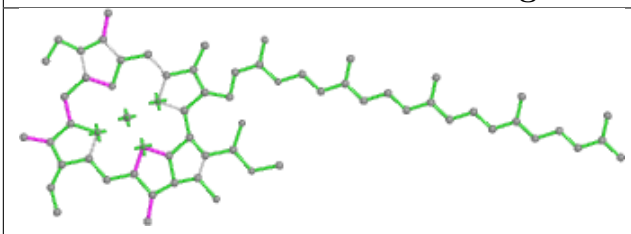


Rings

Ligand CLA 19 308



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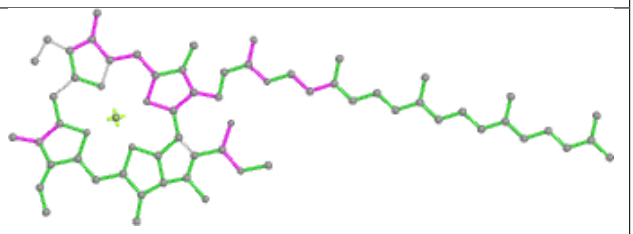
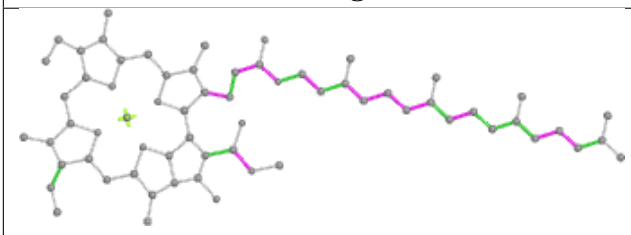


Bond angles



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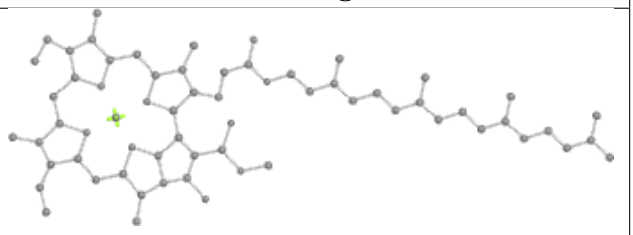
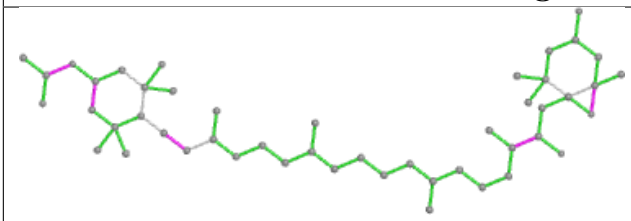


Rings

Ligand A86 7 301



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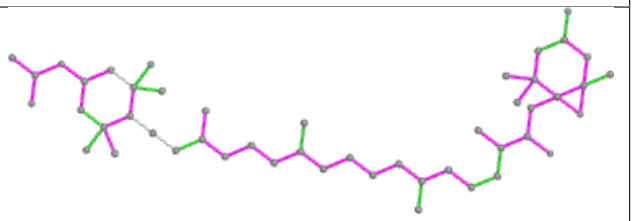
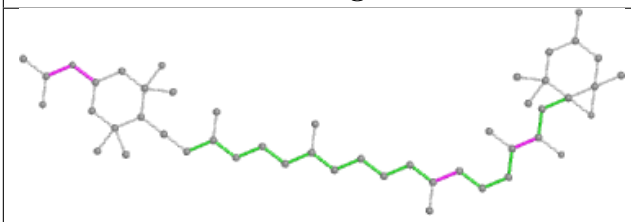


Bond angles



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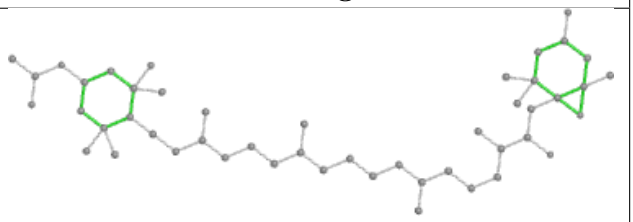
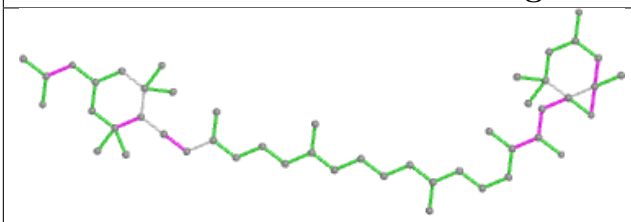


Rings

Ligand A86 11 306



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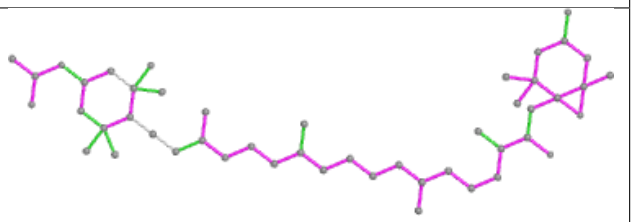

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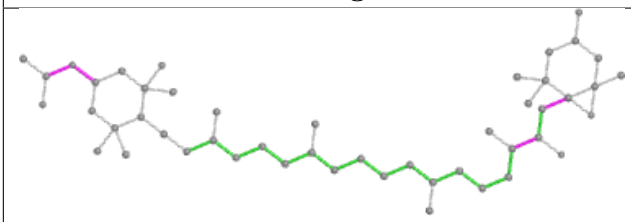
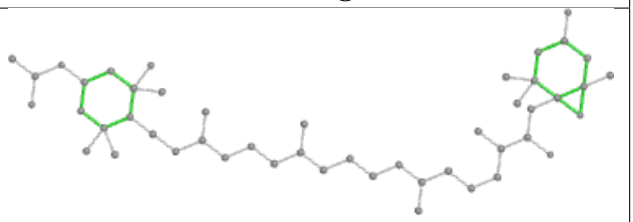
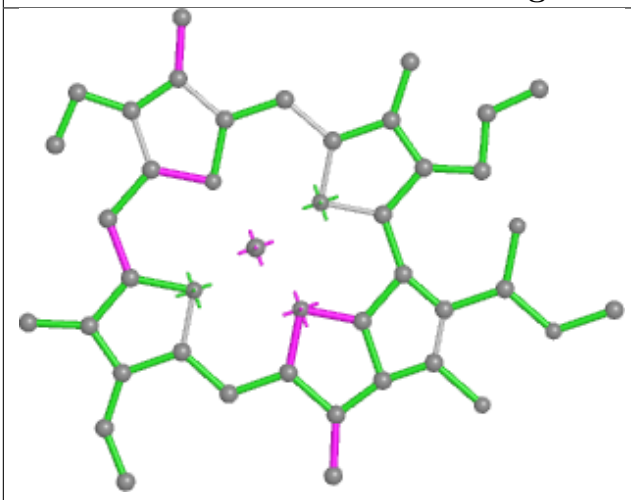


Torsions



Rings

Ligand CLA 1 307



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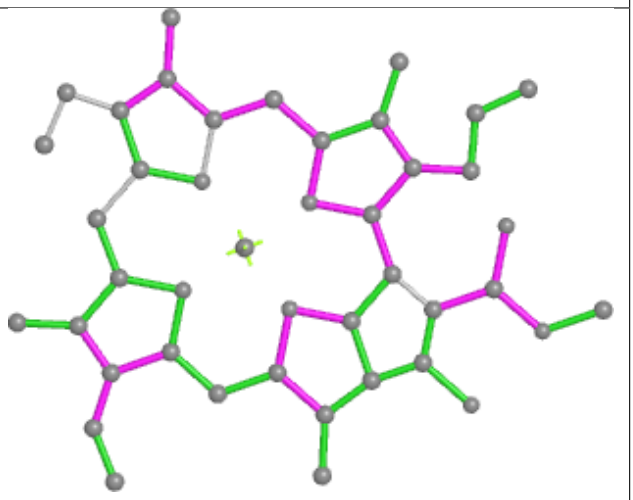

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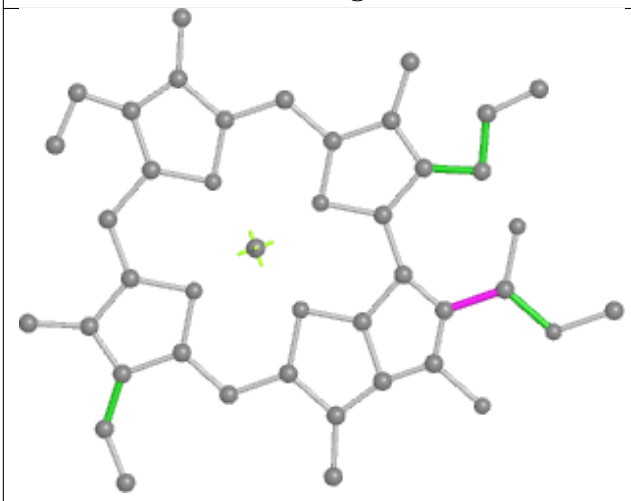

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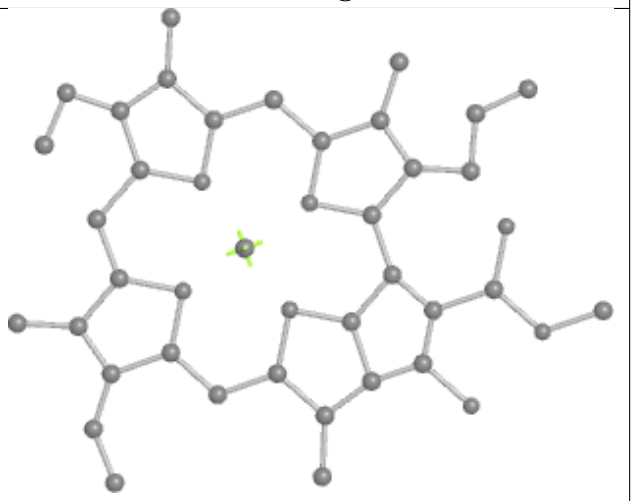
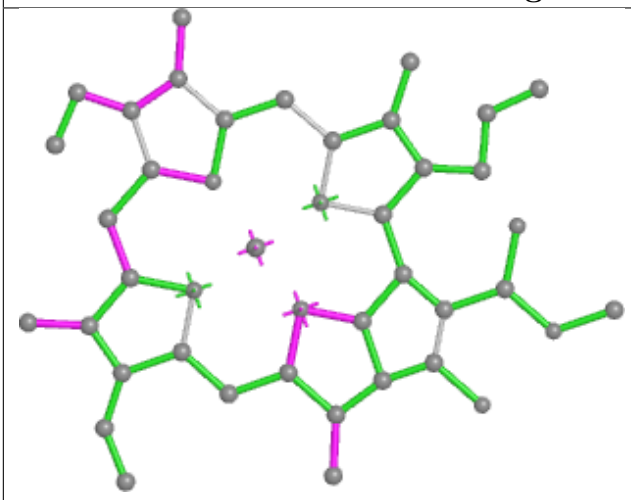


Rings

Ligand CLA P 607



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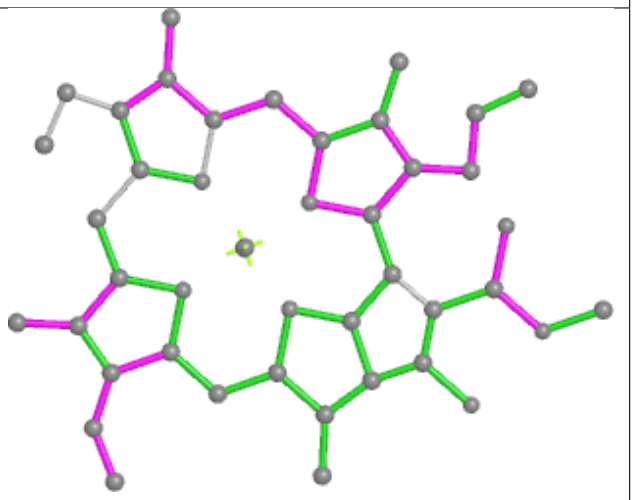

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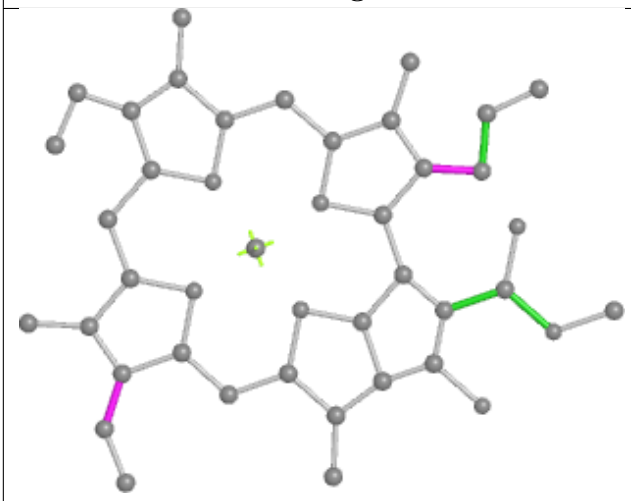

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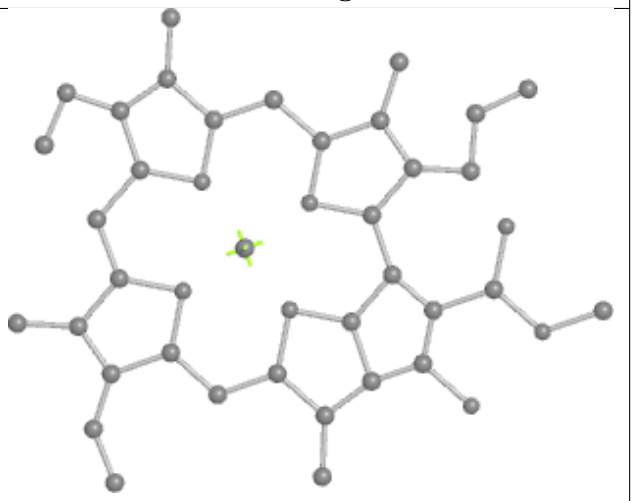
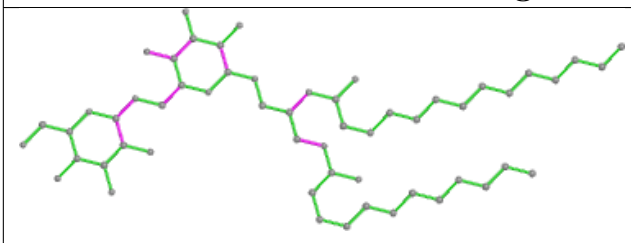


Rings

Ligand DGD W 203



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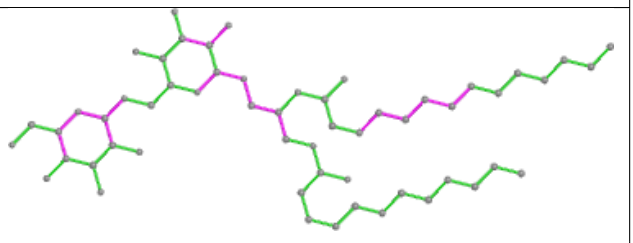

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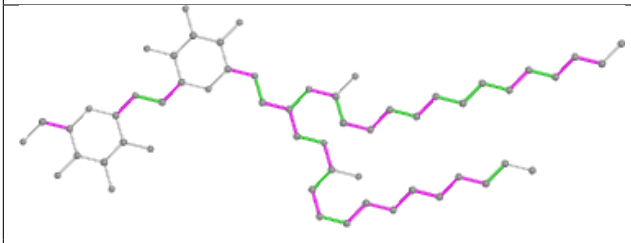

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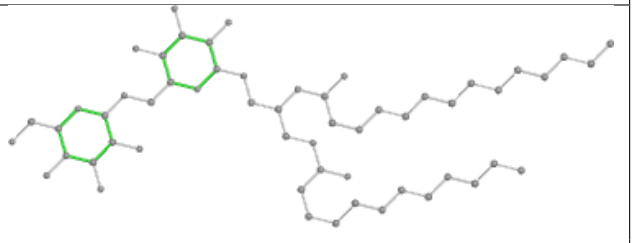
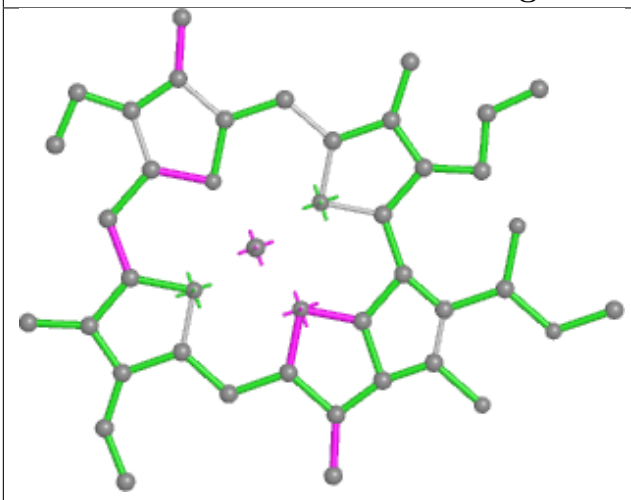


Rings

Ligand CLA 11 307



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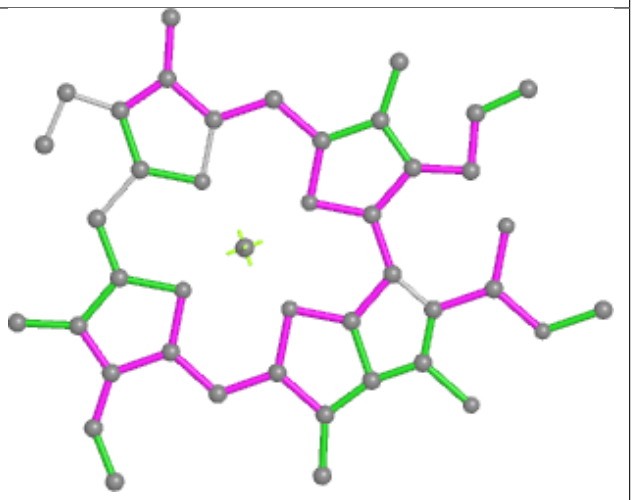

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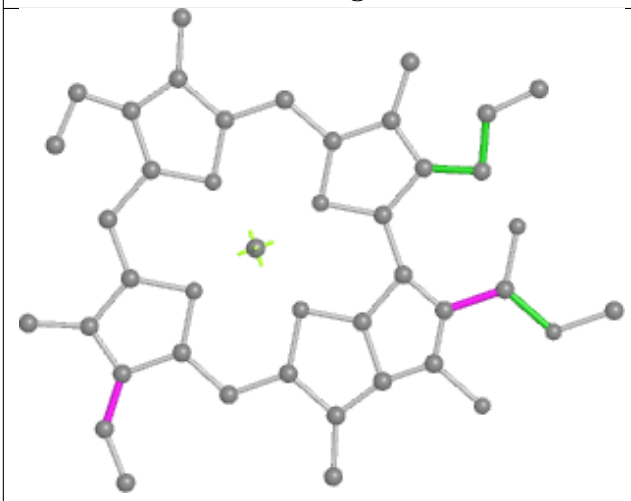

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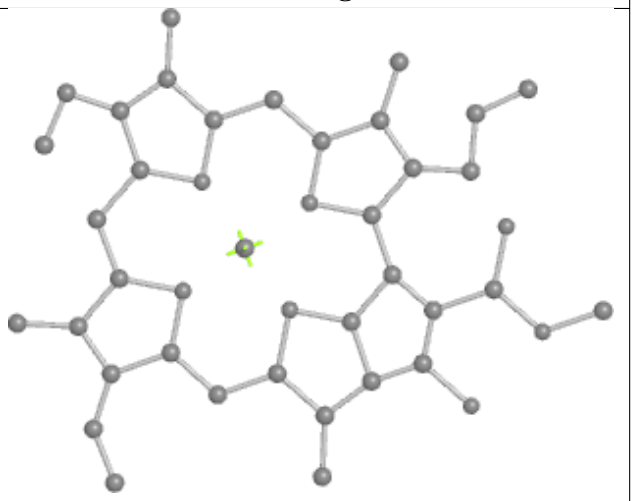
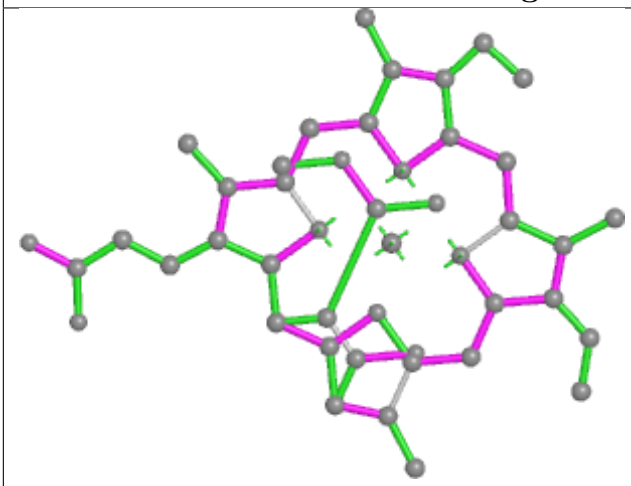


Rings

Ligand KC1 14 313



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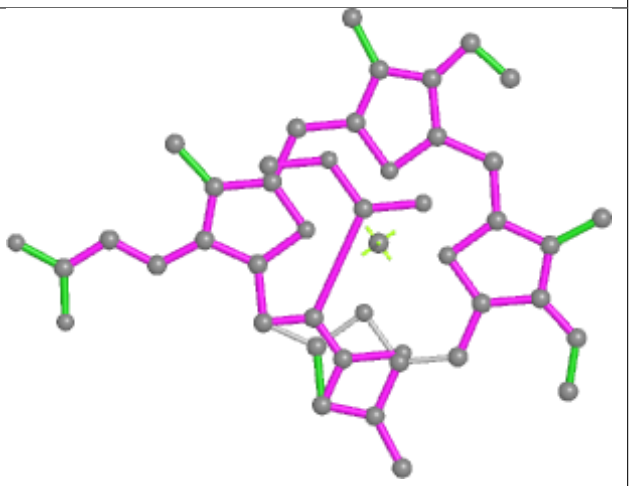

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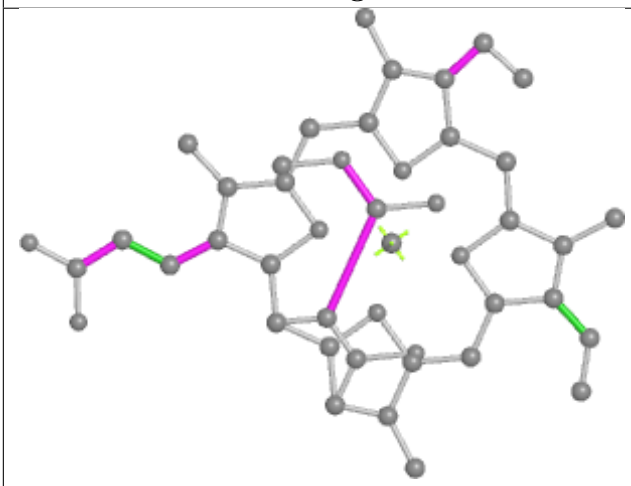

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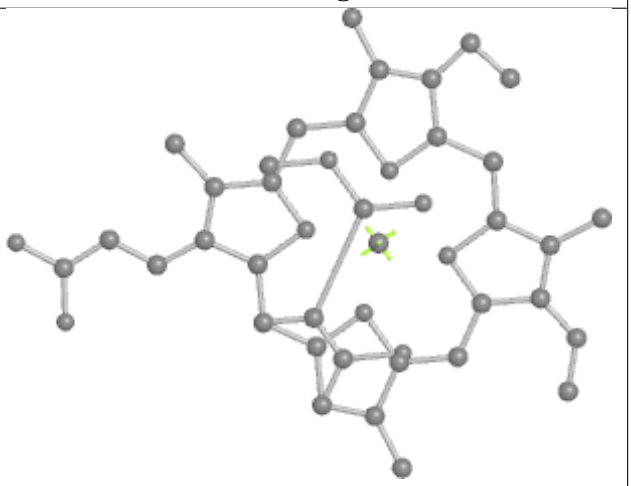
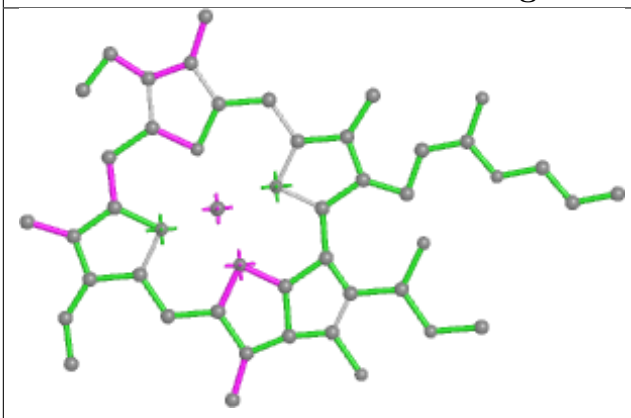


Rings

Ligand CLA 12 313



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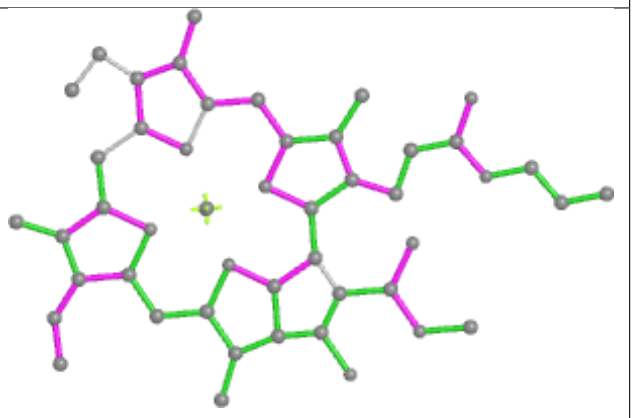

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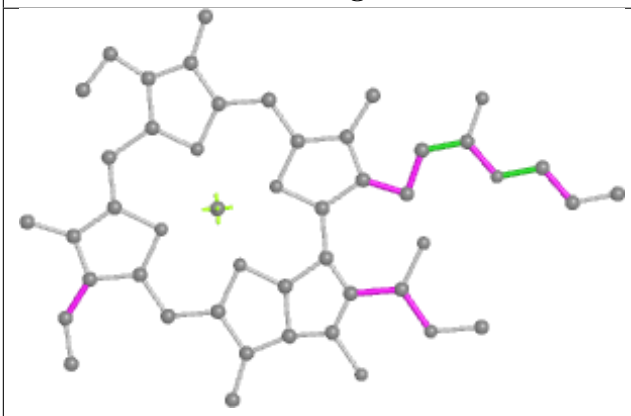

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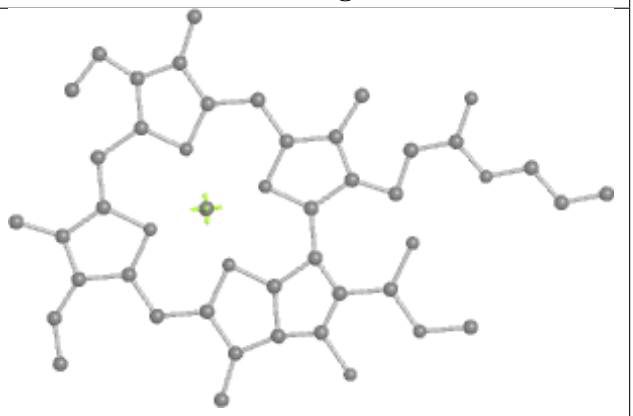
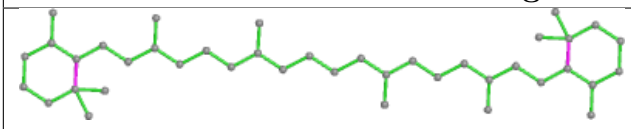


Rings

Ligand BCR B 618



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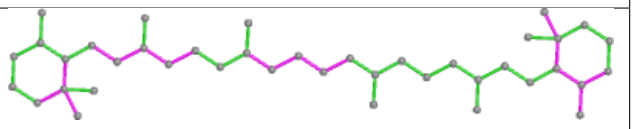

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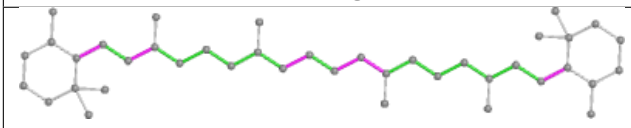
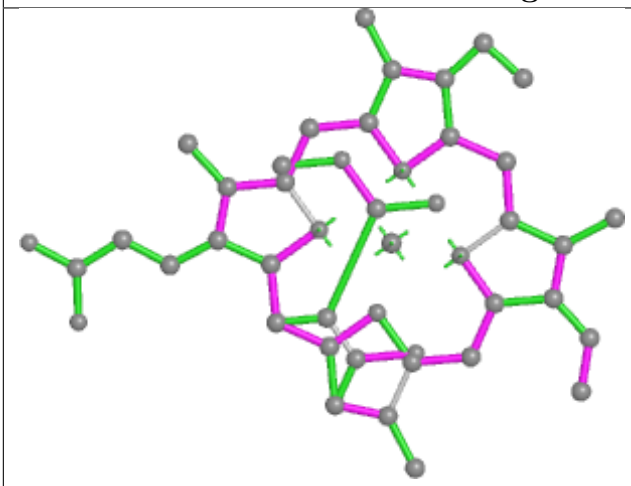


Torsions

Rings

Ligand KC2 14 308



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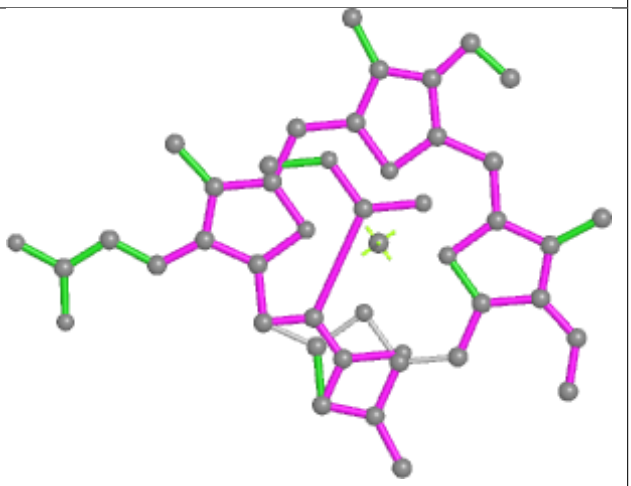

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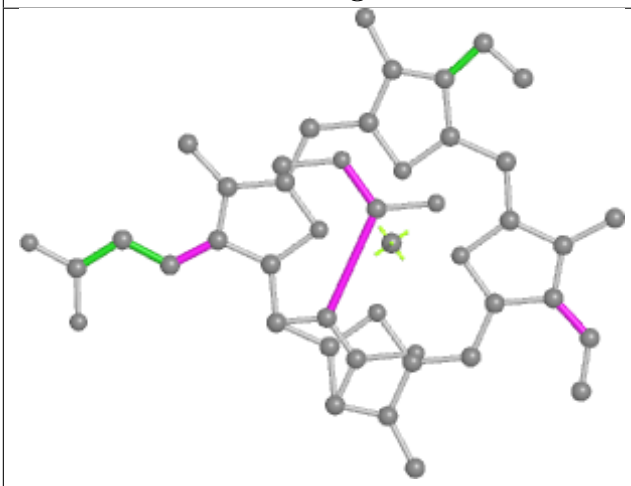

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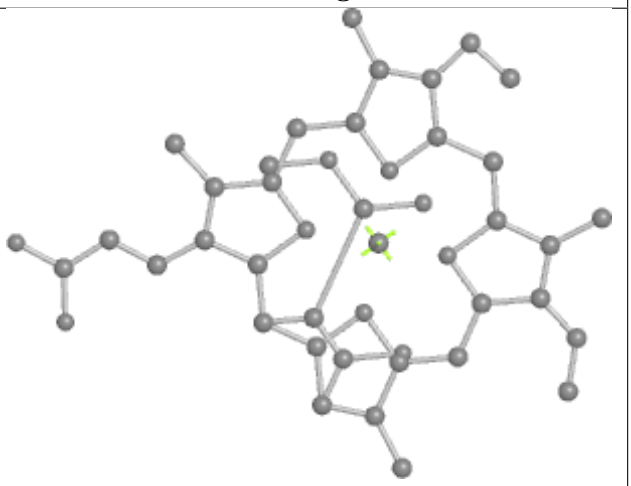
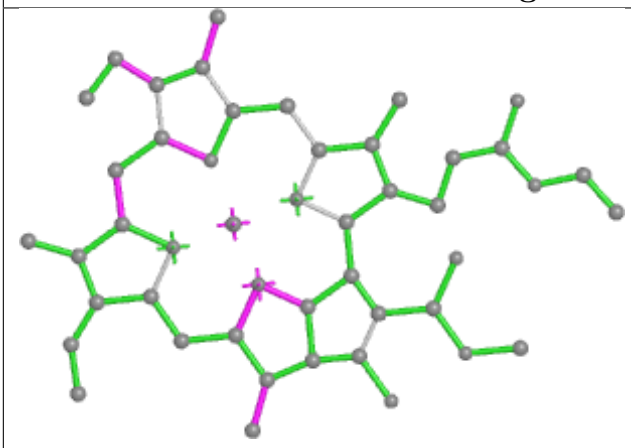


Rings

Ligand CLA 16 313



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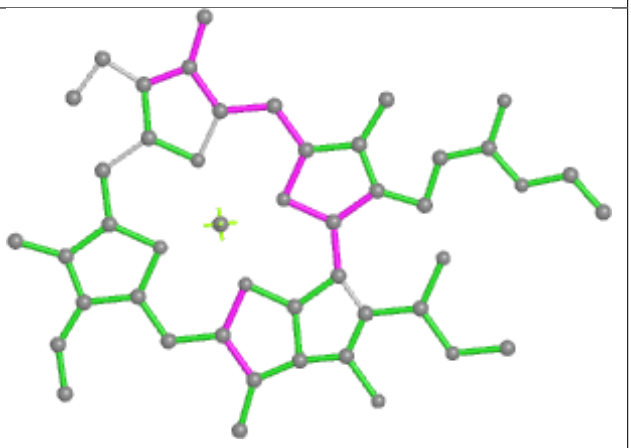

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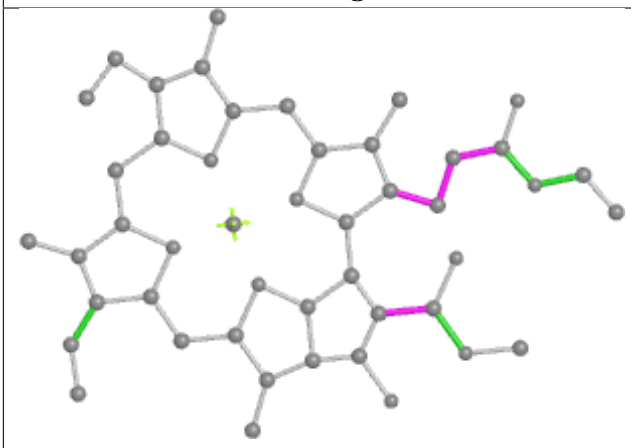

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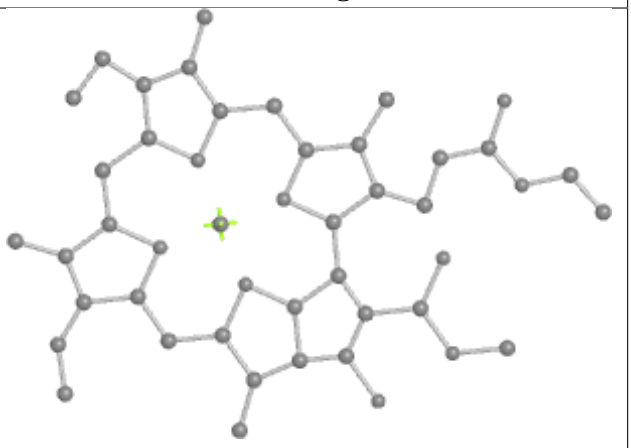
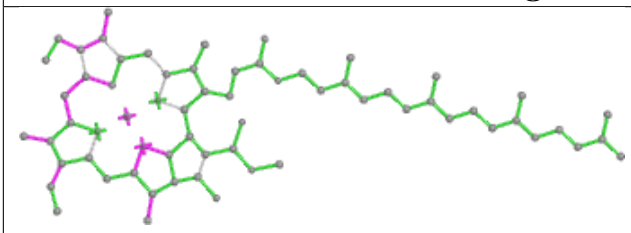


Rings

Ligand CLA B 605



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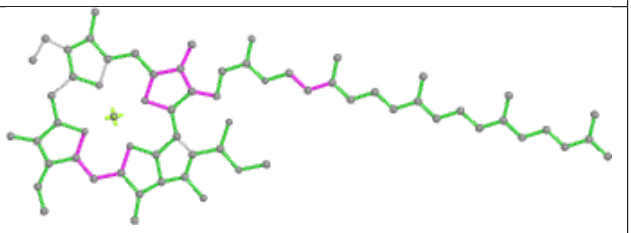

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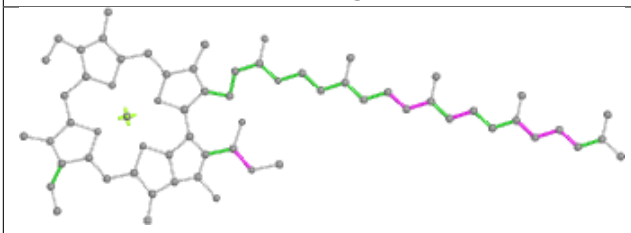

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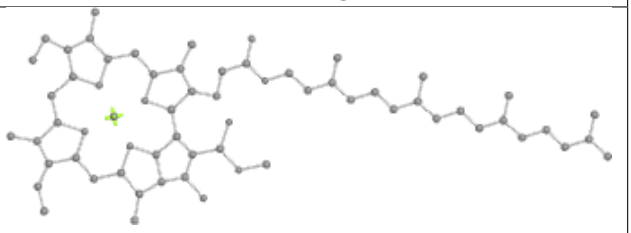
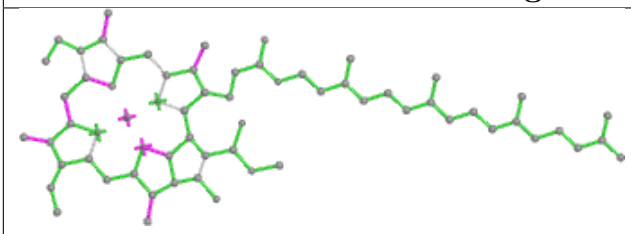


Rings

Ligand CLA B 612



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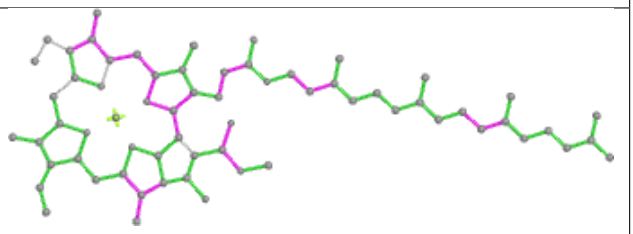
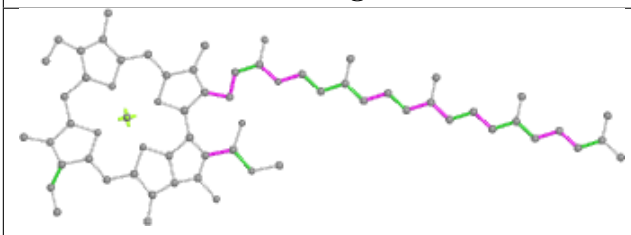


Bond angles



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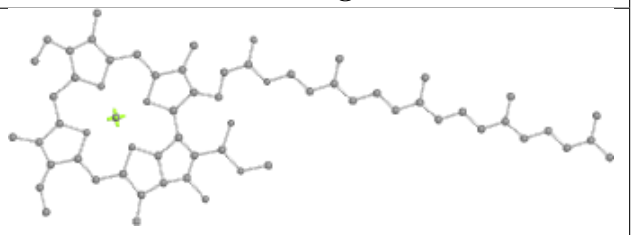
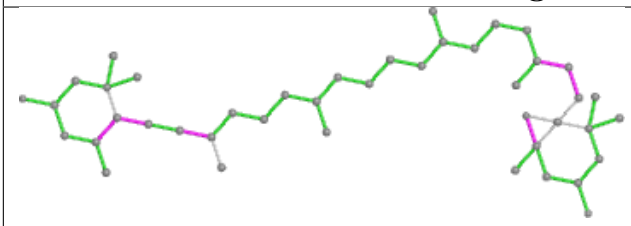


Rings

Ligand DD6 p 612



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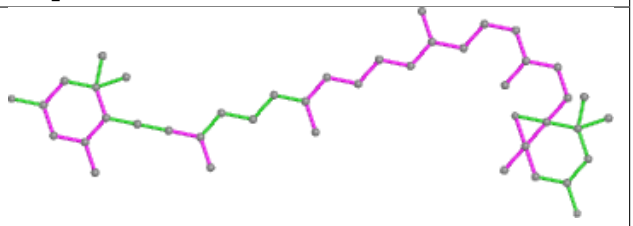
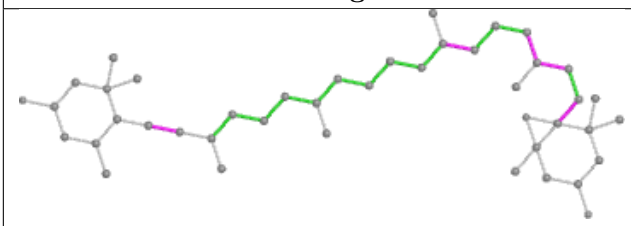


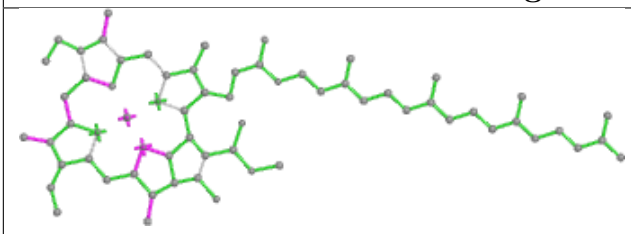
Bond angles



Torsions

Rings

Ligand CLA C 510



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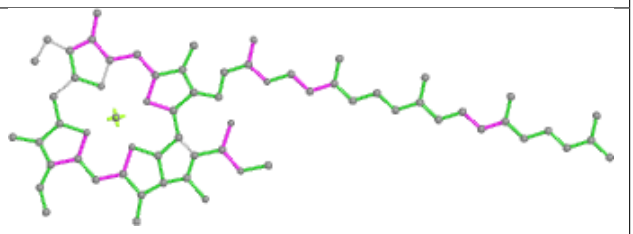
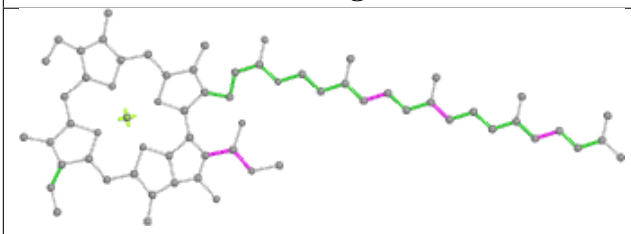


Bond angles



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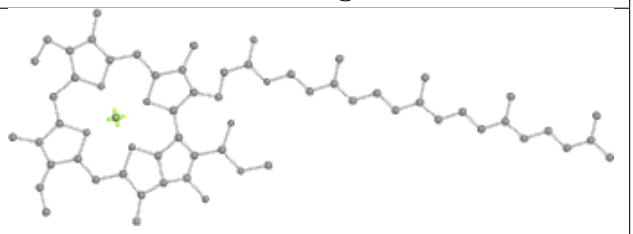
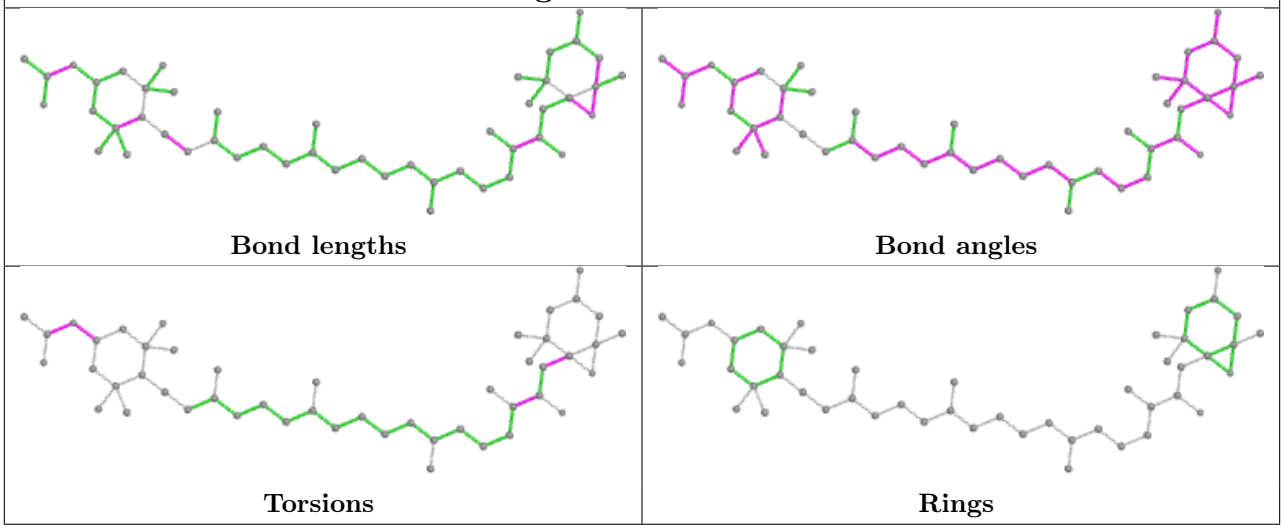


Rings

Ligand A86 1 306



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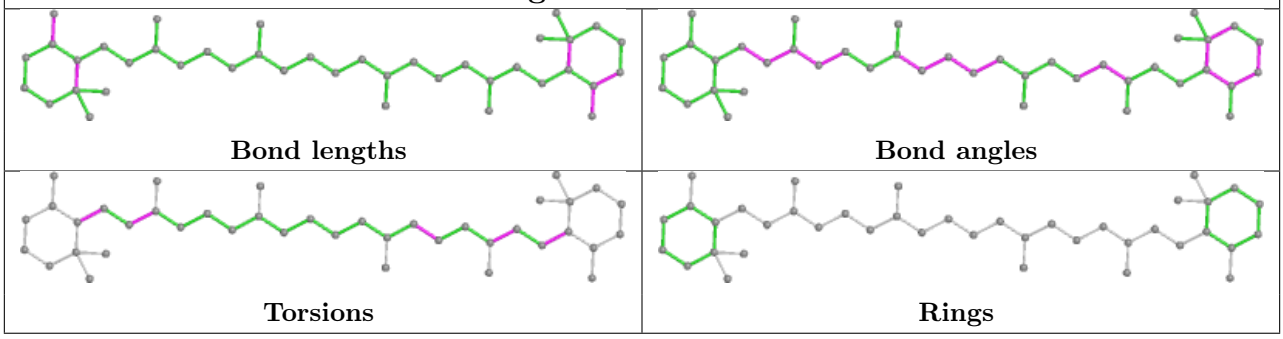
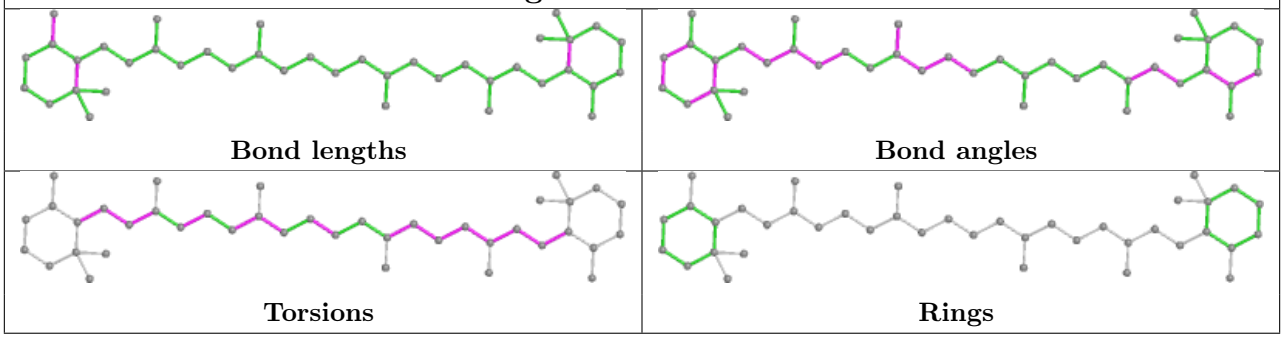


Ligand BCR F 101



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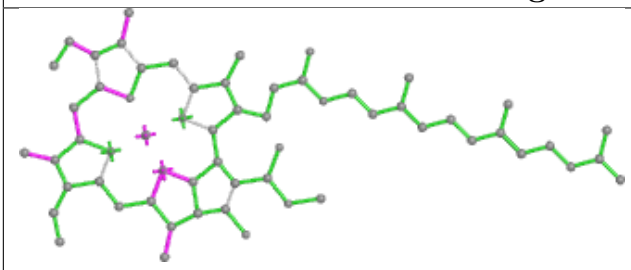
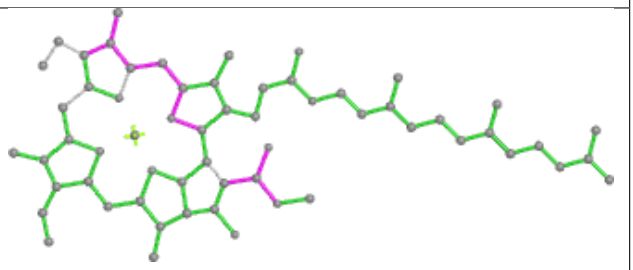
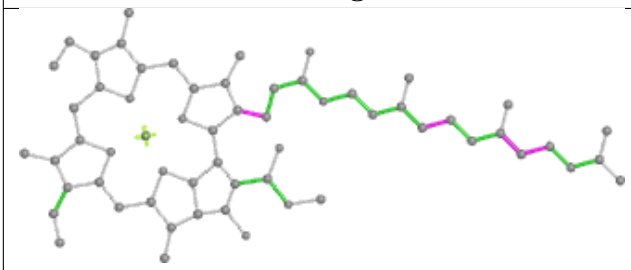
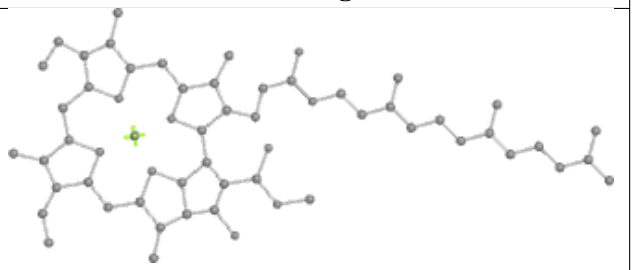
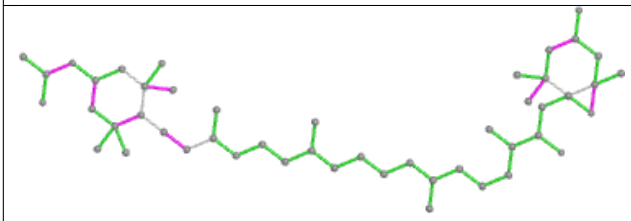
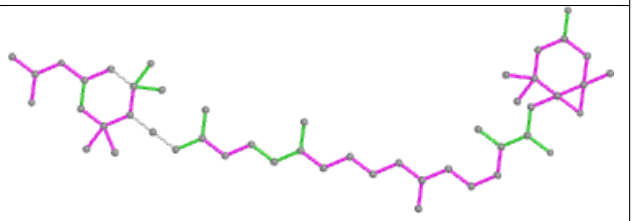
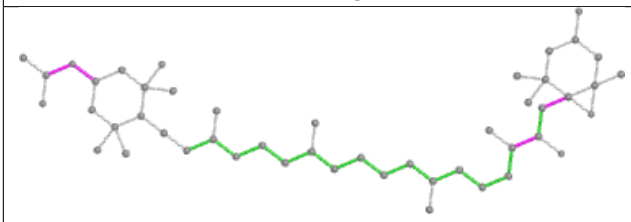
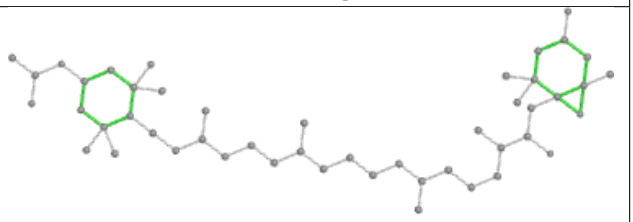
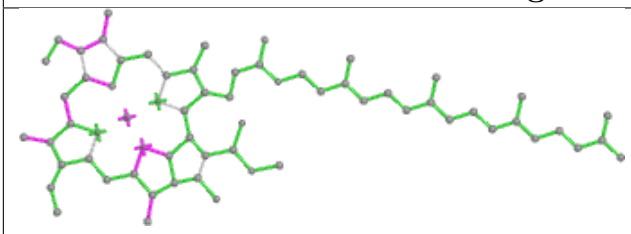
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 10 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 602



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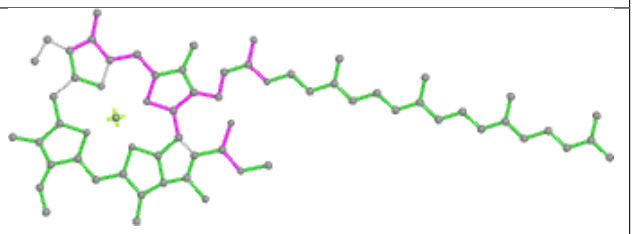

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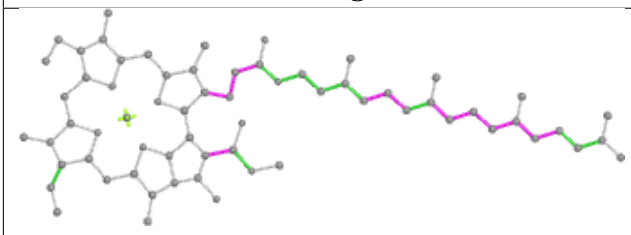

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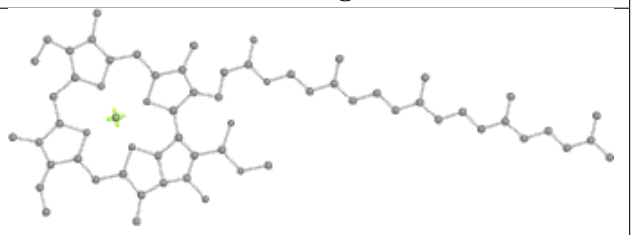
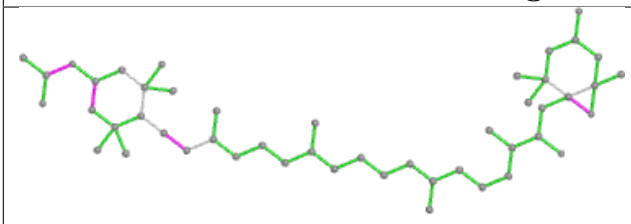


Rings

Ligand A86 12 301



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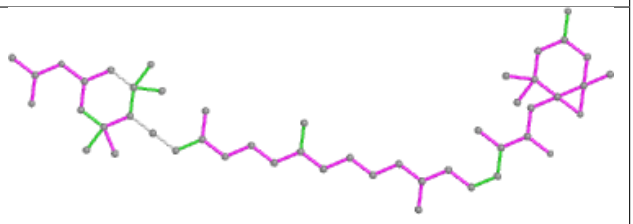

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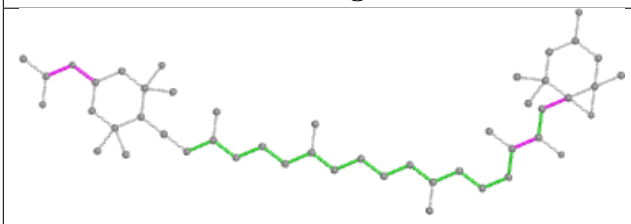

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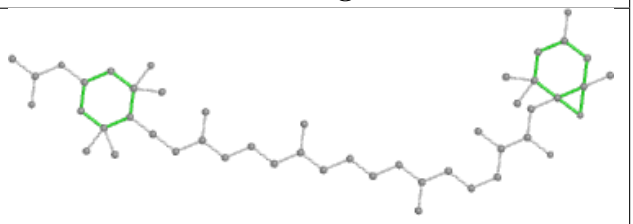
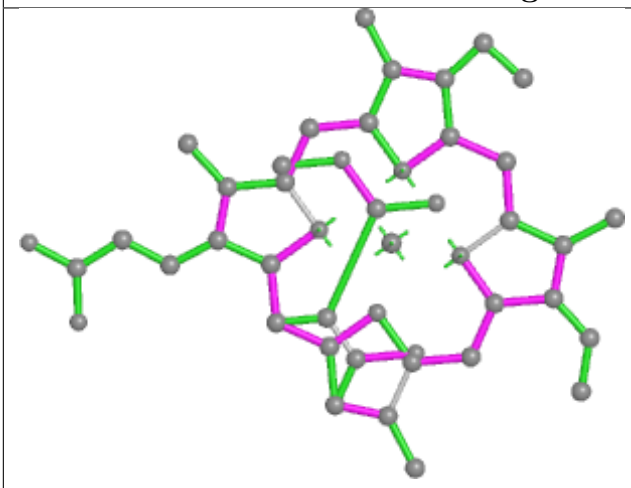


Rings

Ligand KC1 12 314



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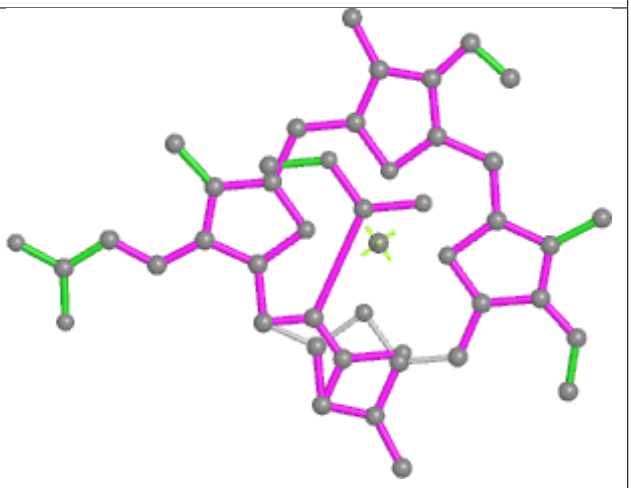

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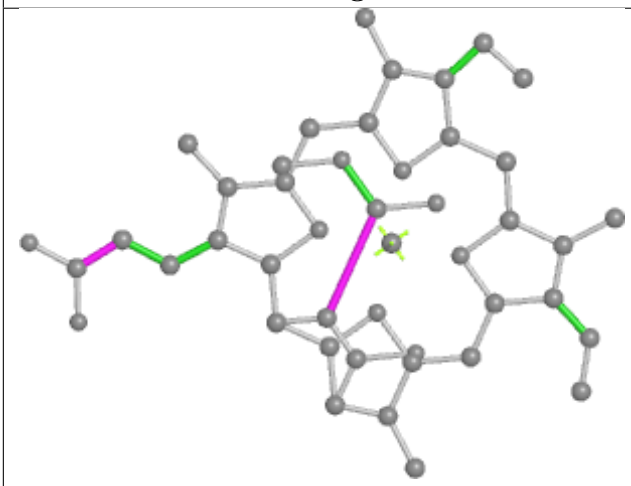

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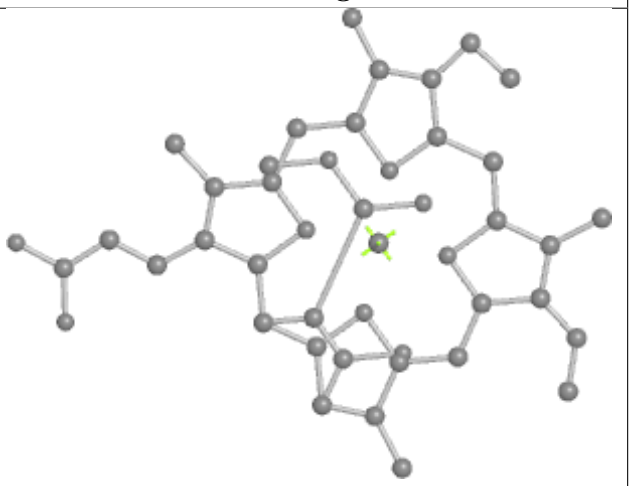
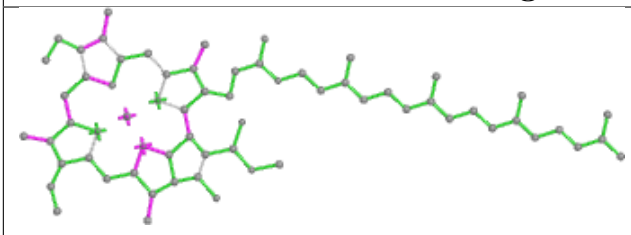


Rings

Ligand CLA 13 313



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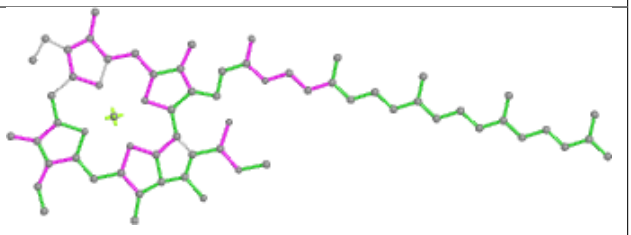

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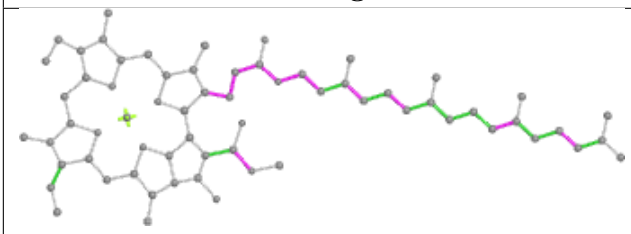

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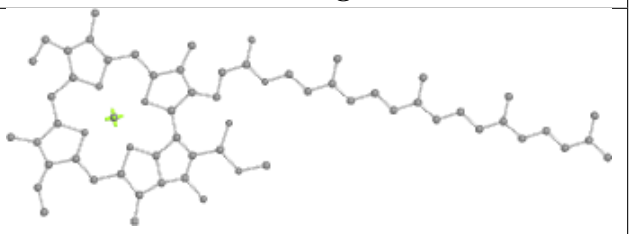
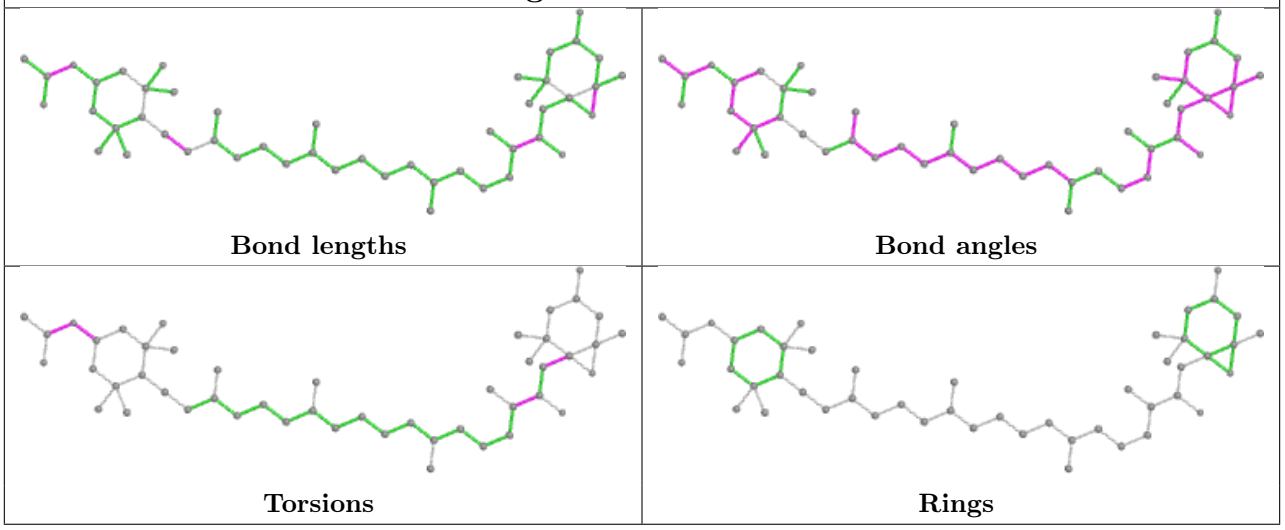


Rings

Ligand A86 14 303



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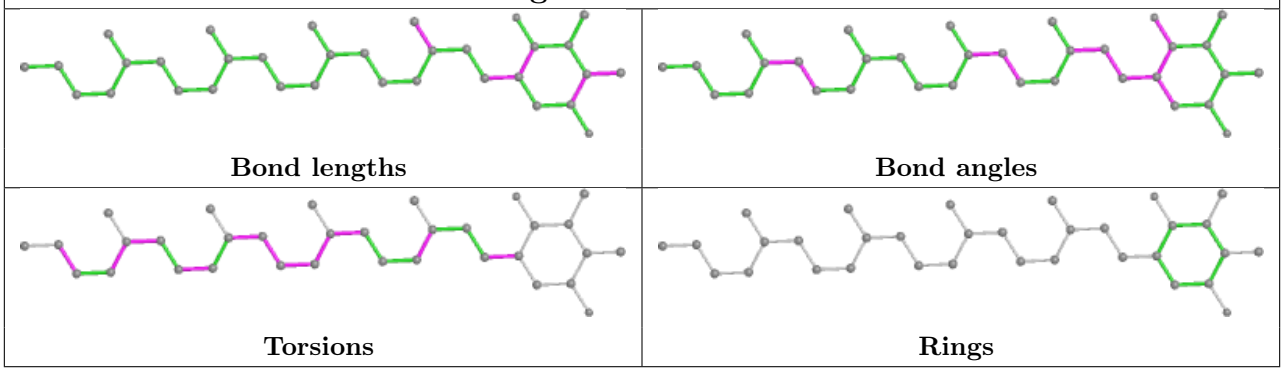

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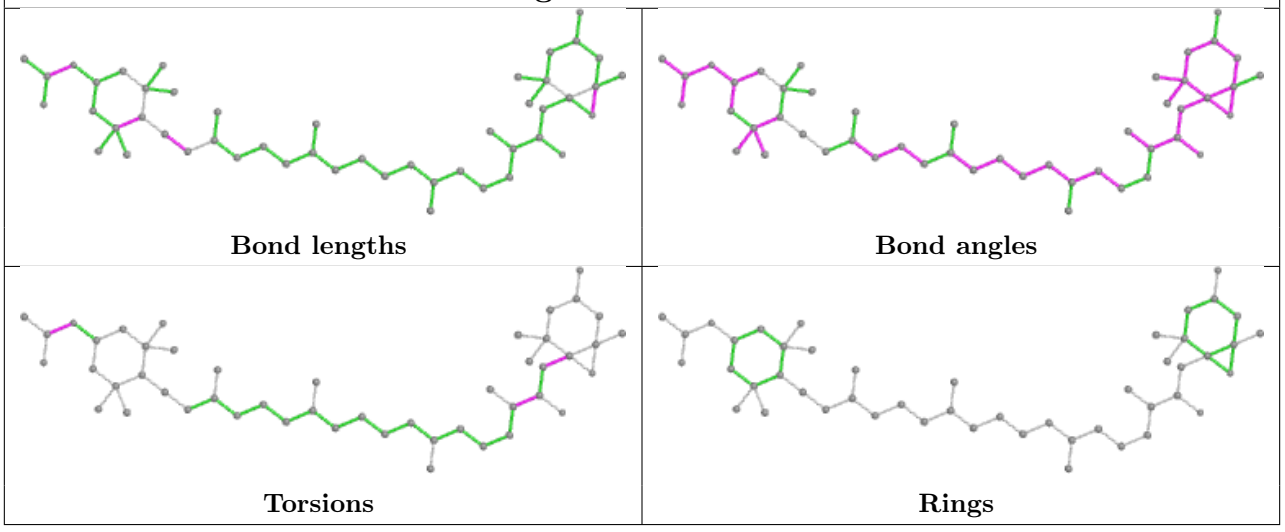
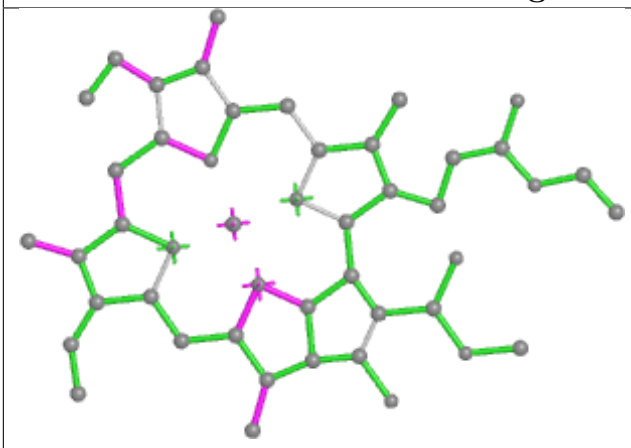


Ligand CLA 0 314



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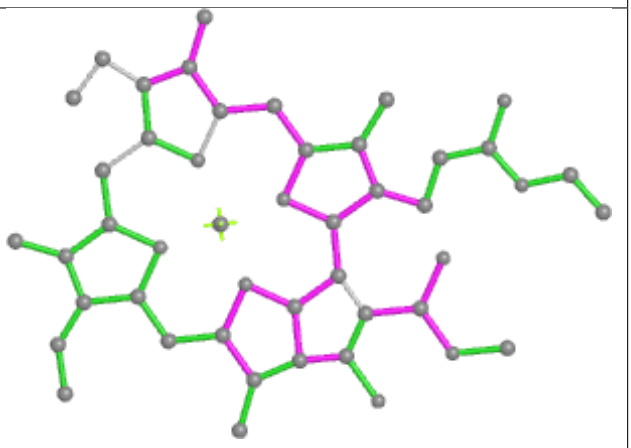
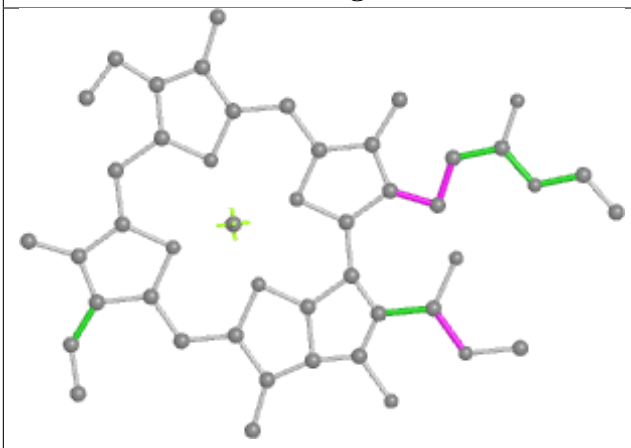


Bond angles



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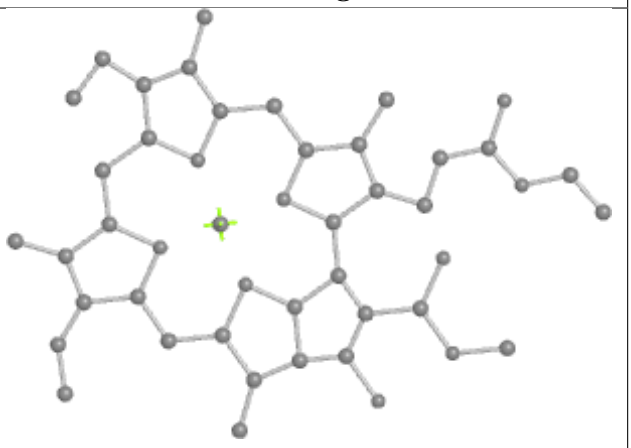
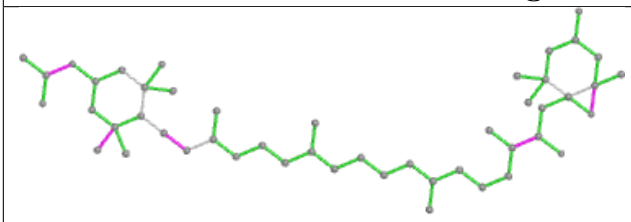


Rings

Ligand A86 15 302



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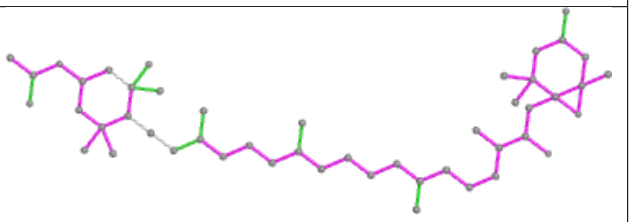

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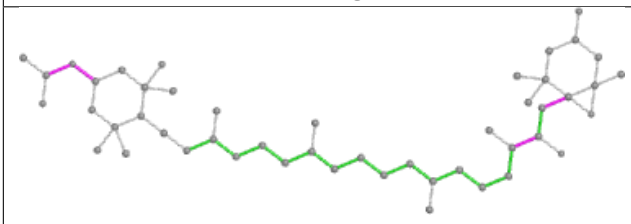

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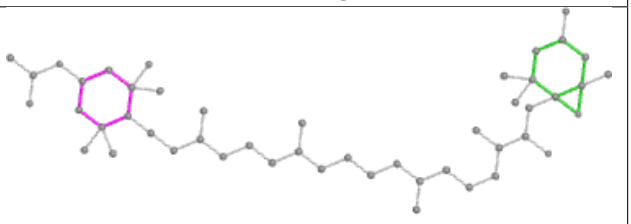
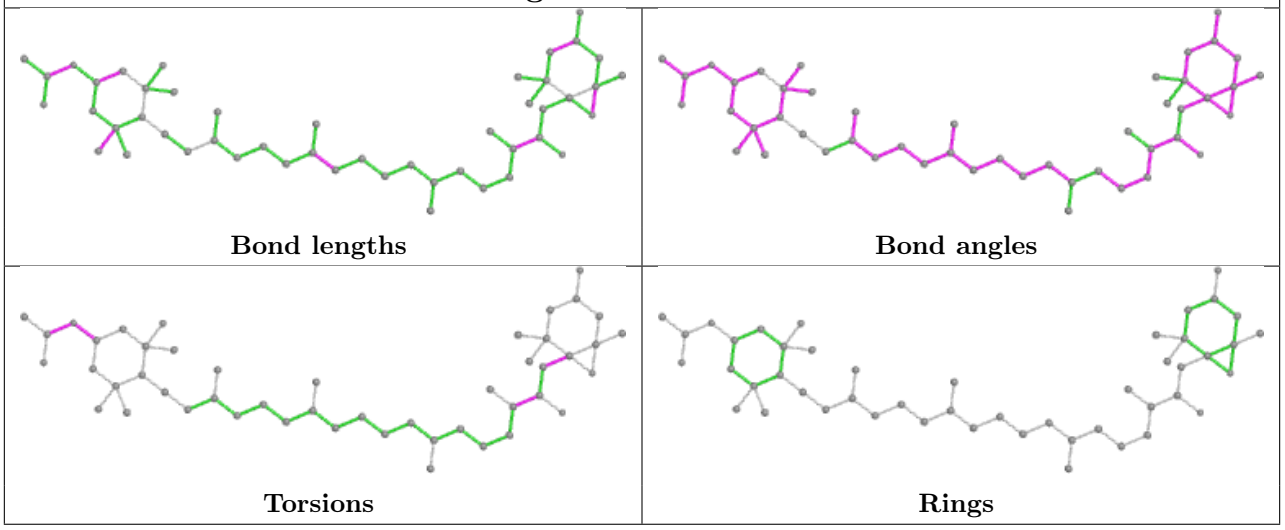
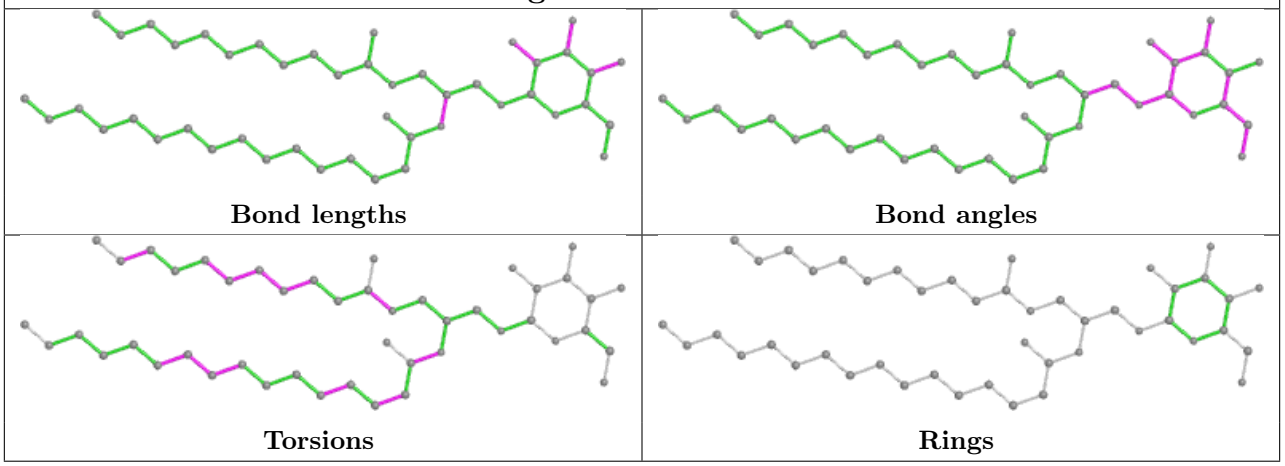


Rings

Ligand A86 17 316



Ligand LMG f 102



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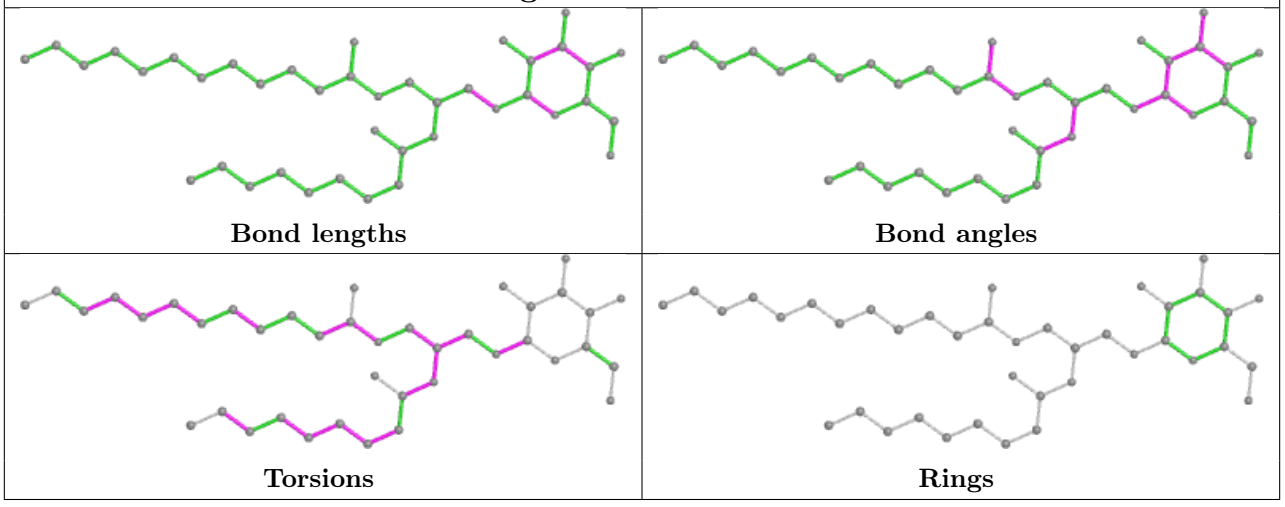
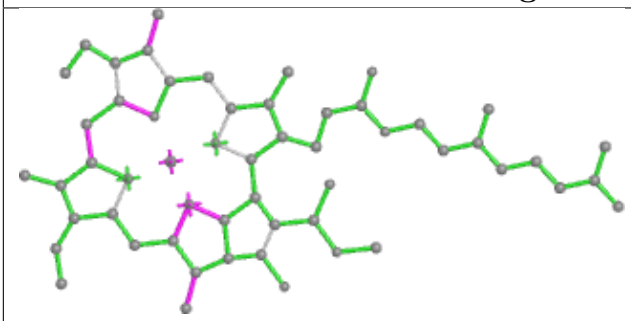
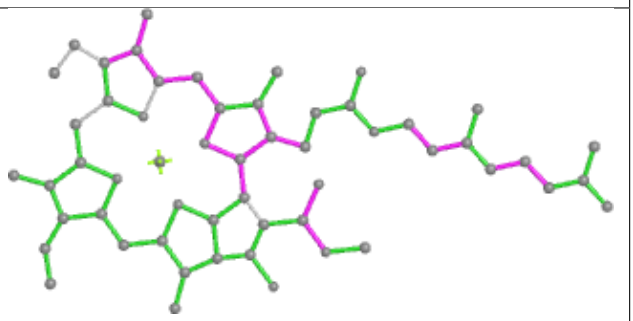


Ligand CLA 15 309



Bond lengths



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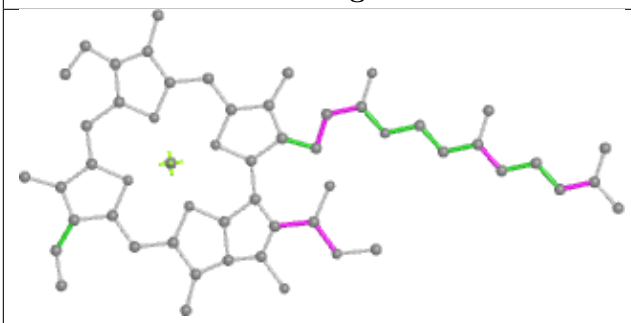
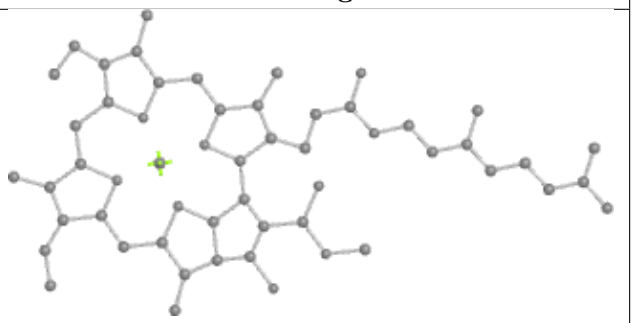
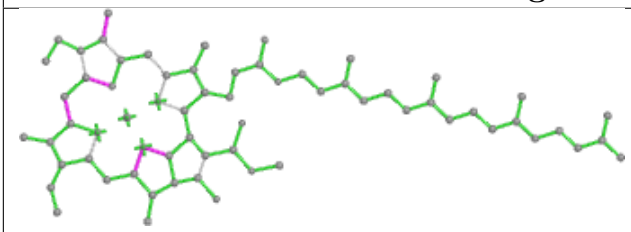


Torsions



Rings

Ligand CLA 9 310



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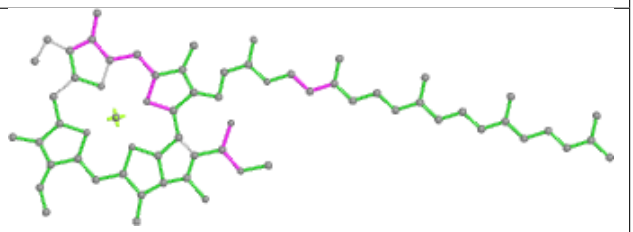

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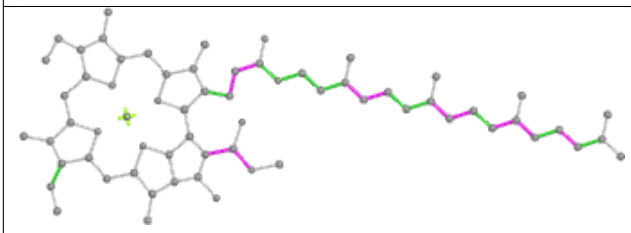

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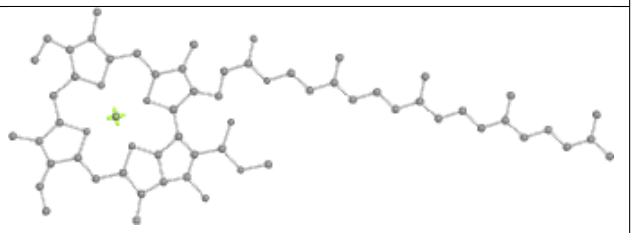
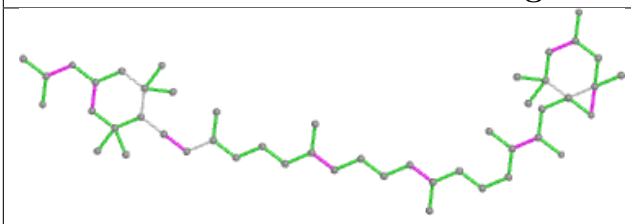


Rings

Ligand A86 14 305



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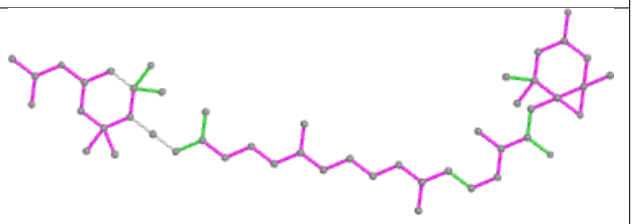

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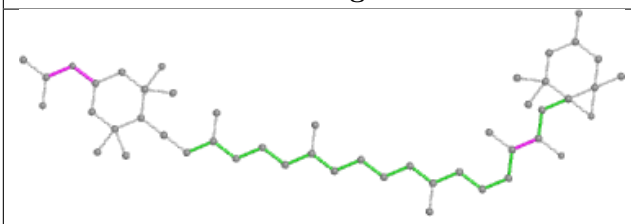

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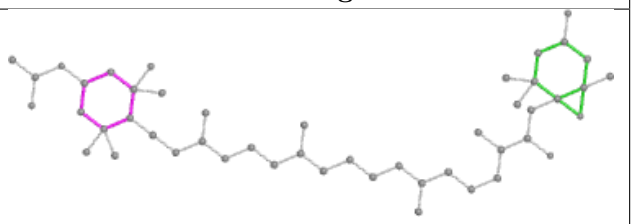
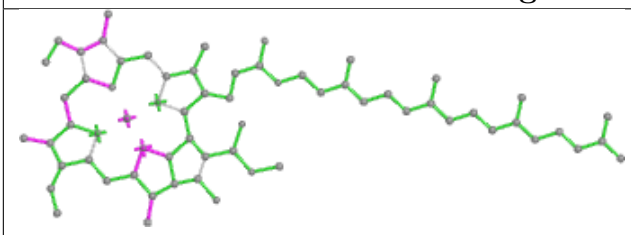


Rings

Ligand CLA 11 313



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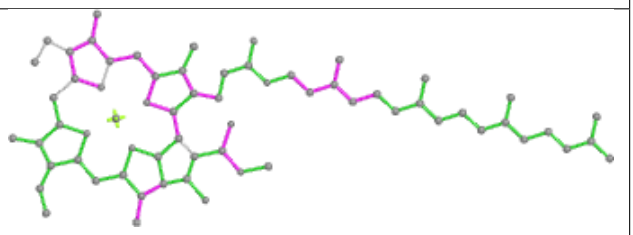
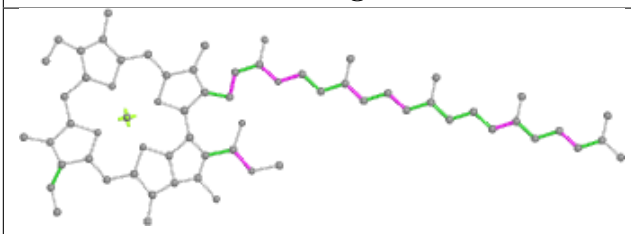


Bond angles



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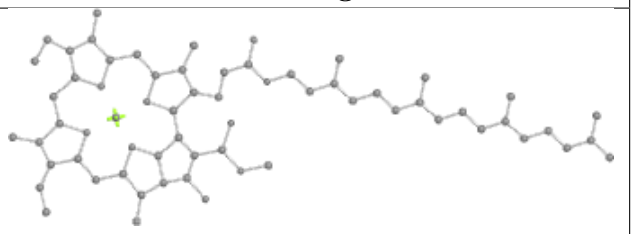
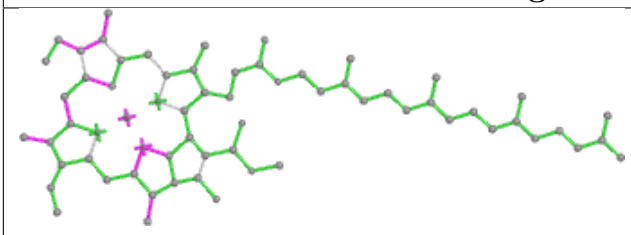


Rings

Ligand CLA 2 307



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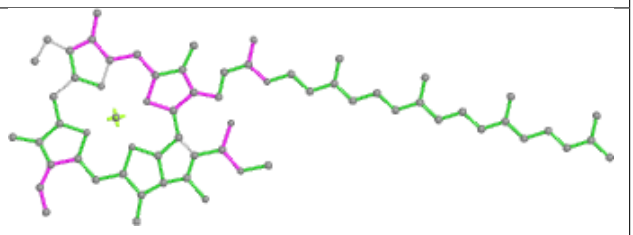

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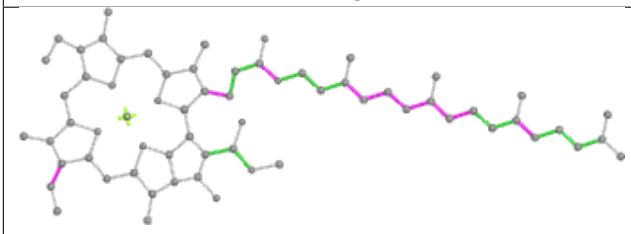
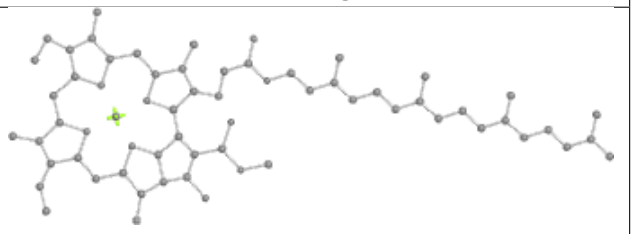
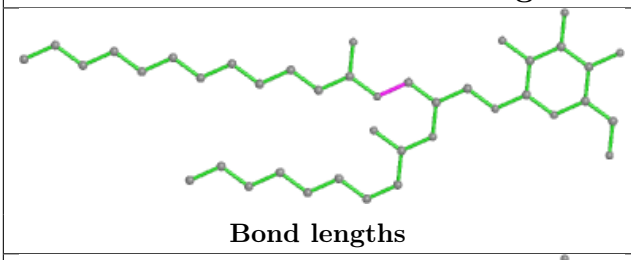


Torsions



Rings

Ligand LMG M 101



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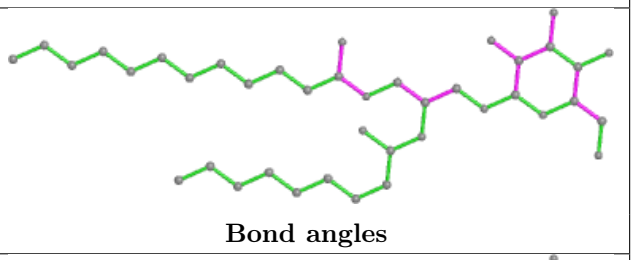

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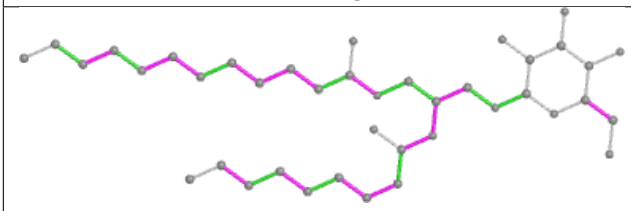

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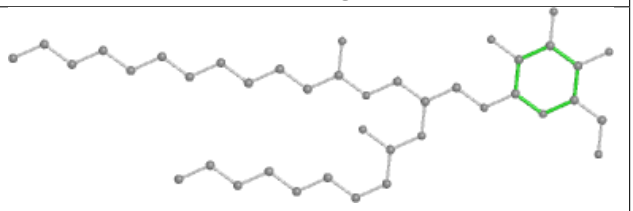
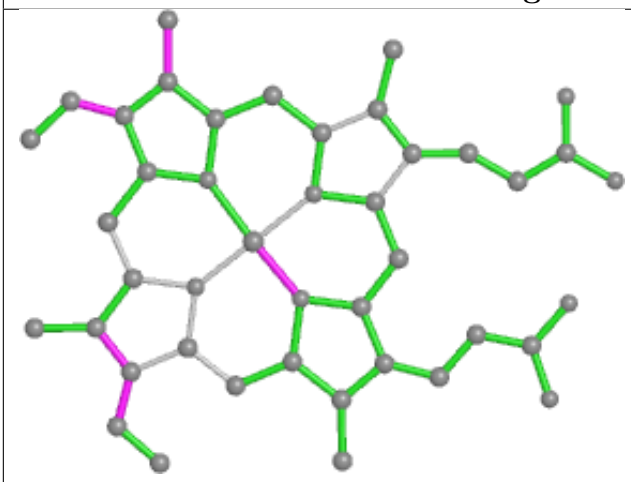


Rings

Ligand HEM e 101



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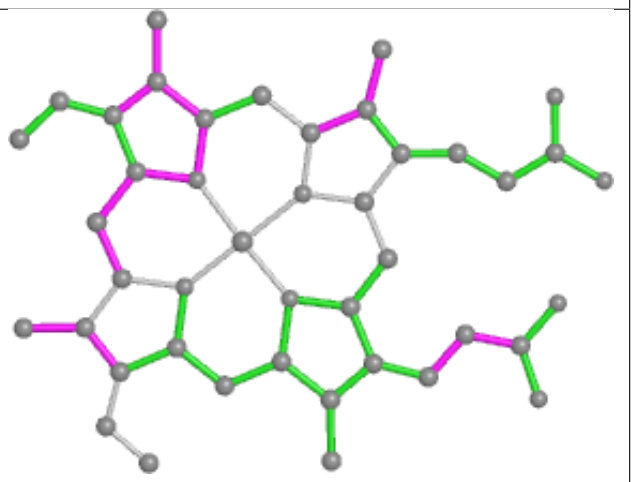

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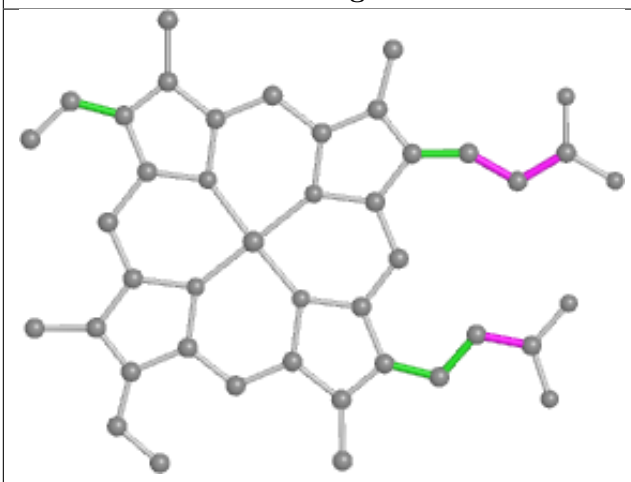

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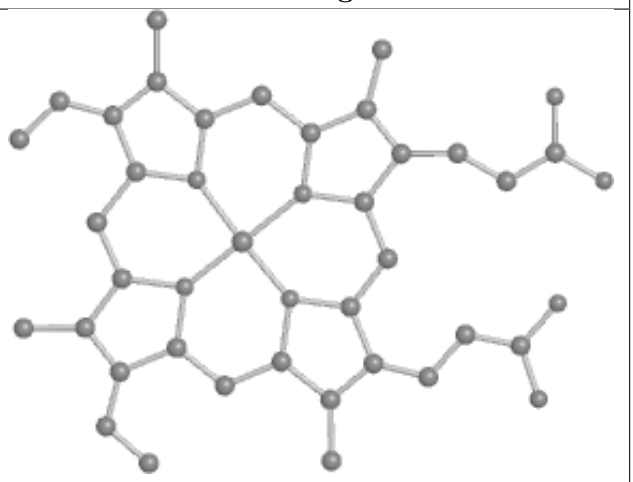
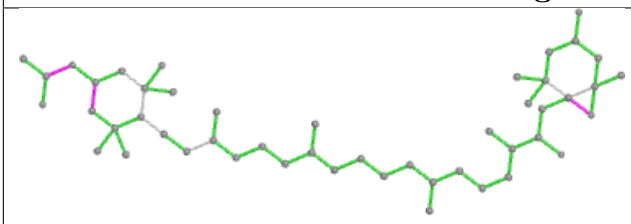


Rings

Ligand A86 9 301



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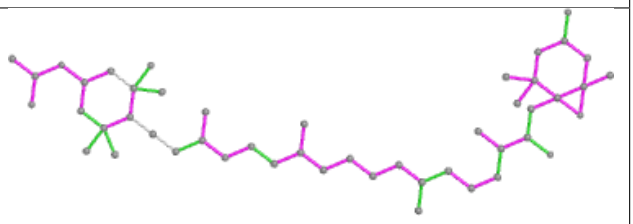

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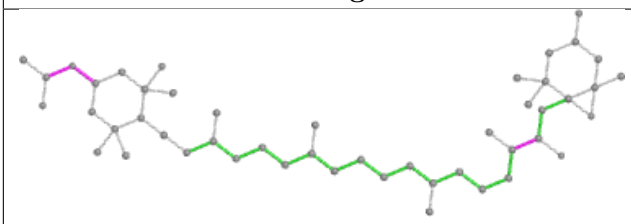

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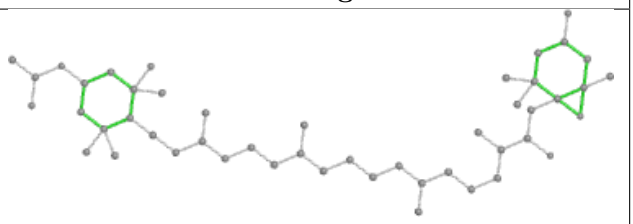
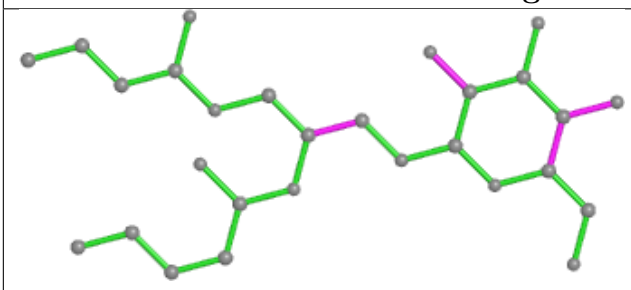


Rings

Ligand LMG n 701



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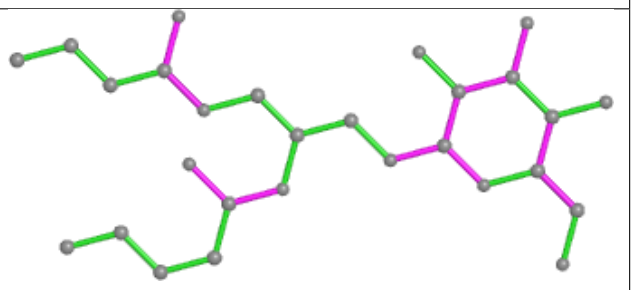

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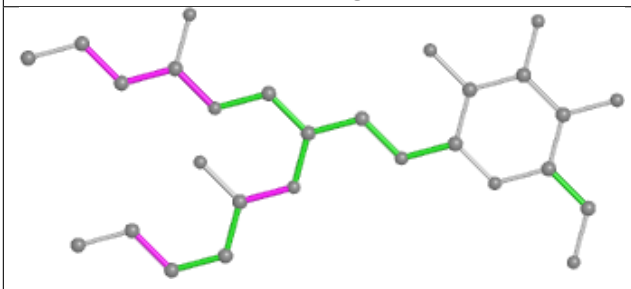

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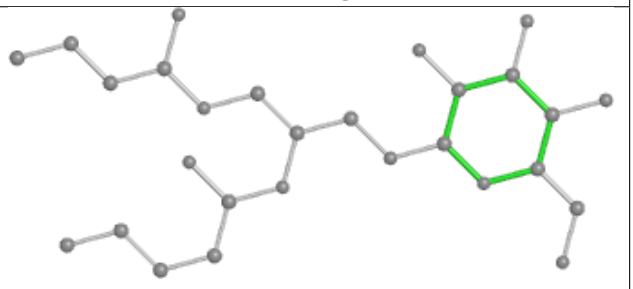
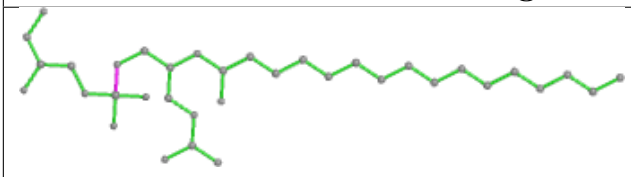


Rings

Ligand LHG 14 317



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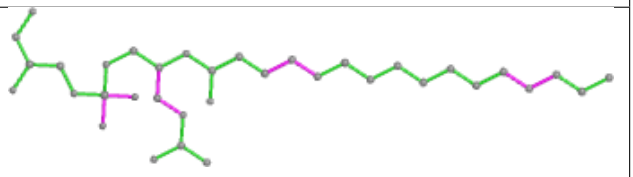

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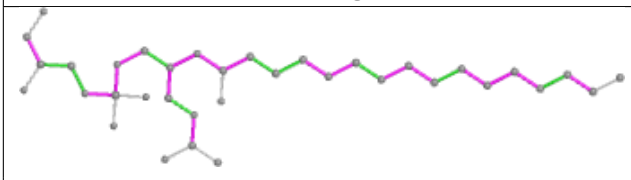

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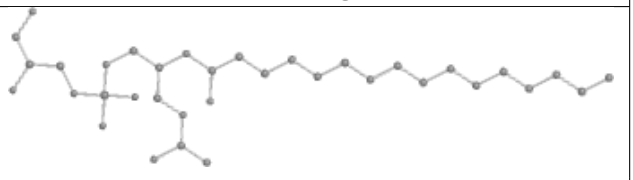

Rings

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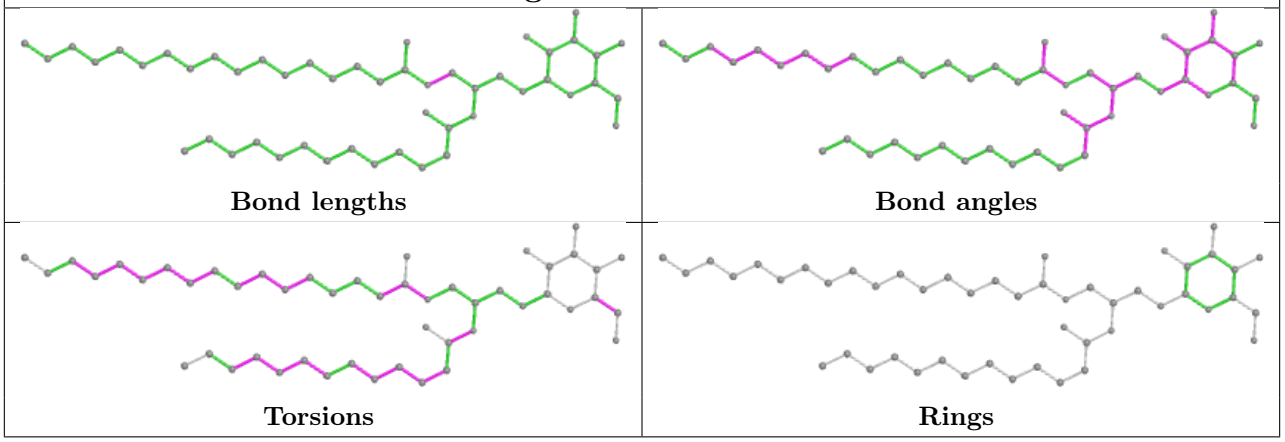

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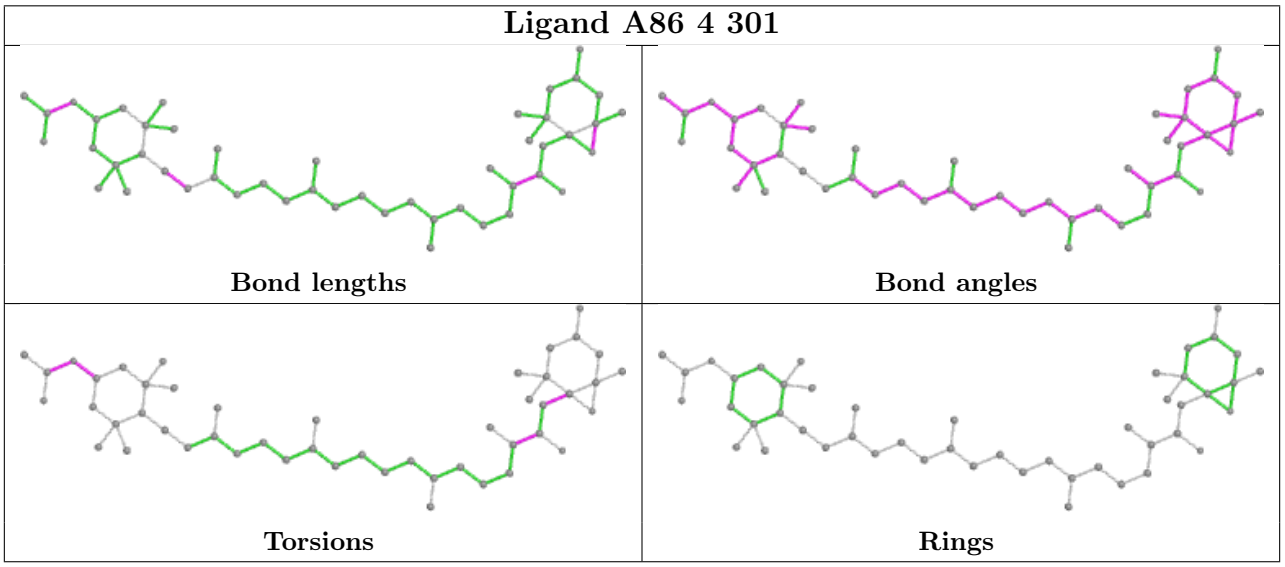

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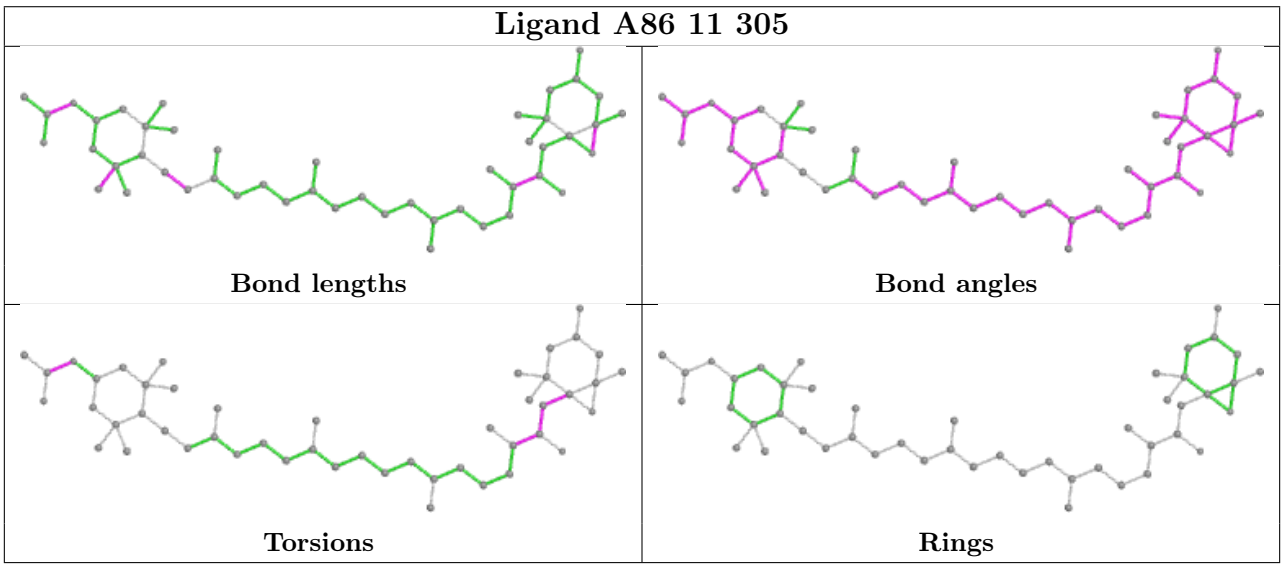
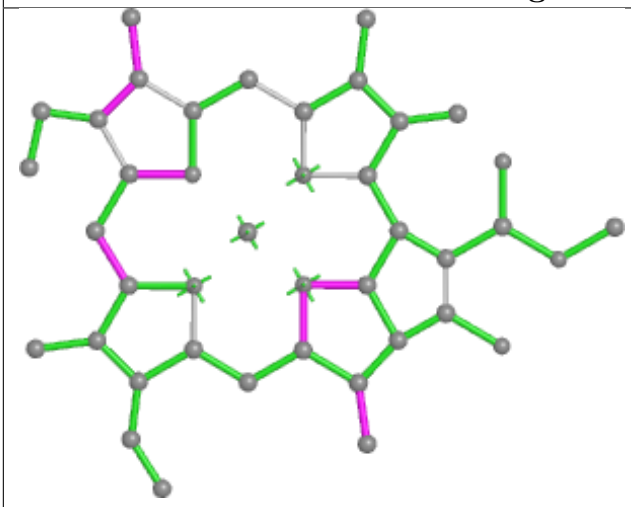


Ligand CLA 5 314



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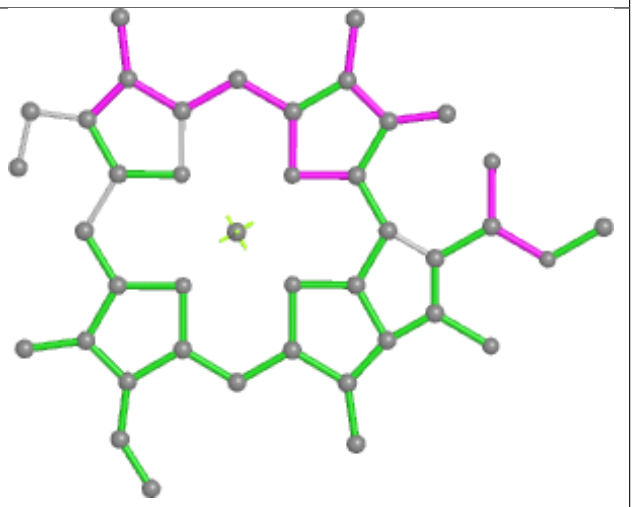

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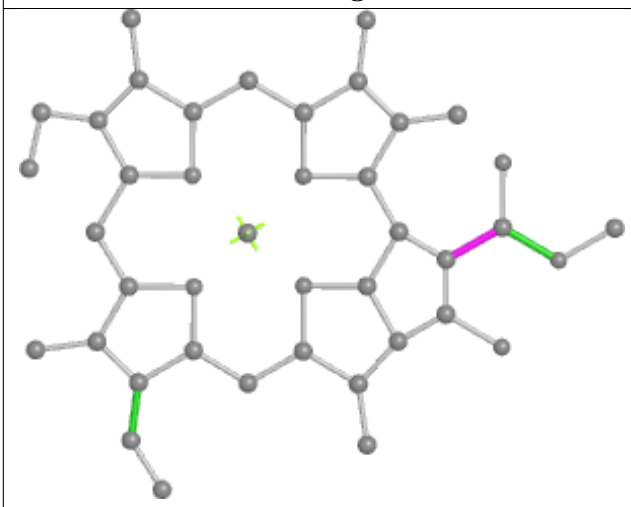

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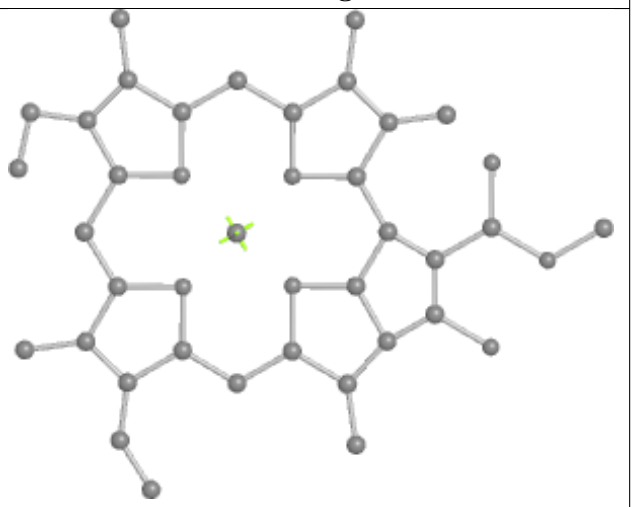
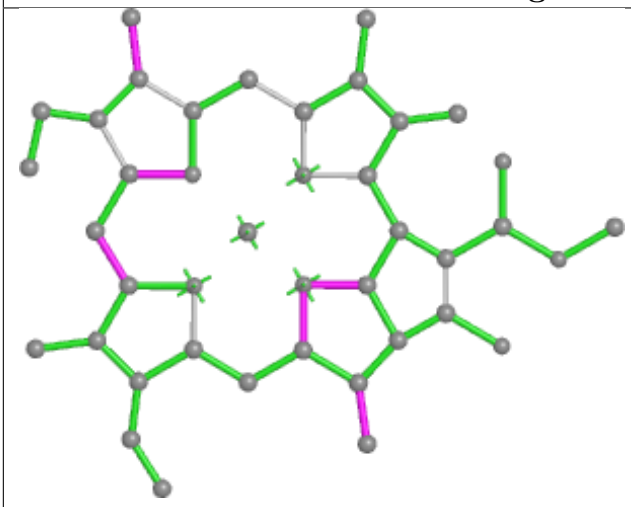


Rings

Ligand CLA 2 314



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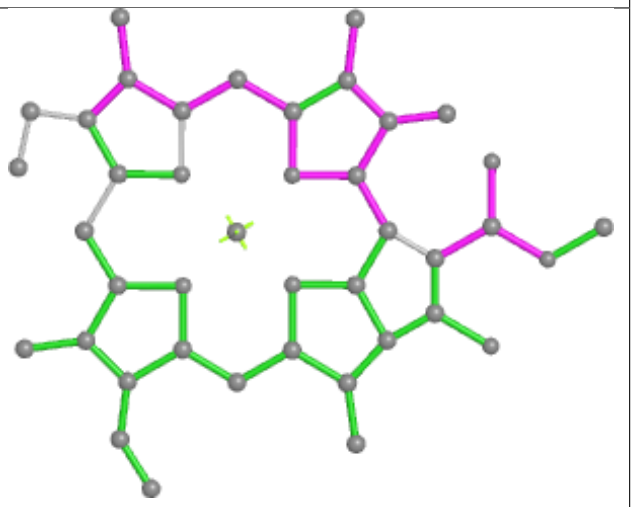

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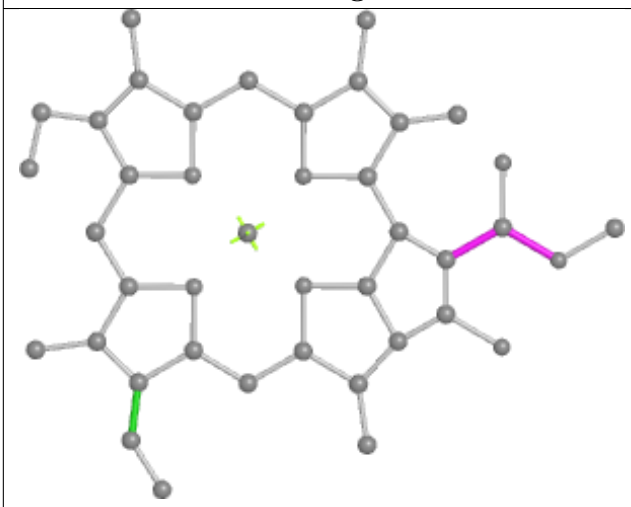

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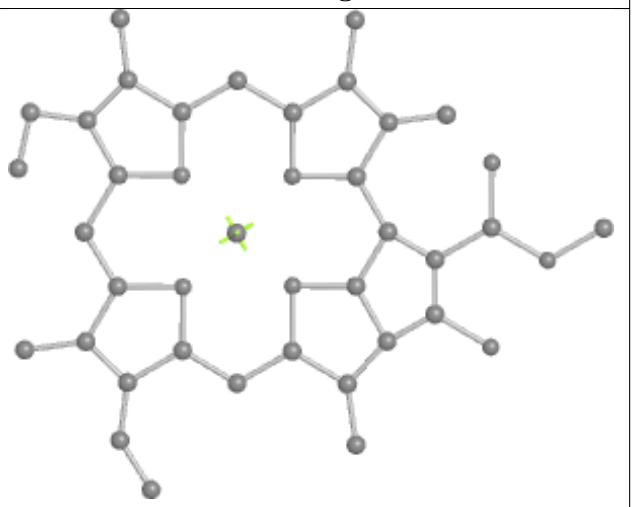
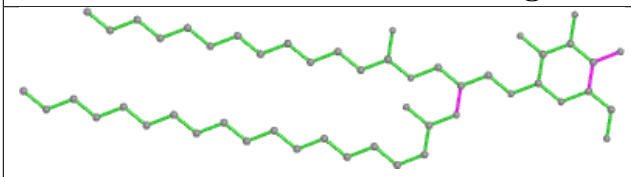


Rings

Ligand LMG J 101



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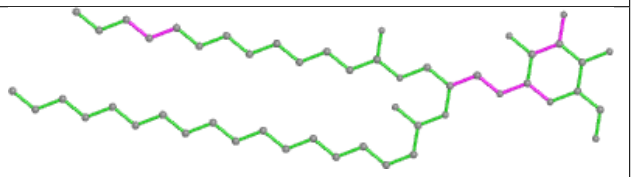

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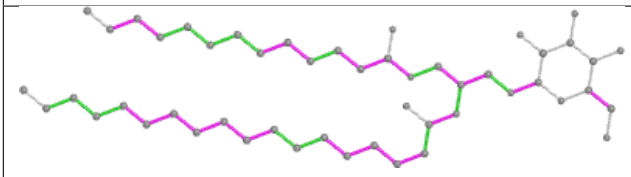

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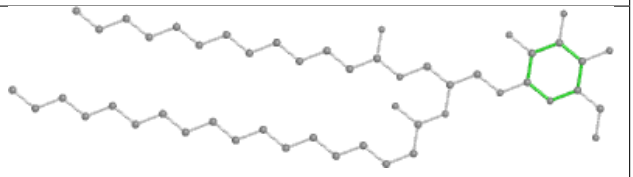
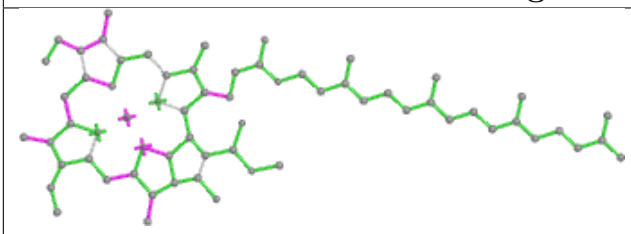


Rings

Ligand CLA d 404



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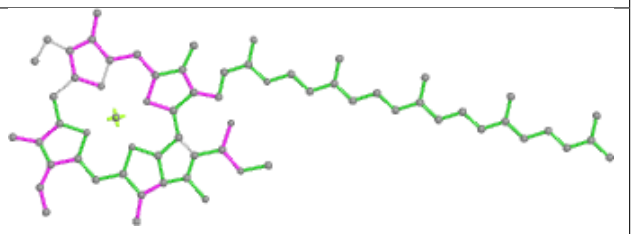
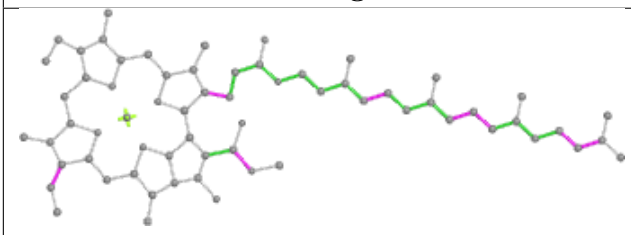


Bond angles



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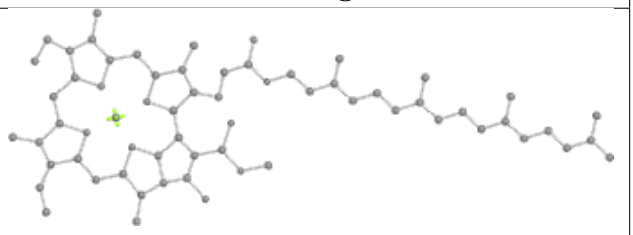
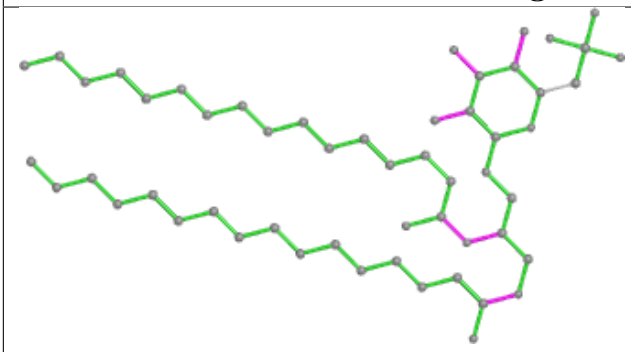


Rings

Ligand SQD a 408



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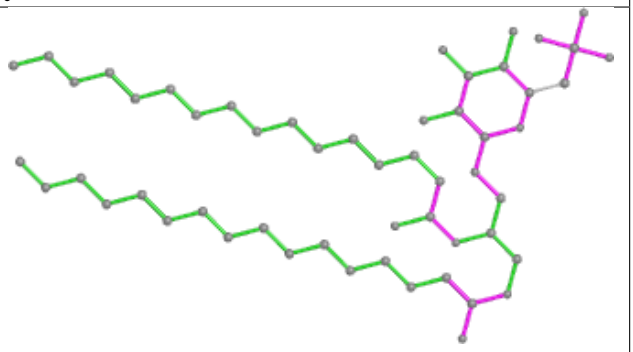

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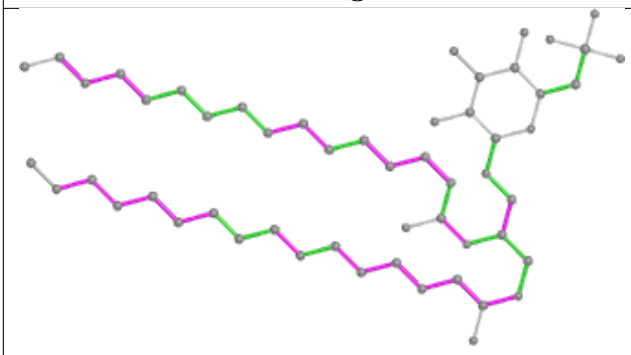

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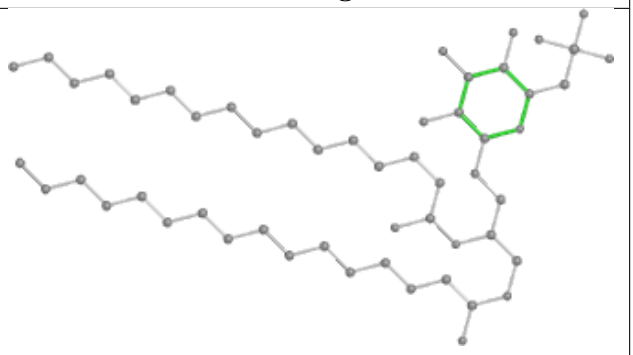
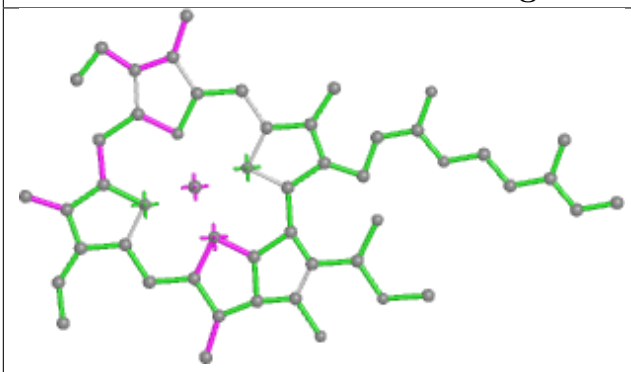


Rings

Ligand CLA 14 312



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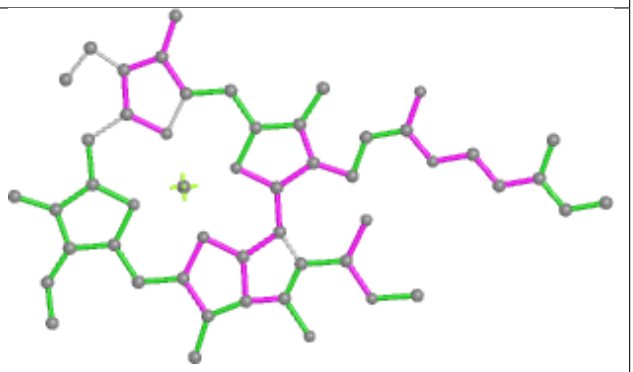
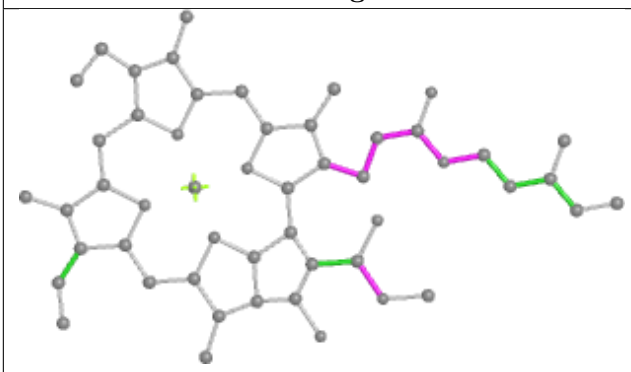


Bond angles



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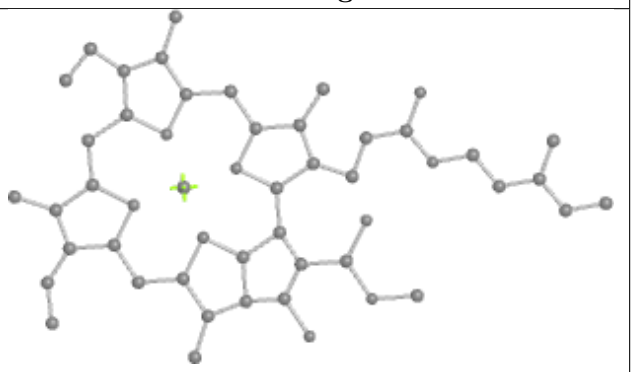
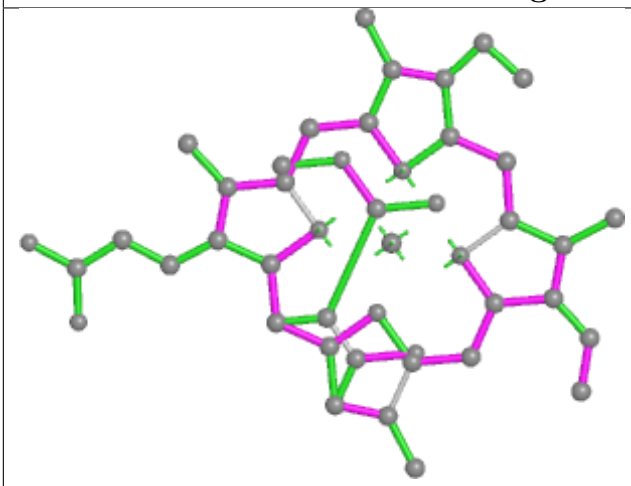


Rings

Ligand KC2 6 312



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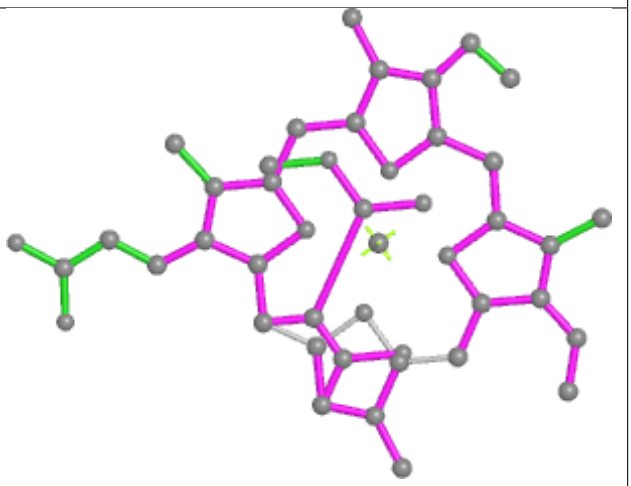

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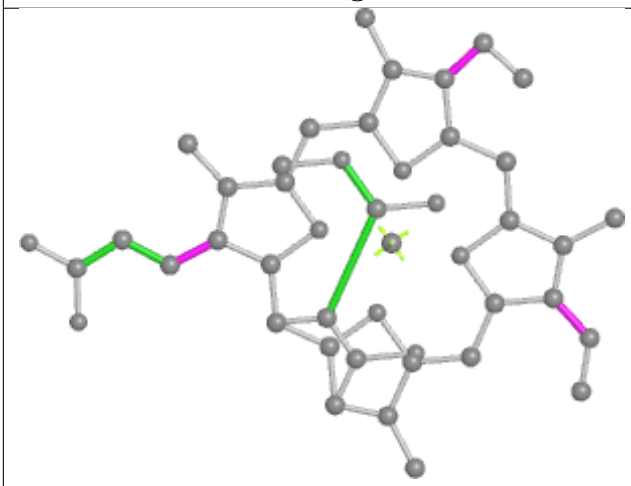

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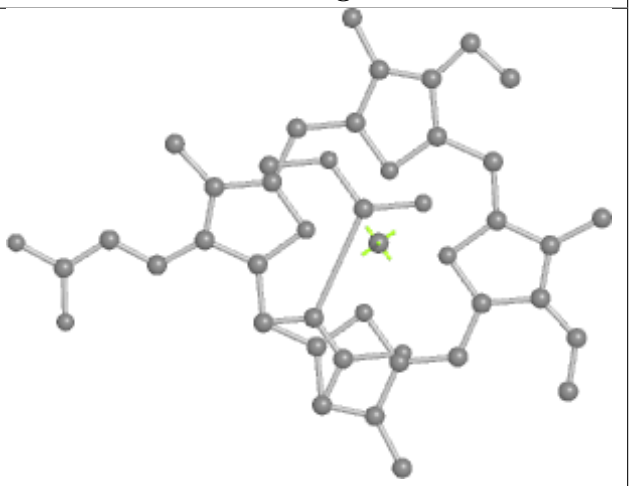
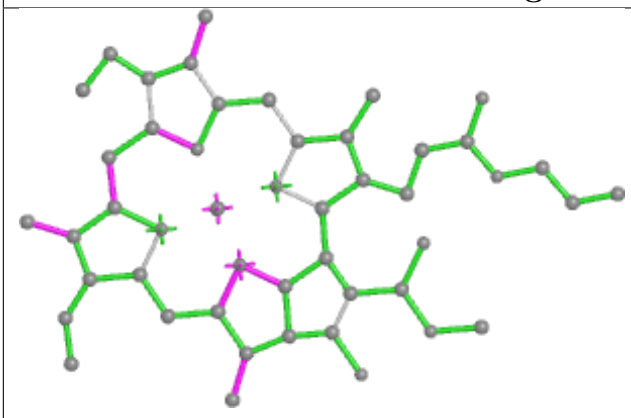
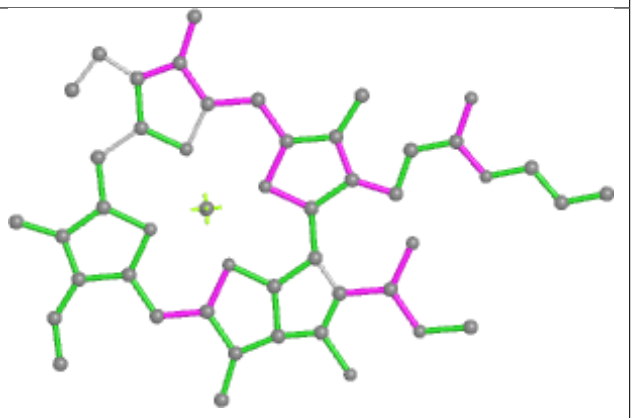


Rings

Ligand CLA P 604



Bond lengths



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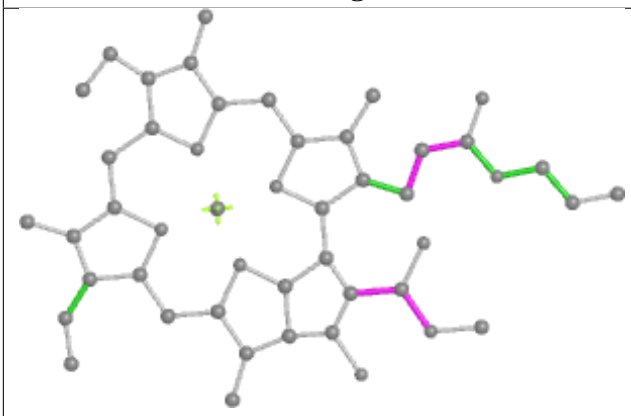
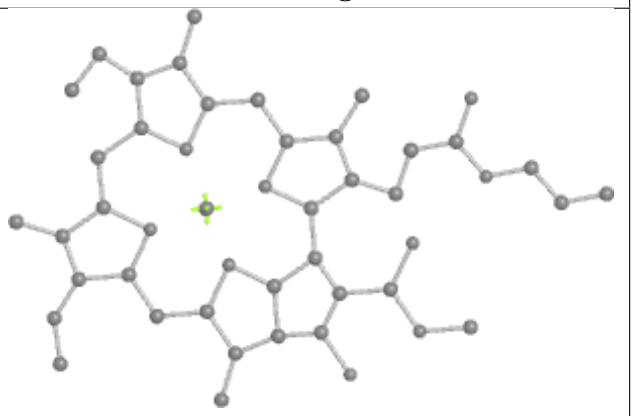
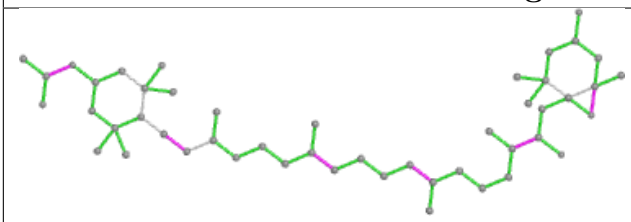


Torsions



Rings

Ligand A86 16 305



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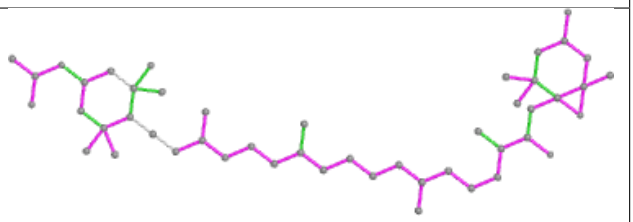

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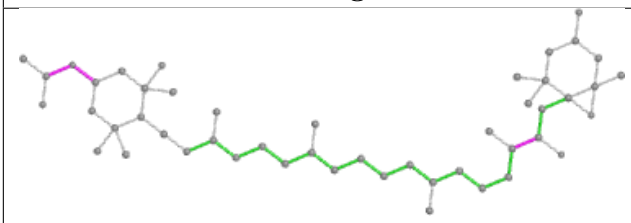

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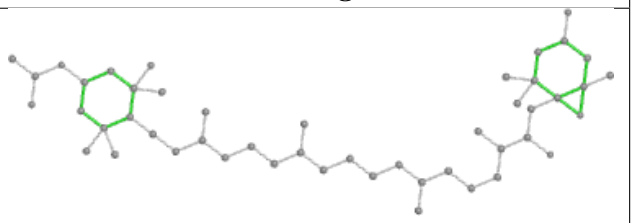
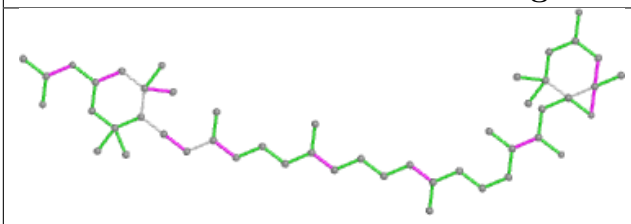


Rings

Ligand A86 P 611



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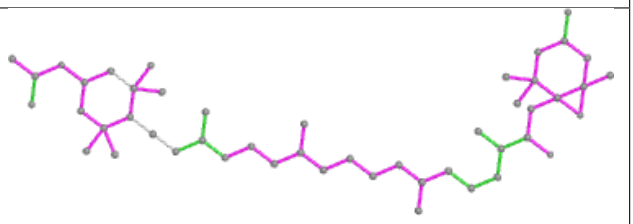

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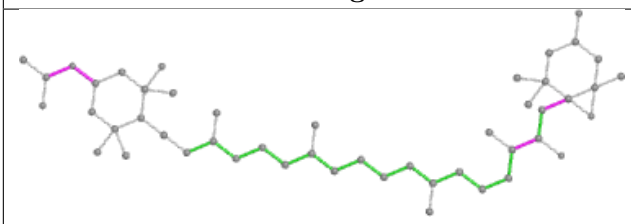

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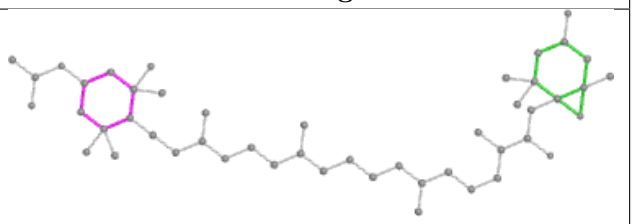
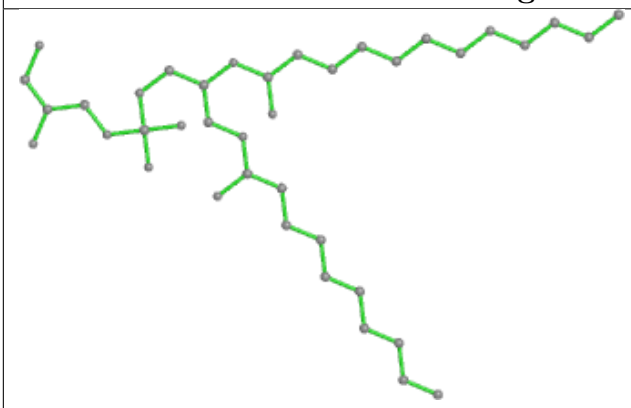


Rings

Ligand LHG 18 315



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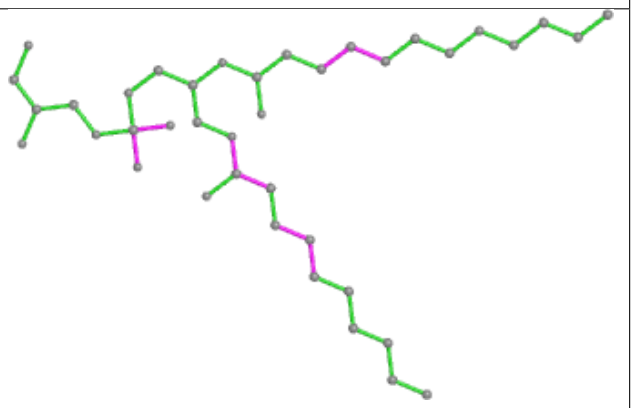

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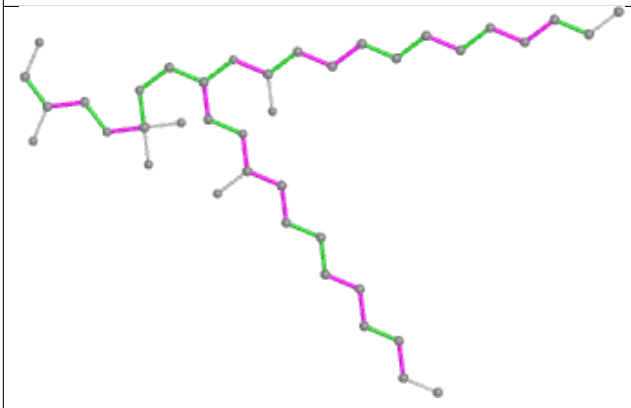

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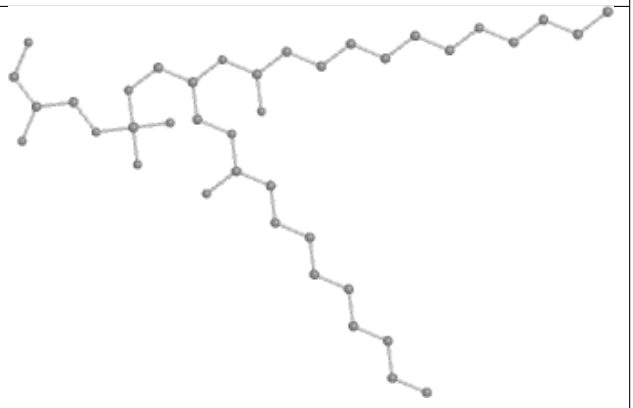
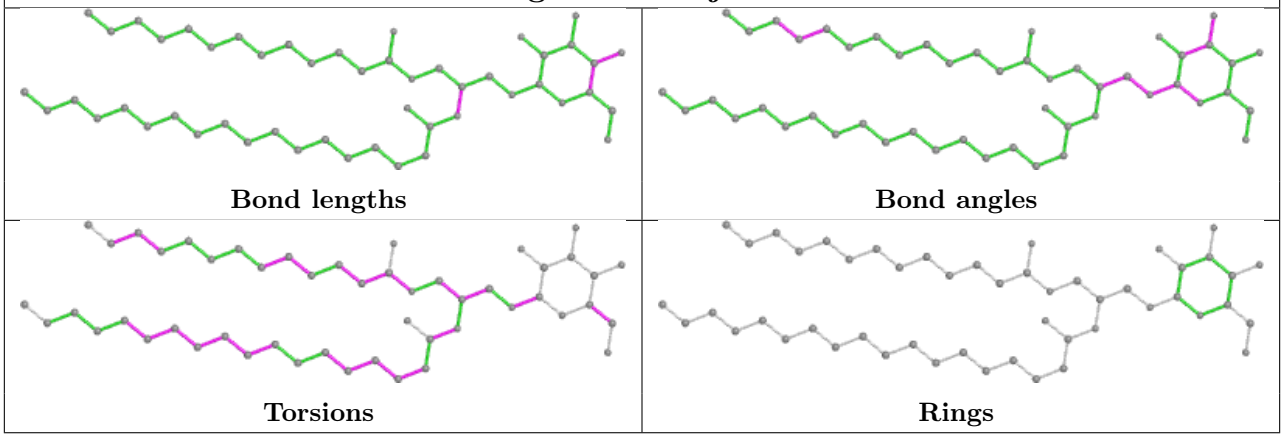


Rings

Ligand LMG j 101



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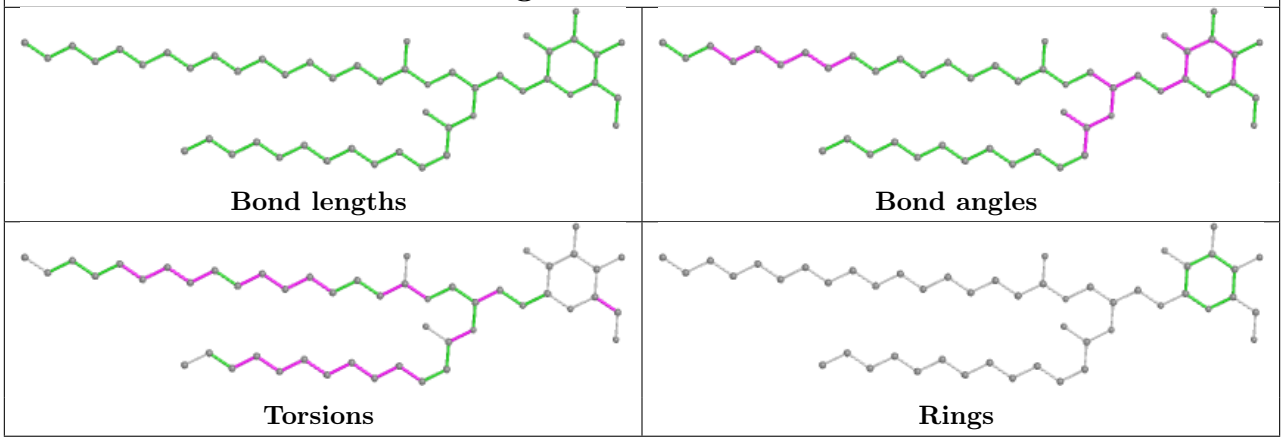
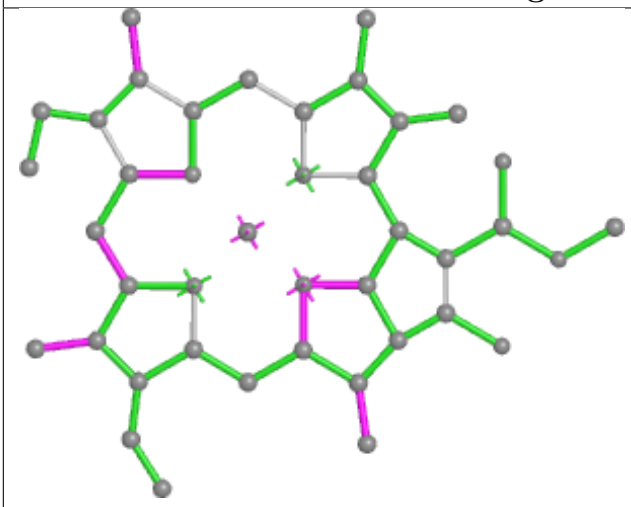


Ligand CLA p 610



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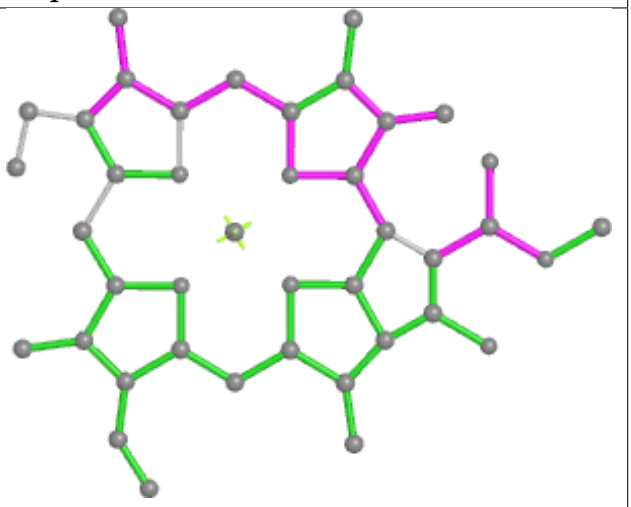

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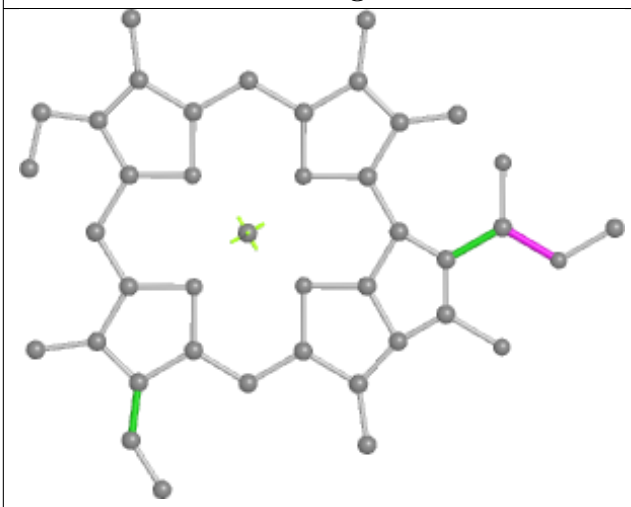

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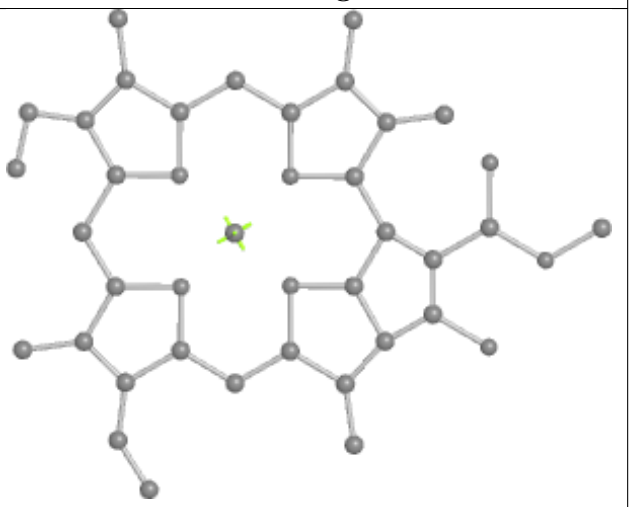

Rings

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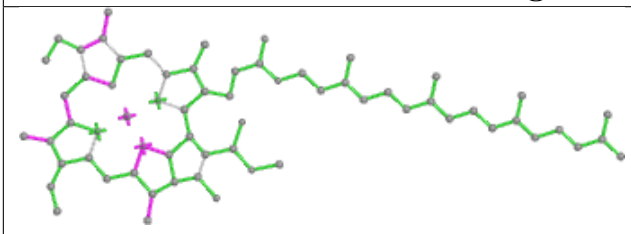

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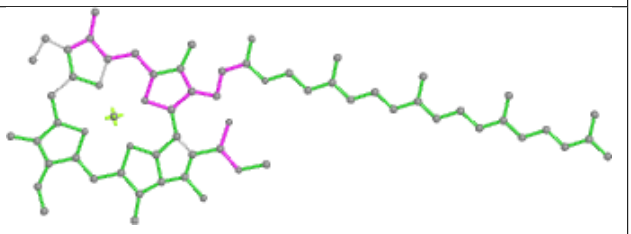

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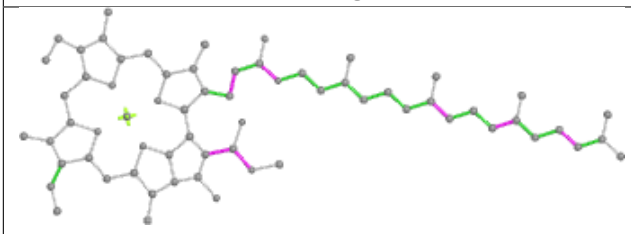

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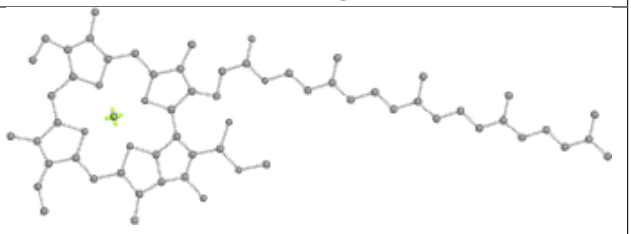

Rings

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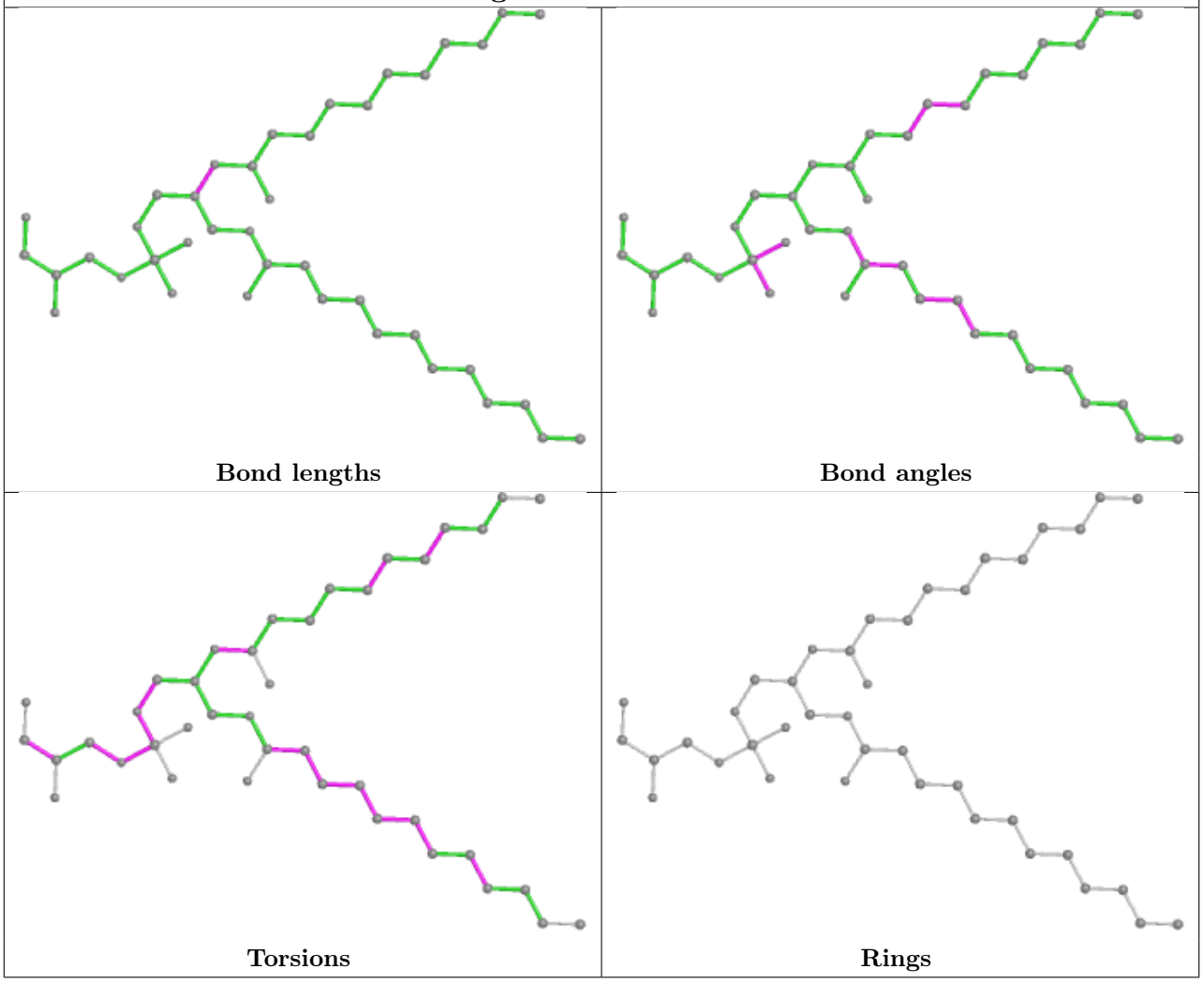
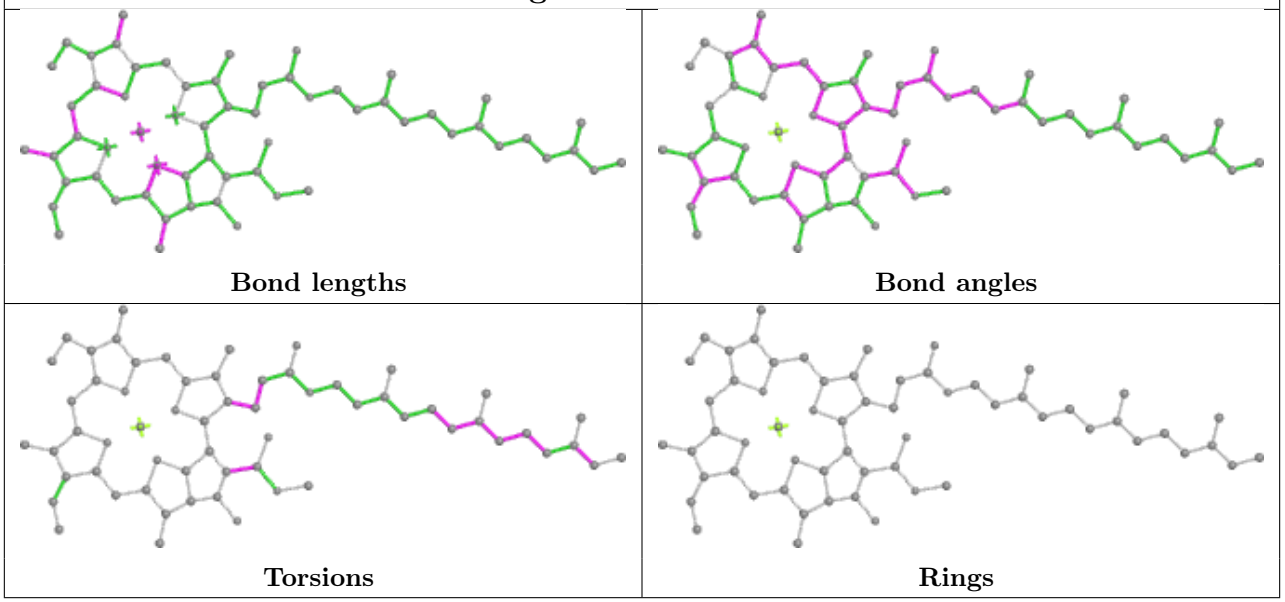
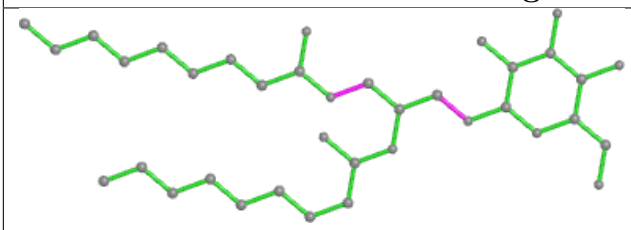


Ligand CLA 1 321



Ligand LMG d 408



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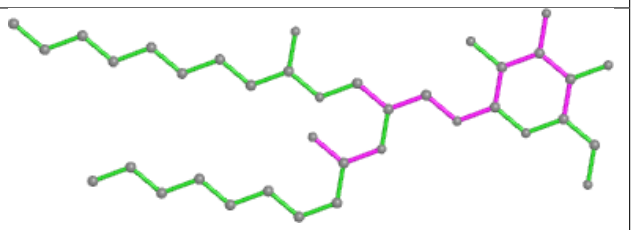

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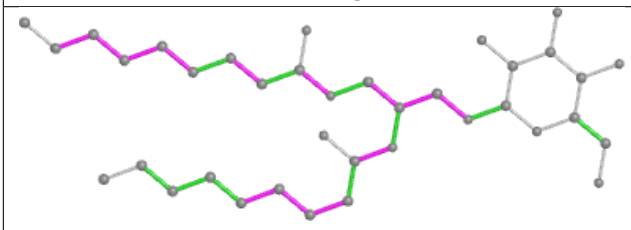

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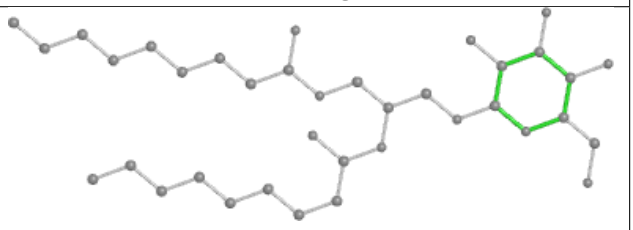
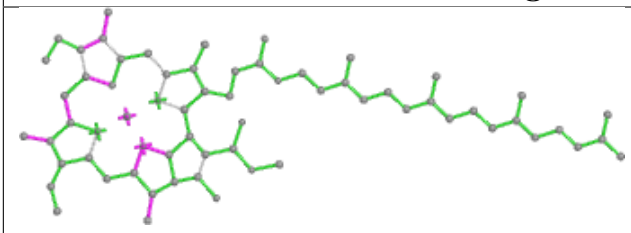


Rings

Ligand CLA B 610



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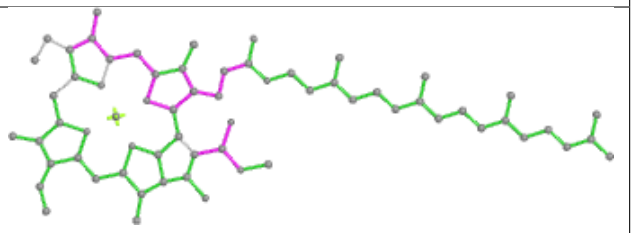

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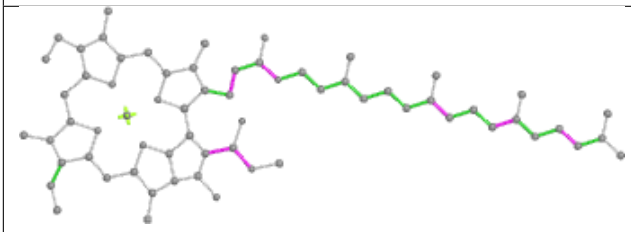

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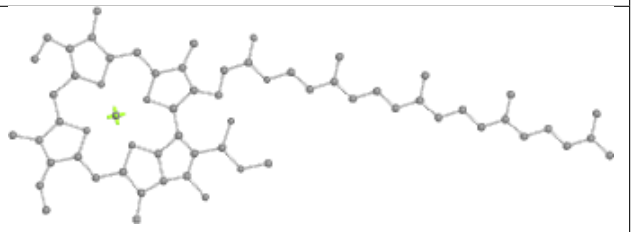
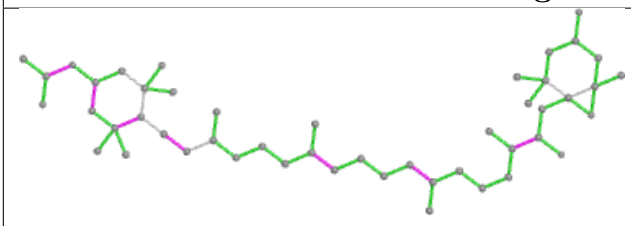


Rings

Ligand A86 8 301



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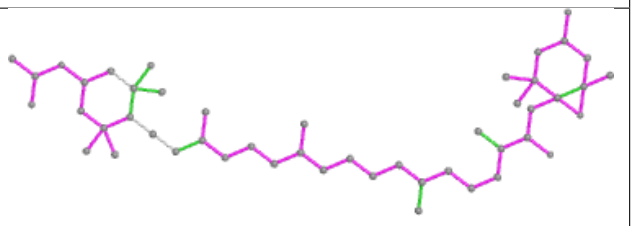

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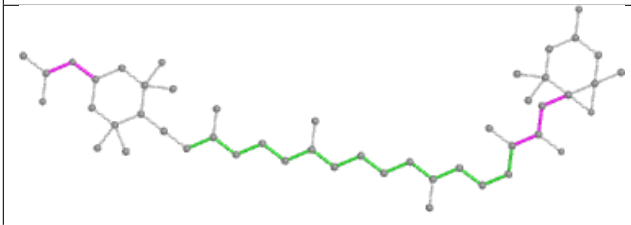

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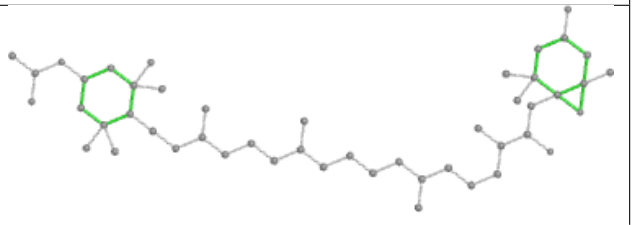
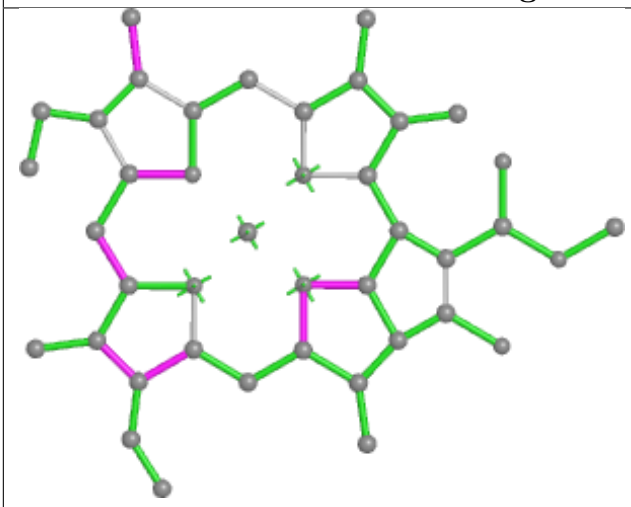


Rings

Ligand CLA 11 315



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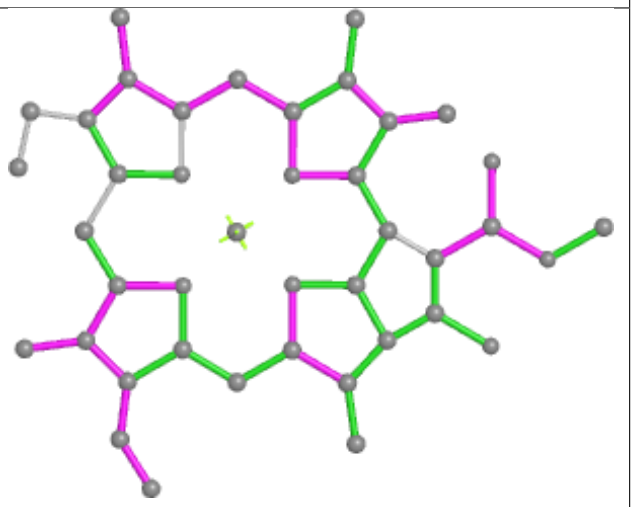

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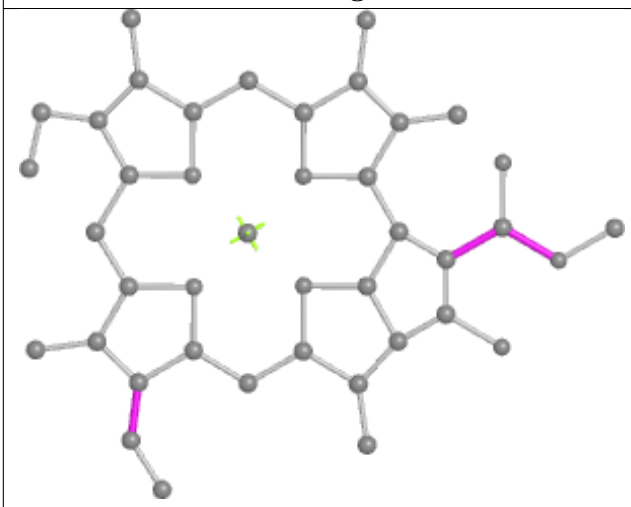

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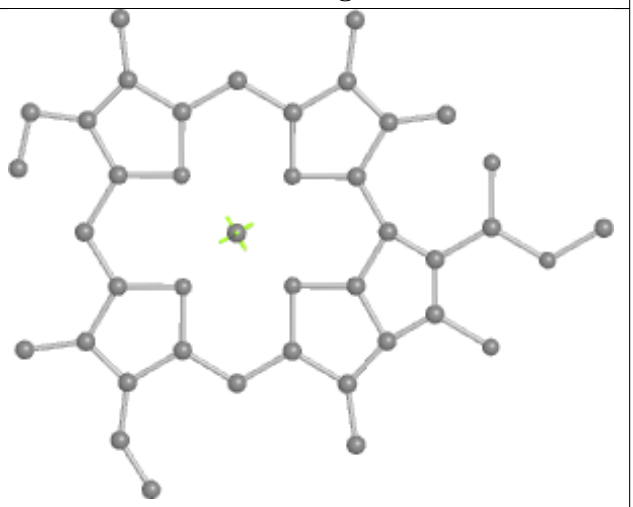
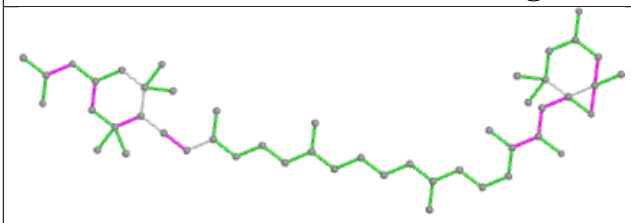


Rings

Ligand A86 17 305



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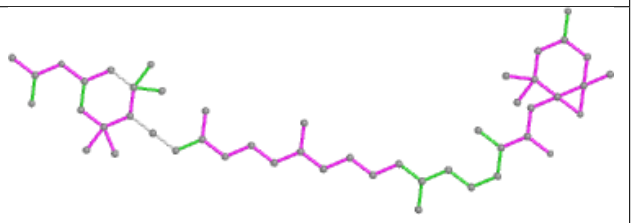

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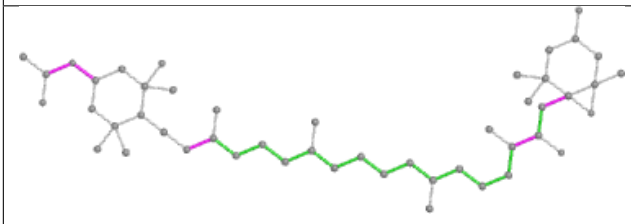

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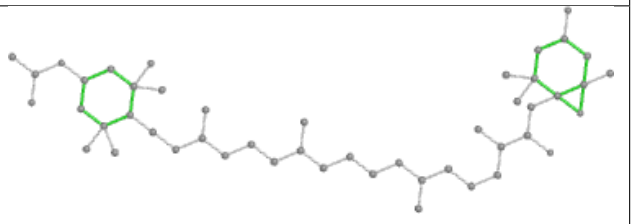
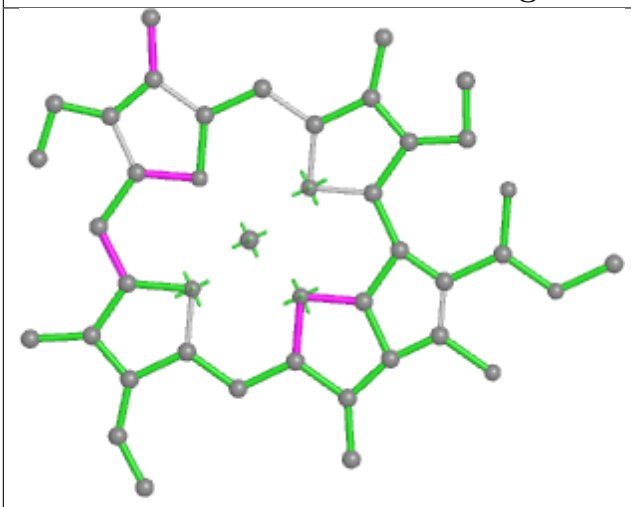


Rings

Ligand CLA 16 308



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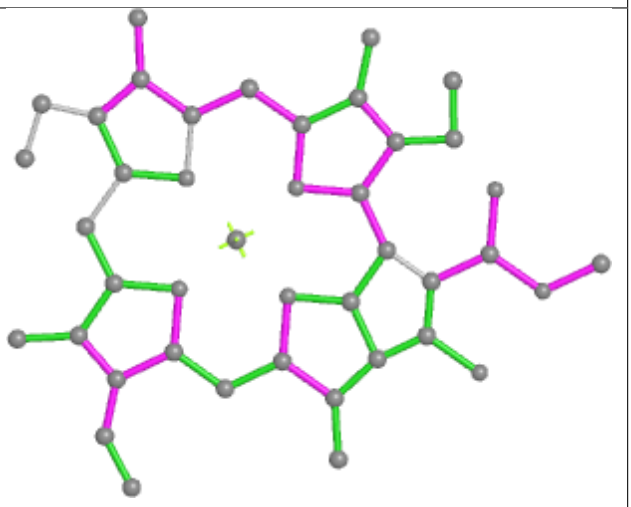

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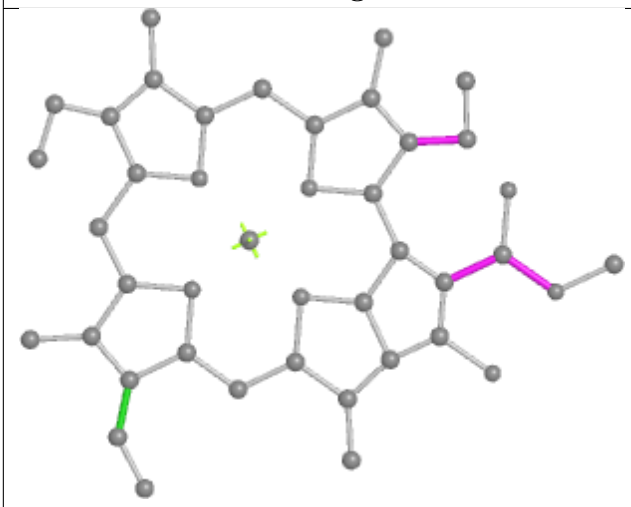

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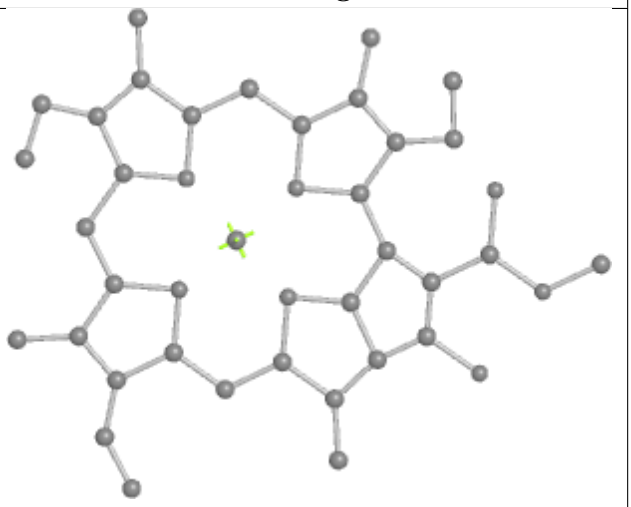

Rings

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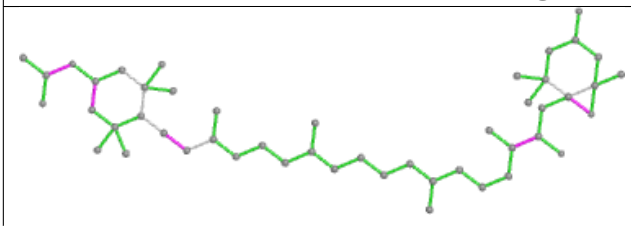

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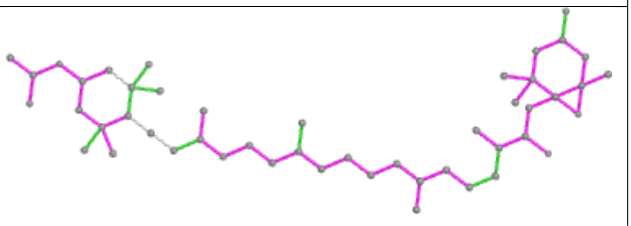
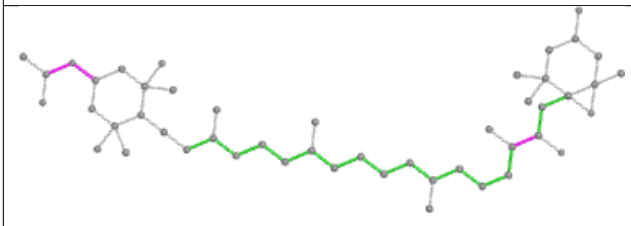


Bond angles



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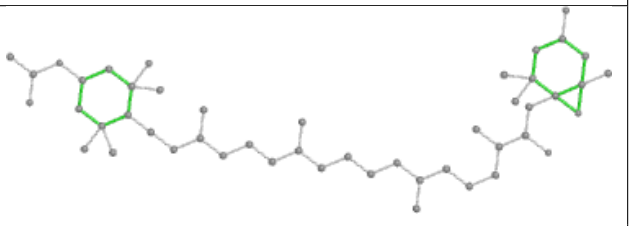
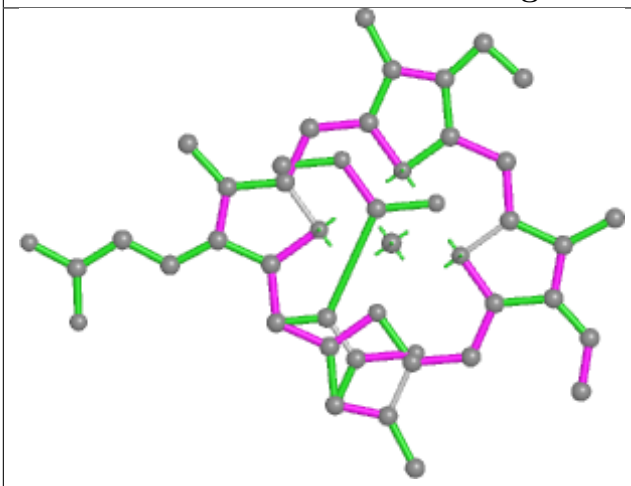


Rings

Ligand KC2 12 309



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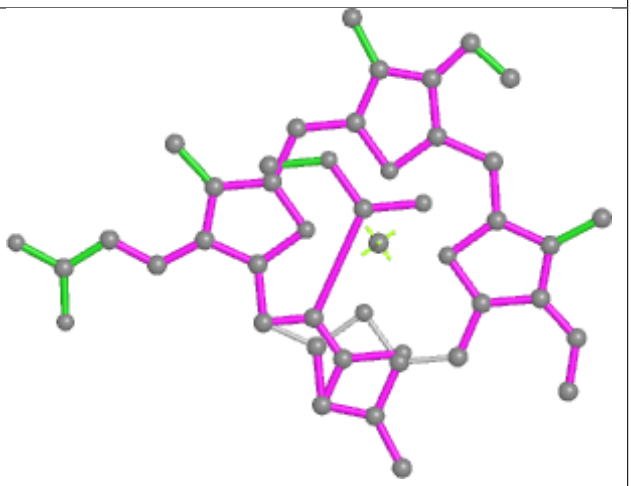

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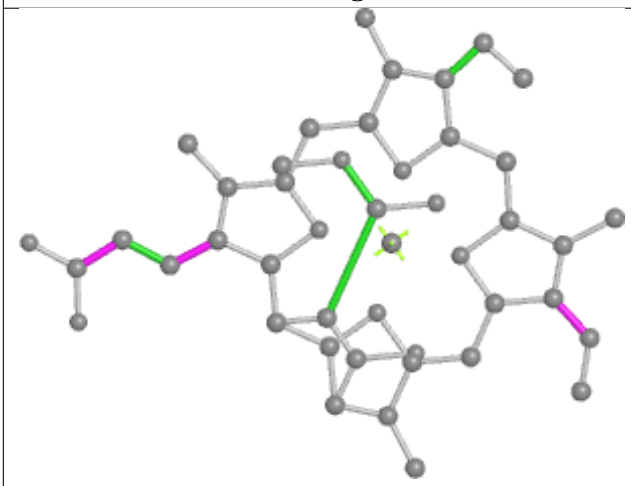

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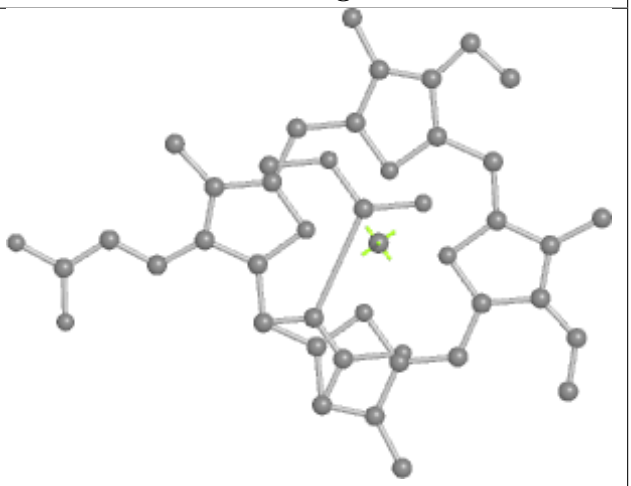

Rings

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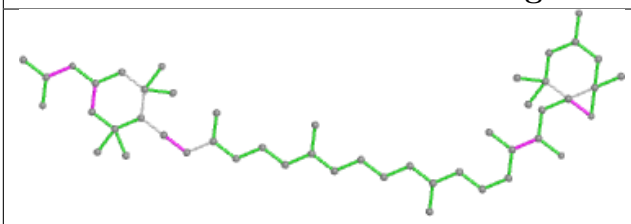

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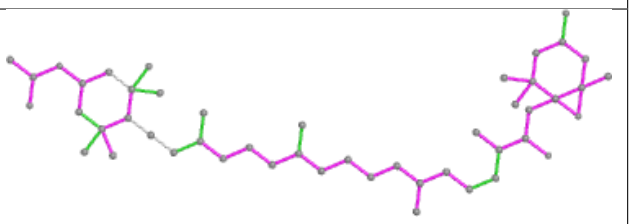

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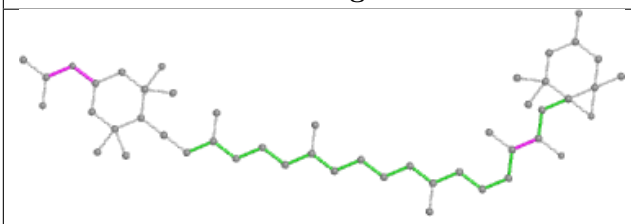

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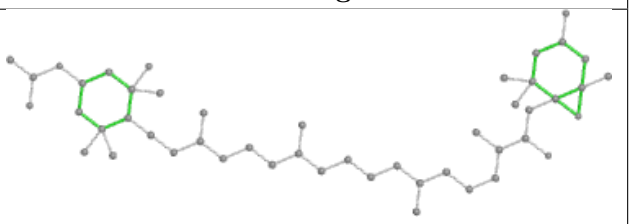

Rings

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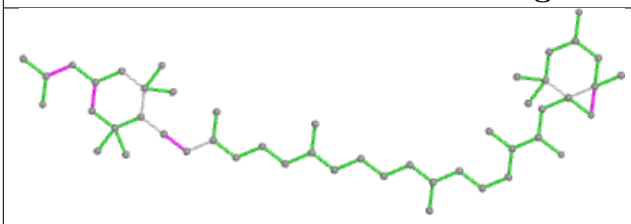

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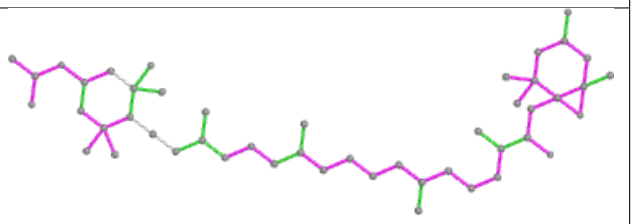

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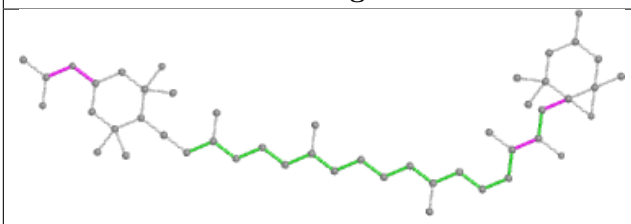

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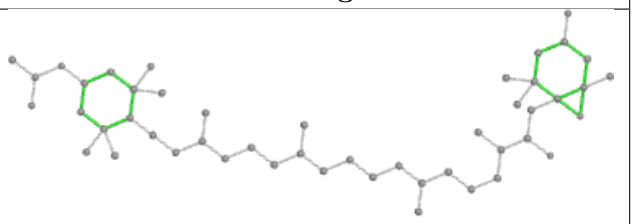

Rings

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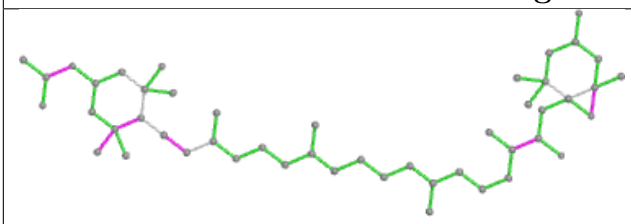

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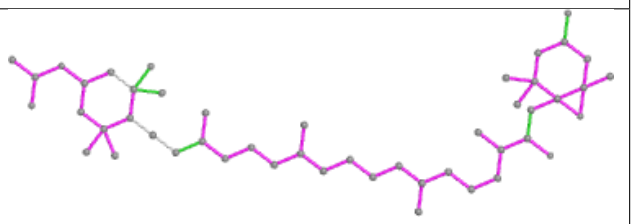

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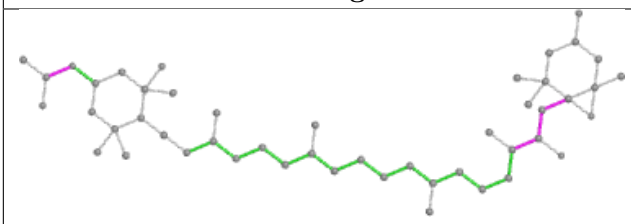

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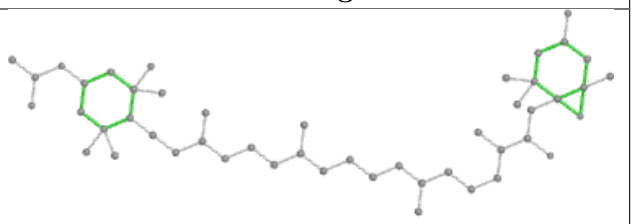
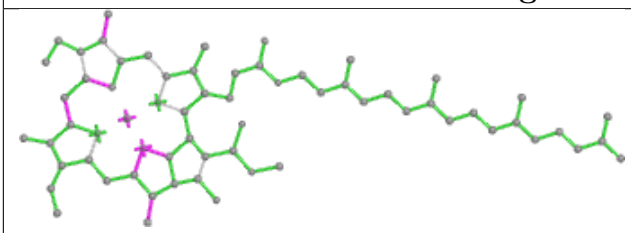


Rings

Ligand CLA 19 312



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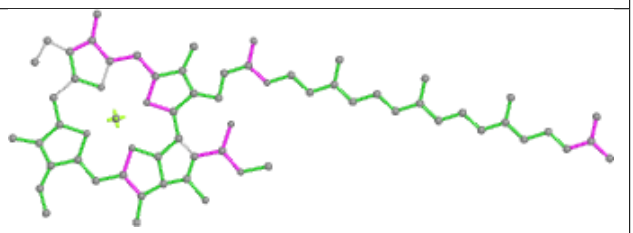

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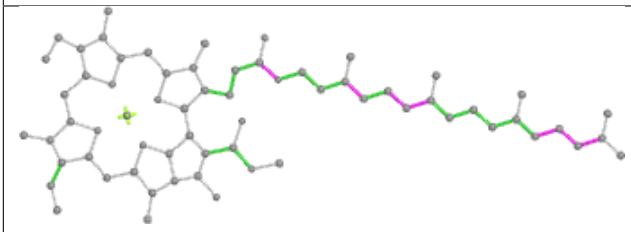

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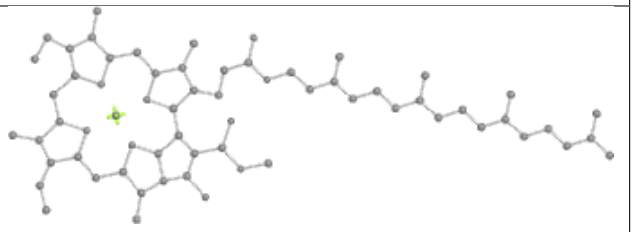

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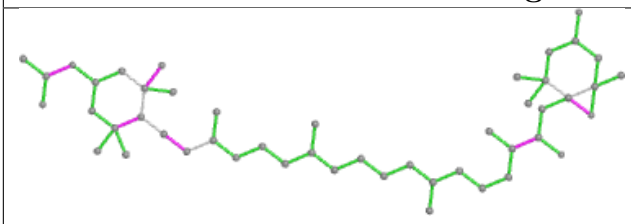

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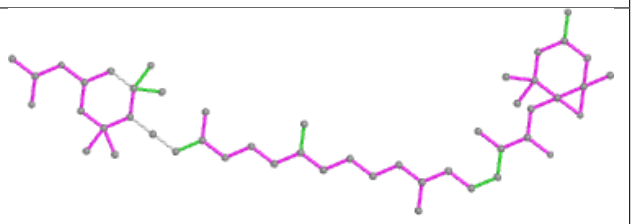

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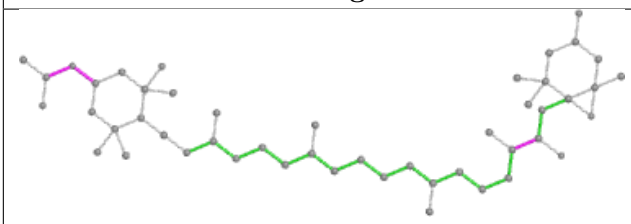

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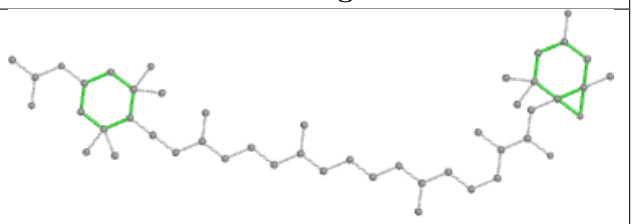

Rings

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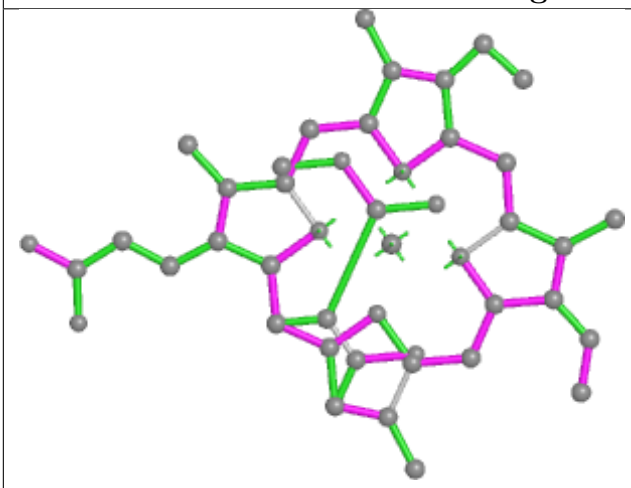

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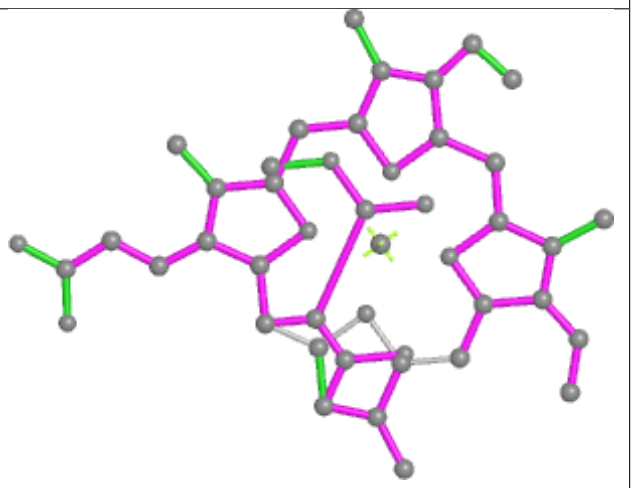

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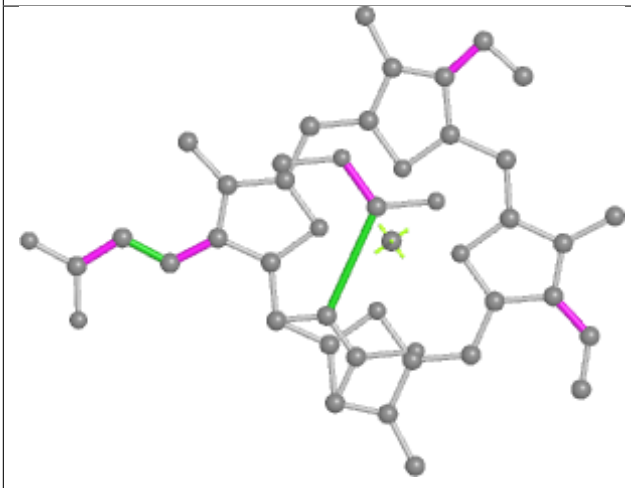

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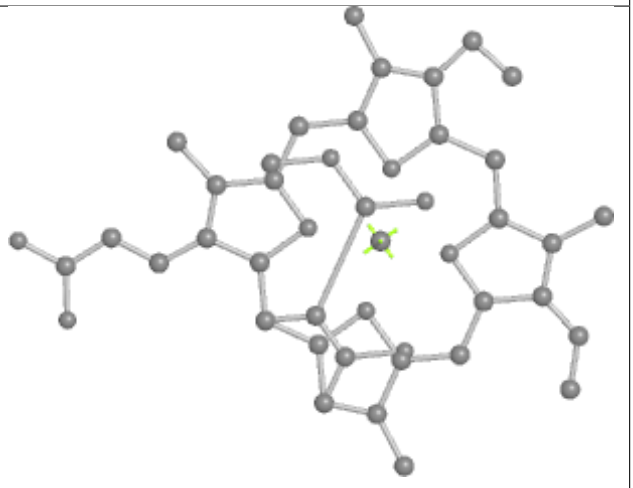
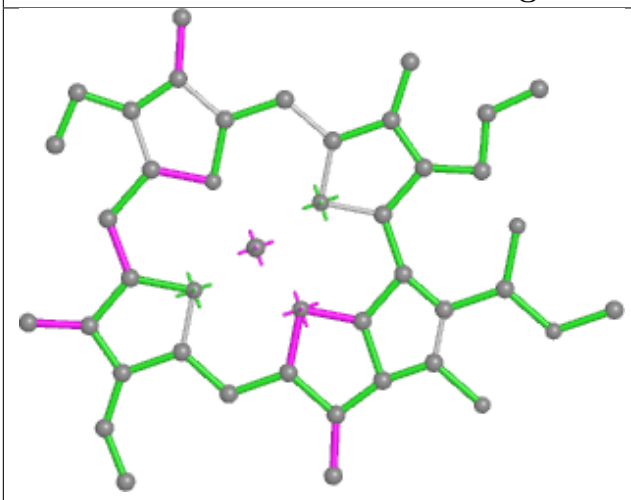


Rings

Ligand CLA 13 308



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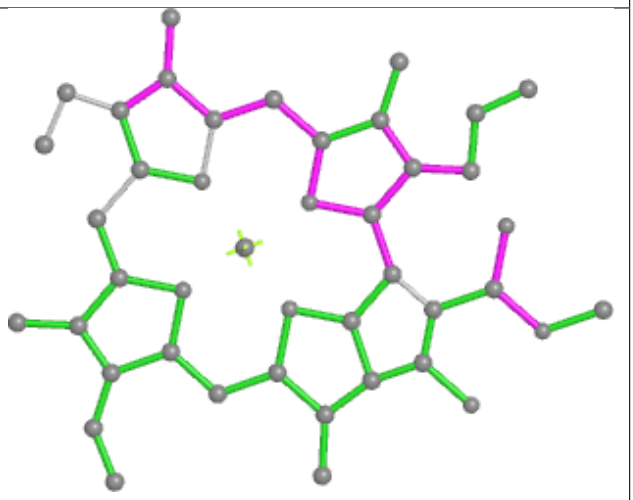

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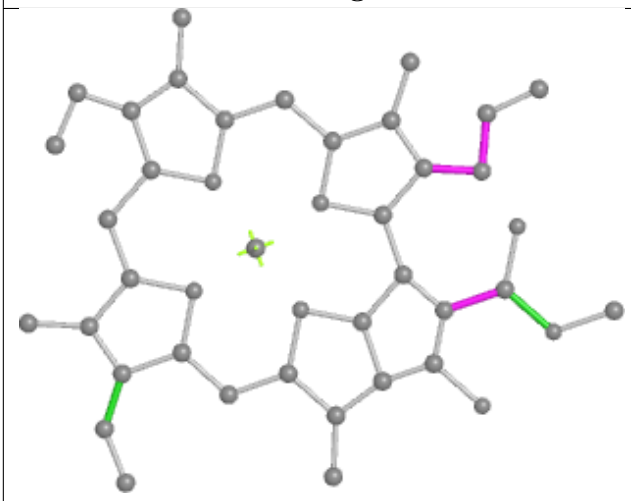

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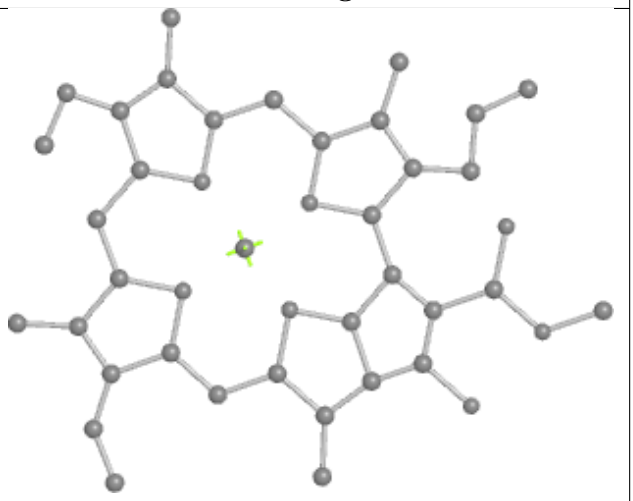
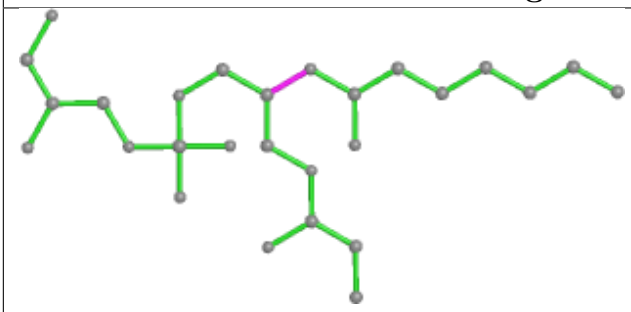


Rings

Ligand LHG p 615



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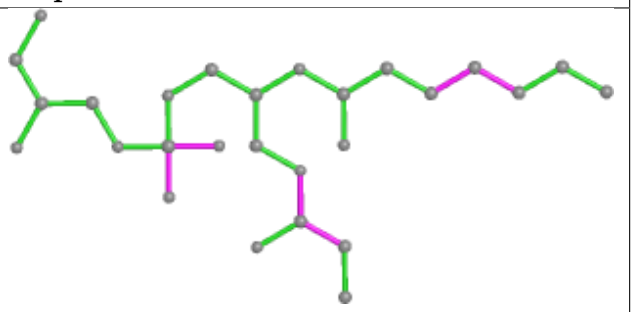

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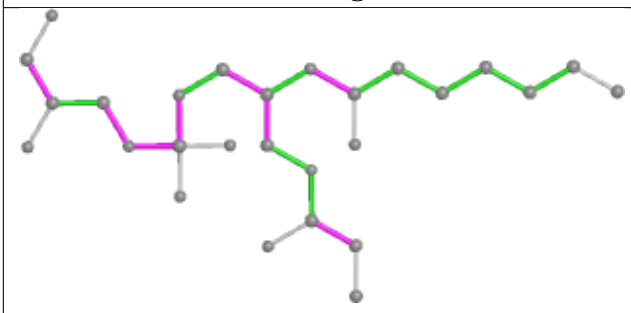

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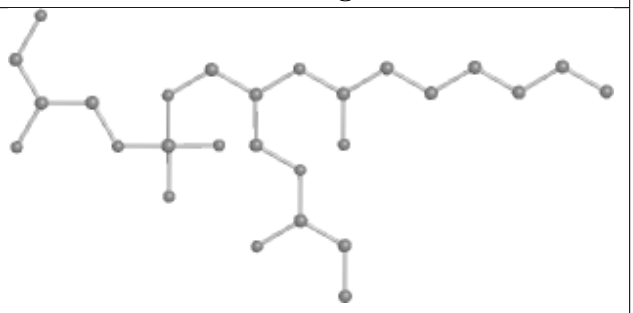
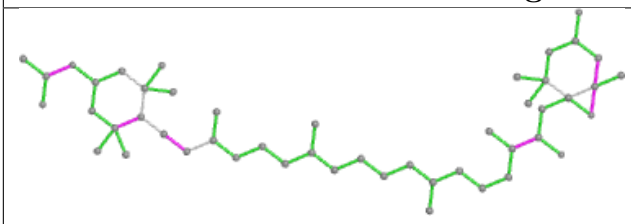


Rings

Ligand A86 17 303



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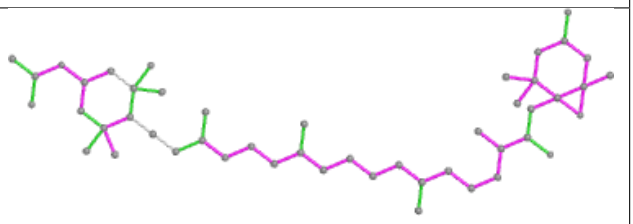

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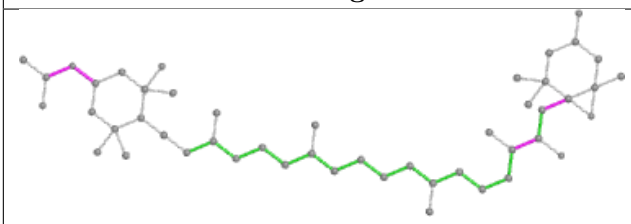

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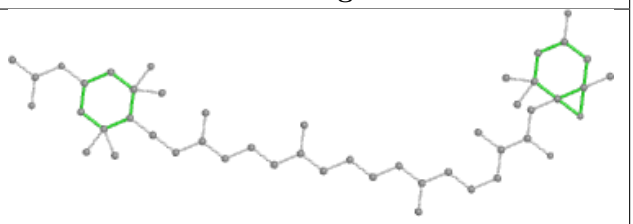
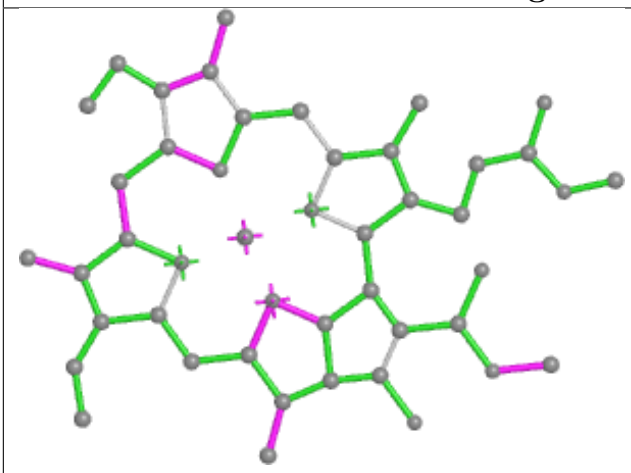


Rings

Ligand CLA 1 312



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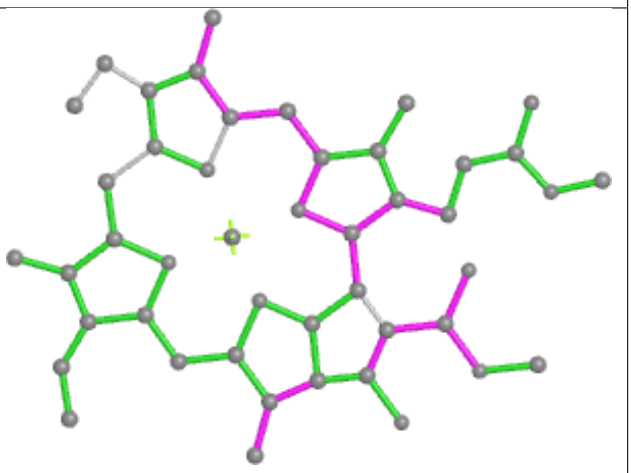

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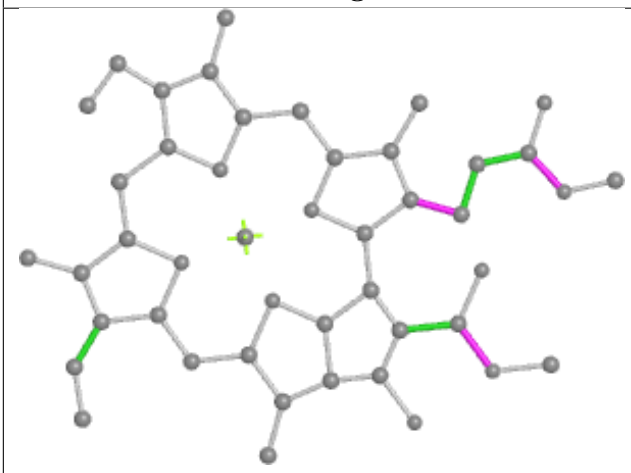

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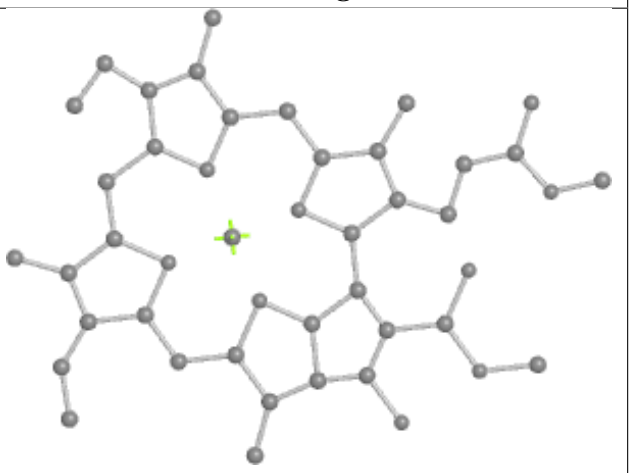
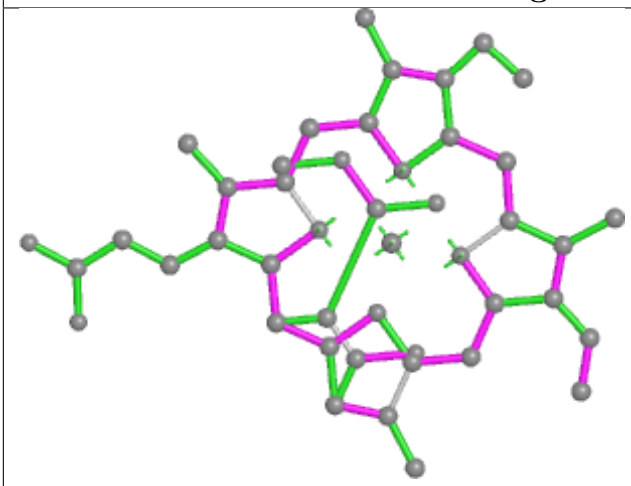


Rings

Ligand KC2 9 309



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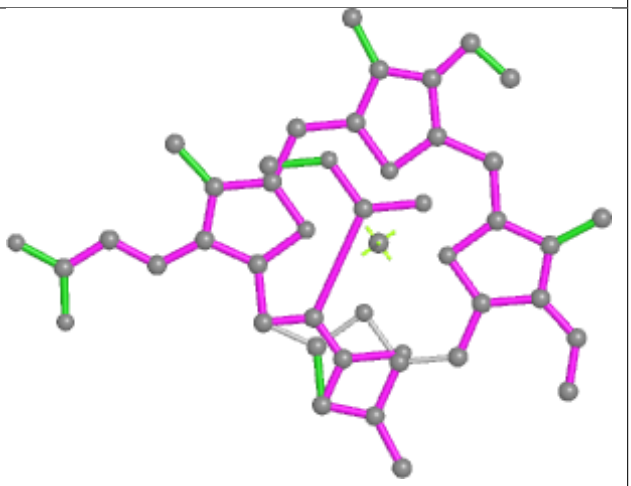

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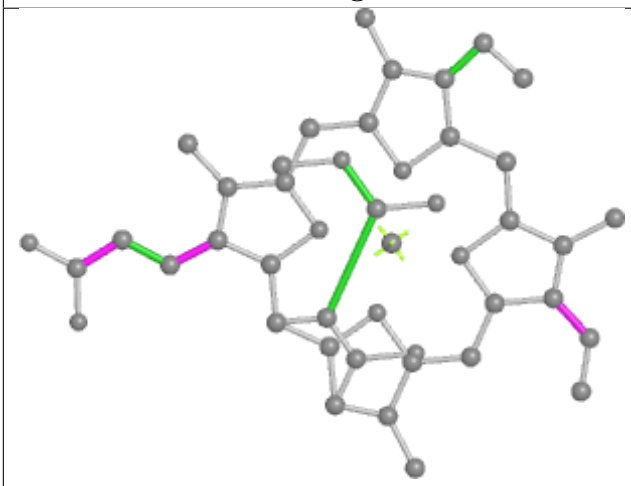

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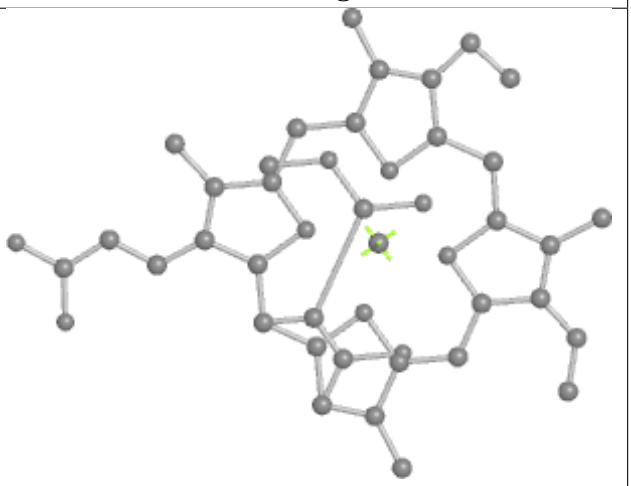
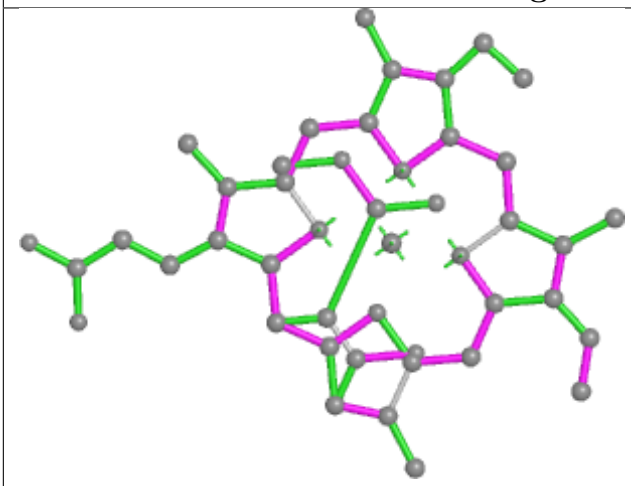


Rings

Ligand KC2 4 308



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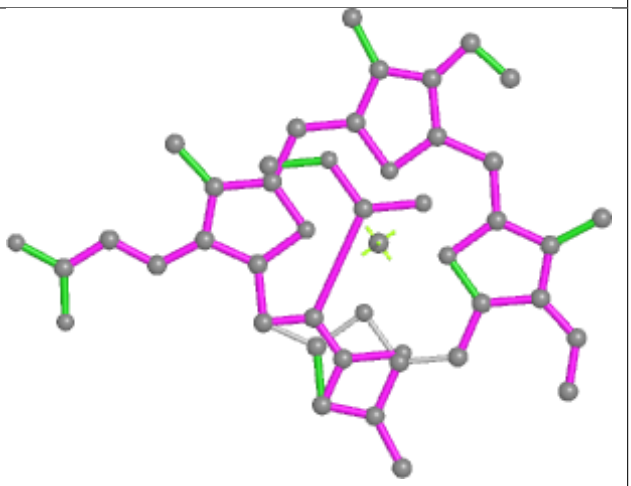

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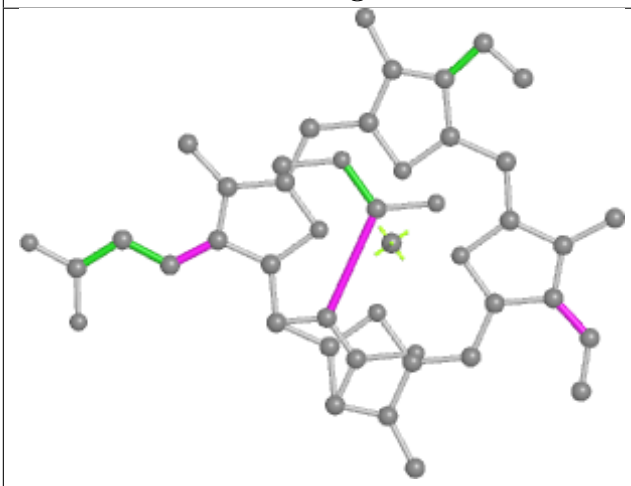

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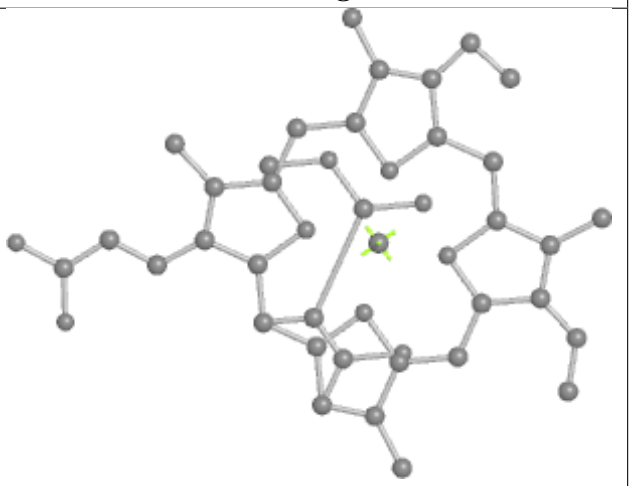
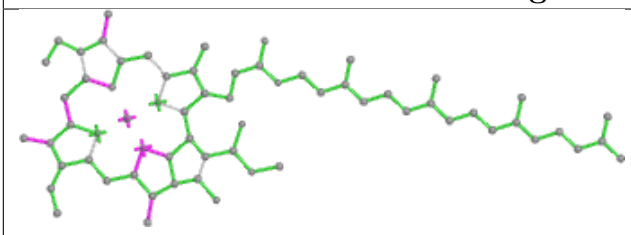


Rings

Ligand CLA c 510



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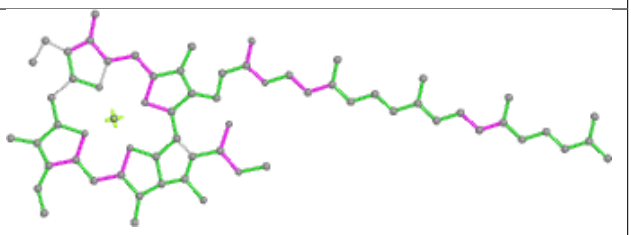

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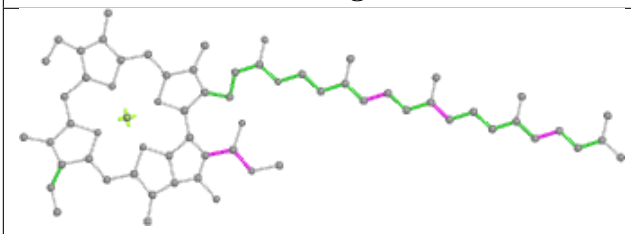

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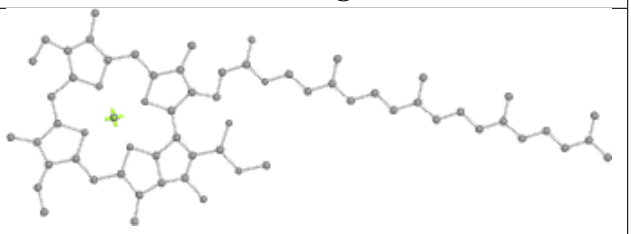
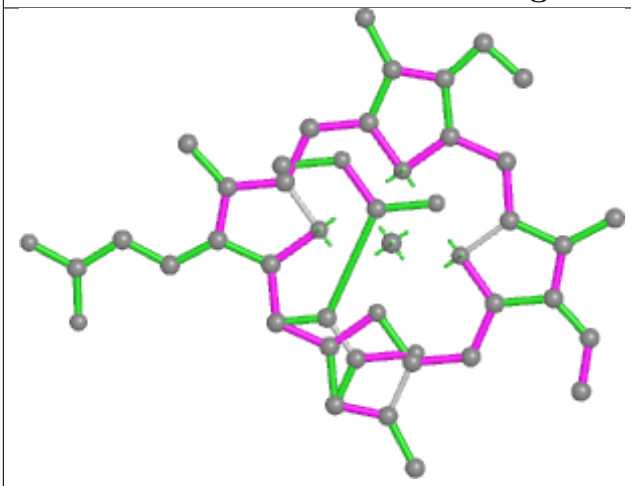


Rings

Ligand KC2 0 310



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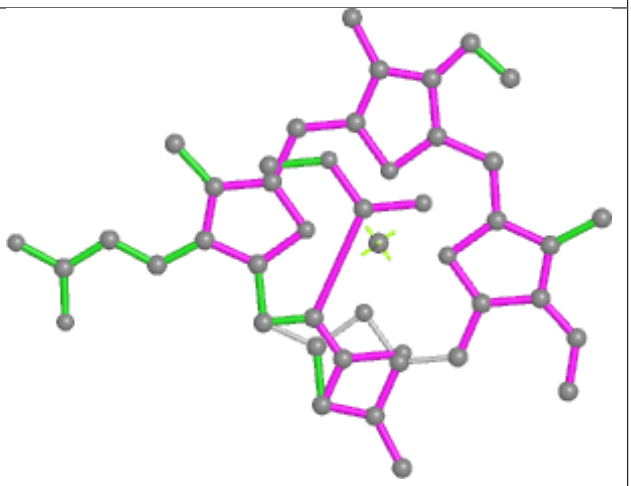

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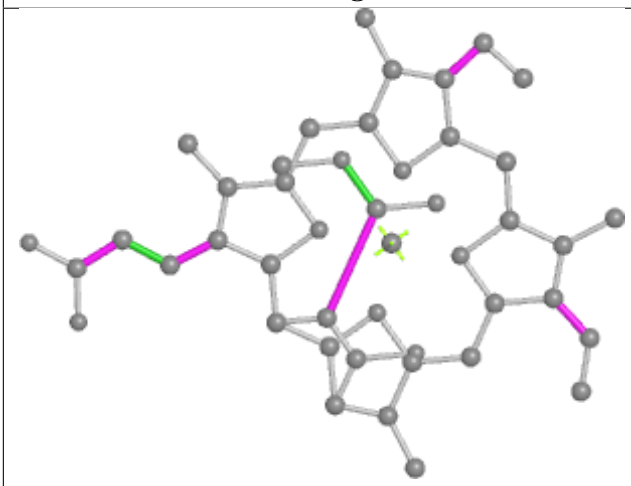
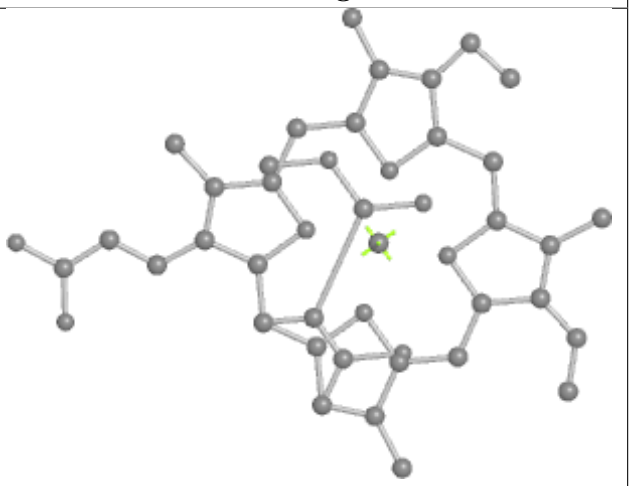
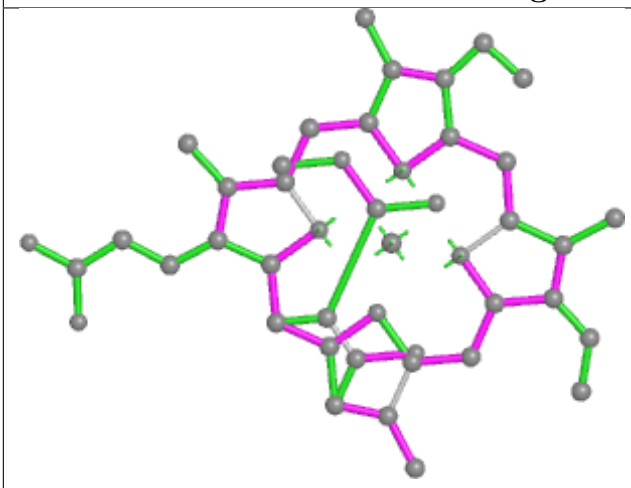


Torsions



Rings

Ligand KC1 6 315



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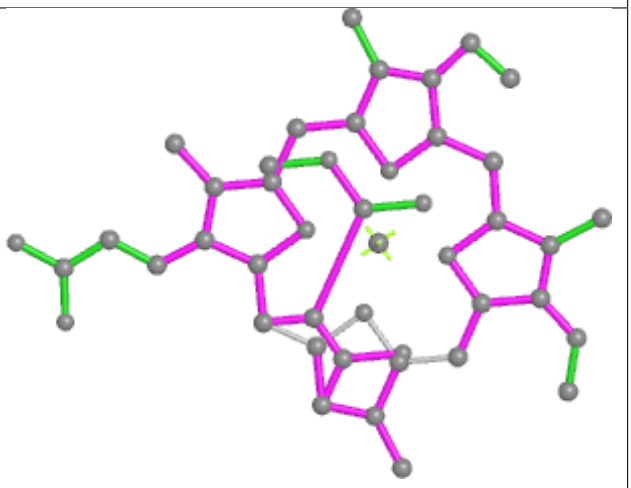

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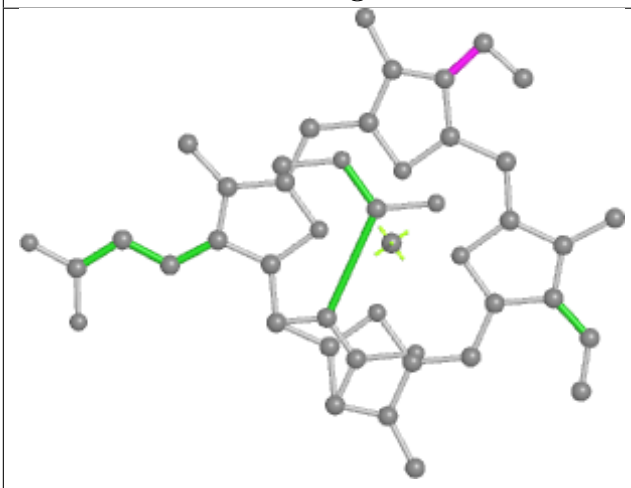

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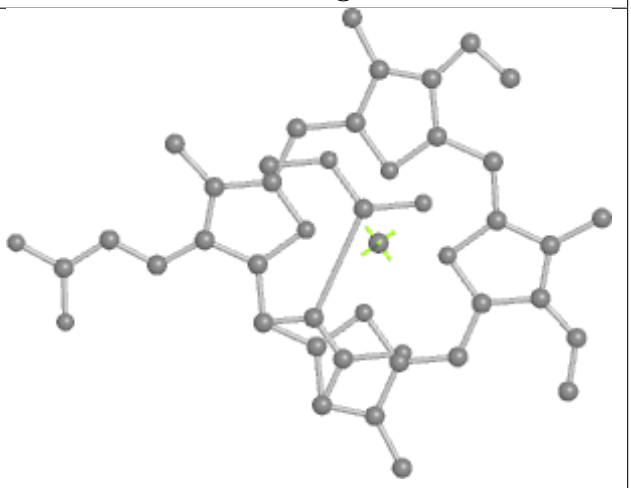
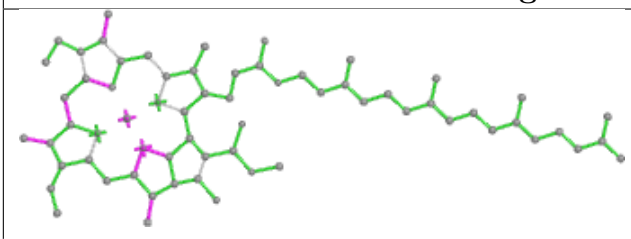


Rings

Ligand CLA 11 308



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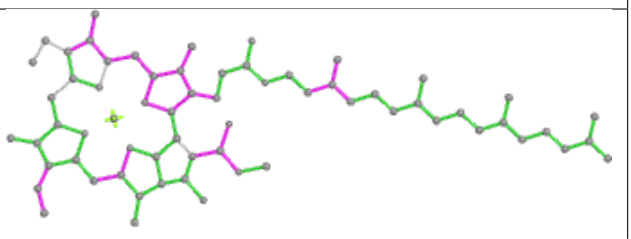

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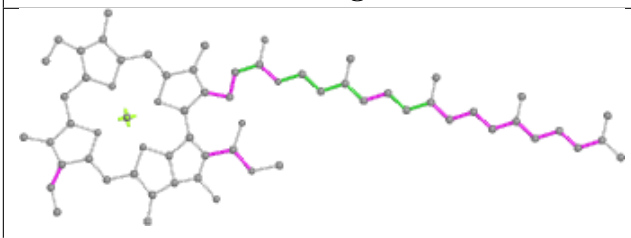

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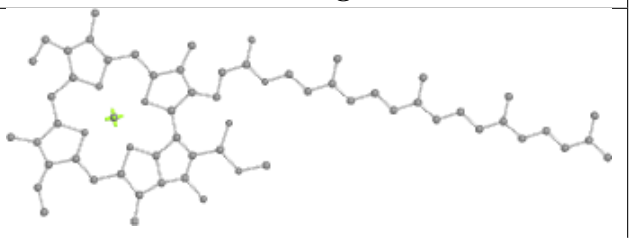
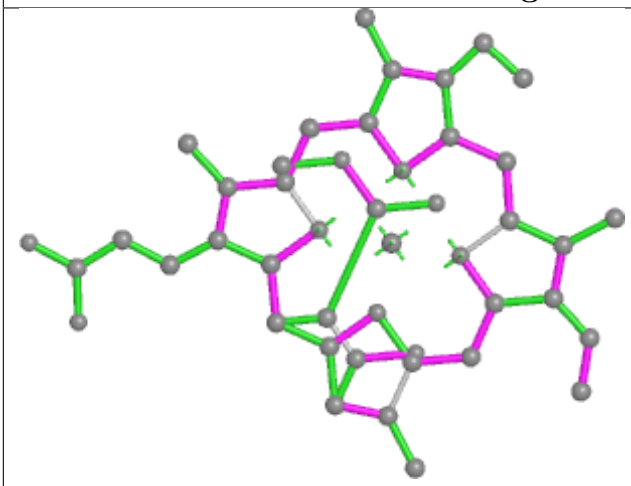


Rings

Ligand KC2 10 310



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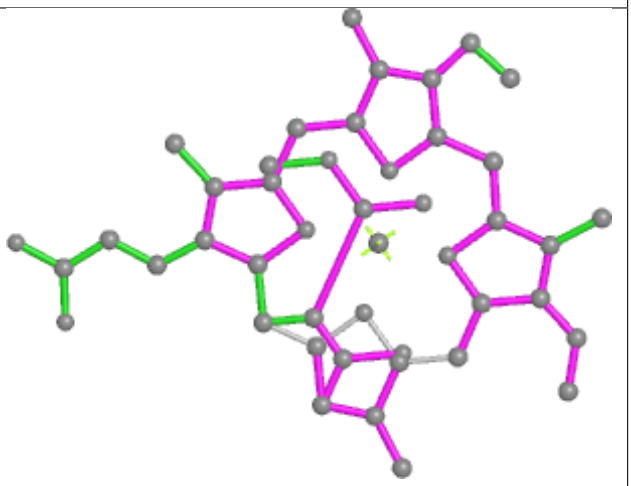

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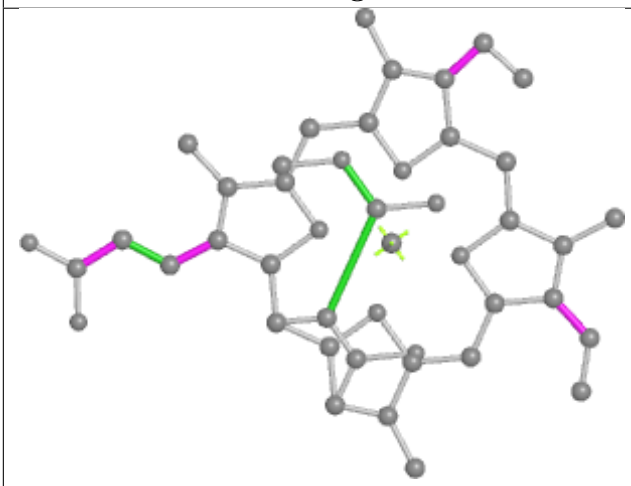

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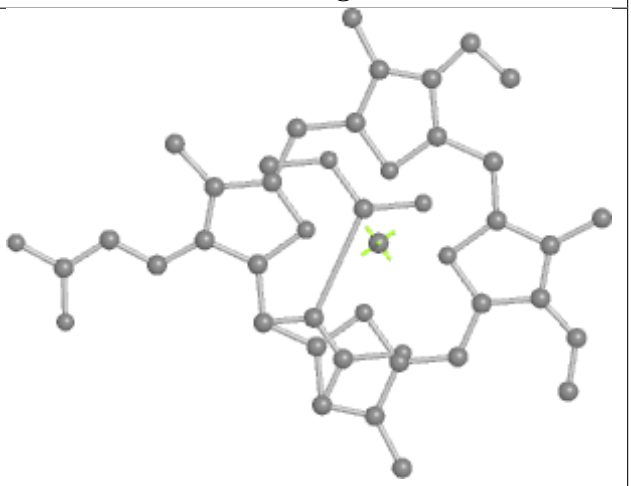
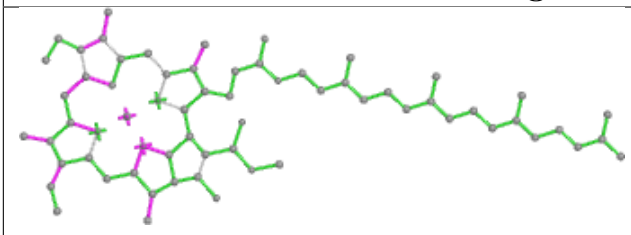


Rings

Ligand CLA b 605



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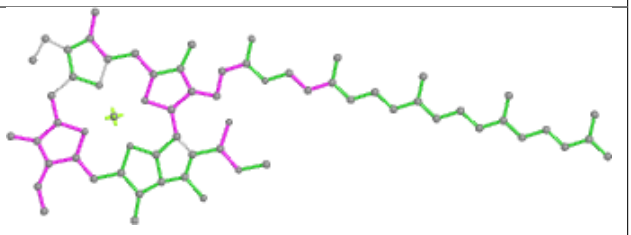

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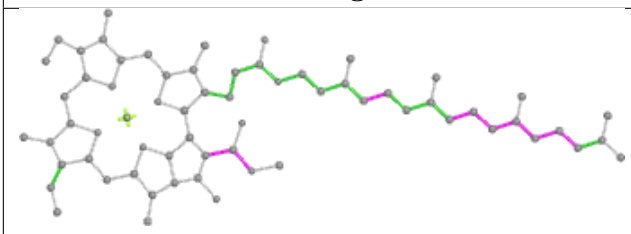

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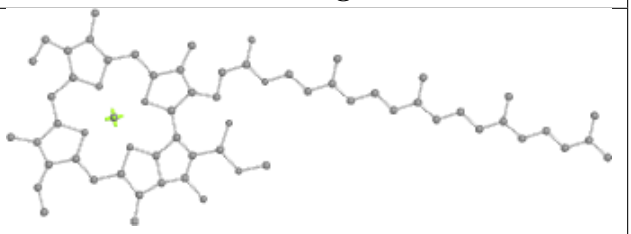
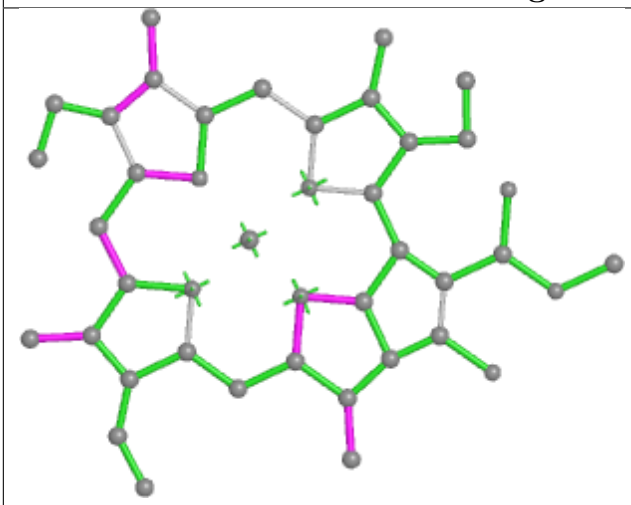


Rings

Ligand CLA 1 316



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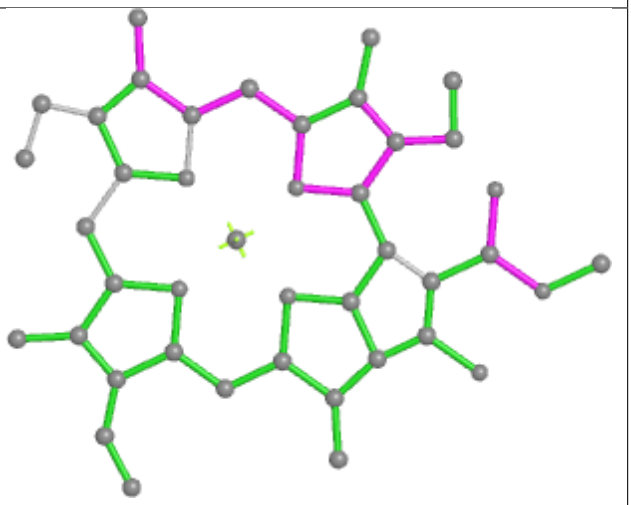

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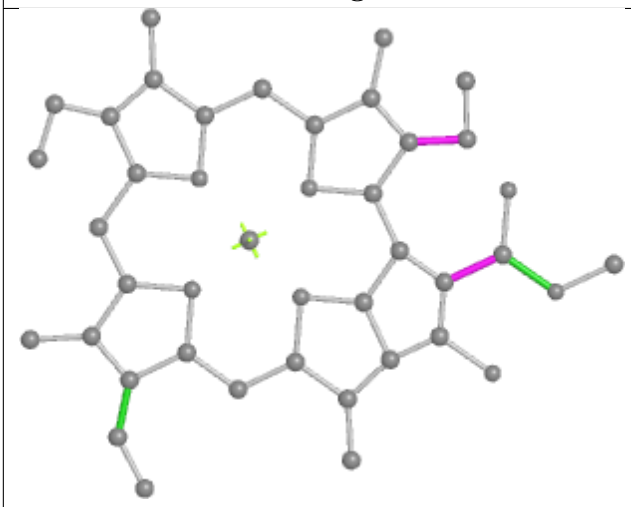

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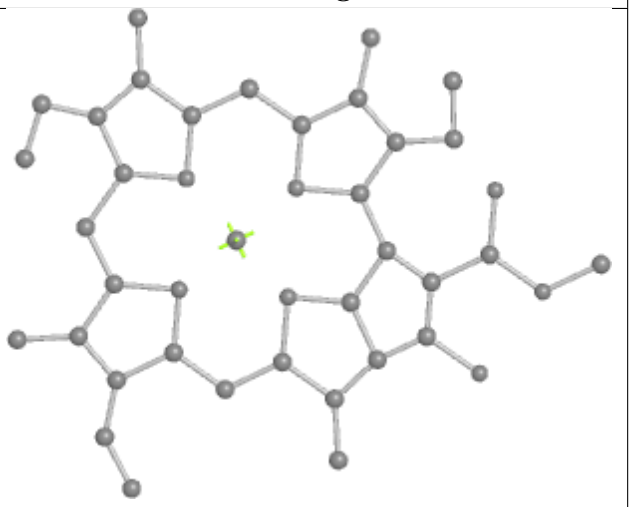
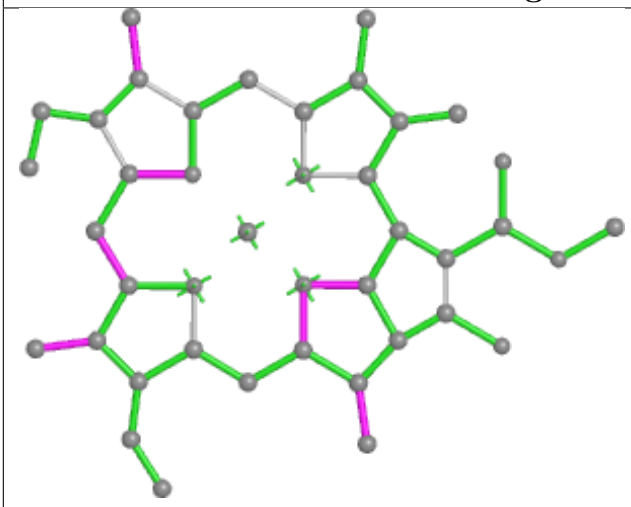


Rings

Ligand CLA P 605



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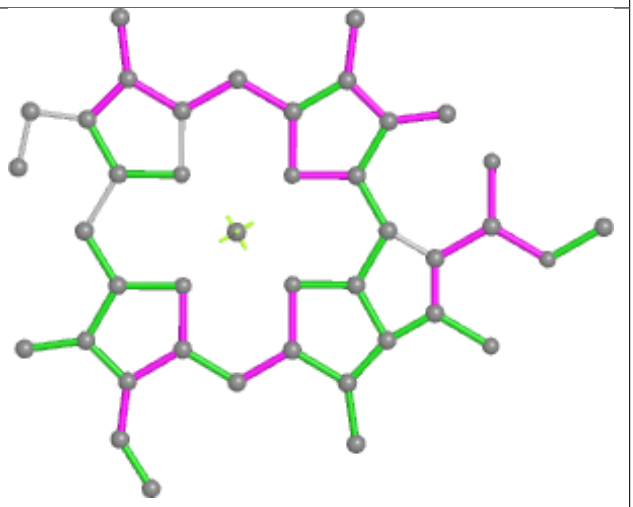

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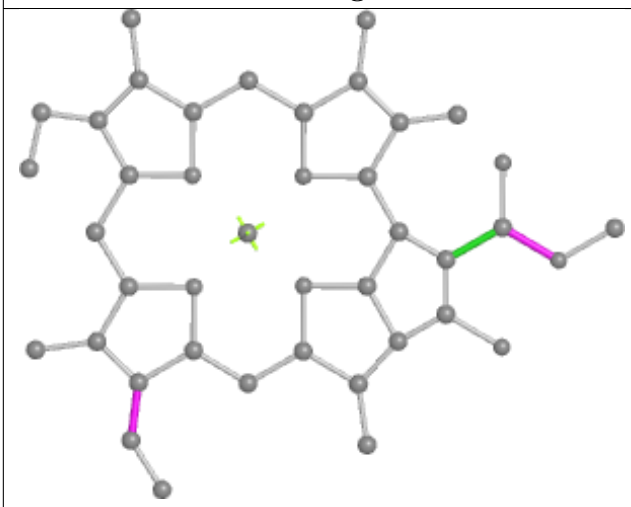

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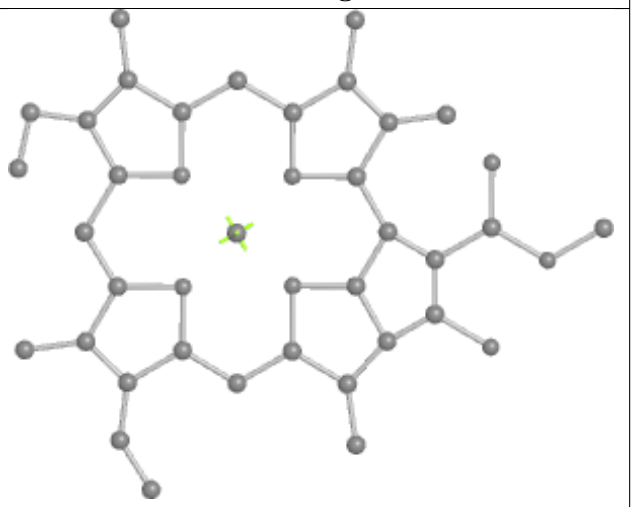
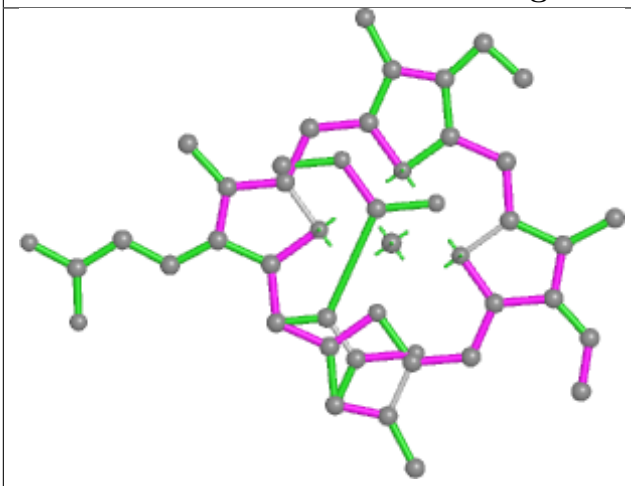


Rings

Ligand KC2 3 311



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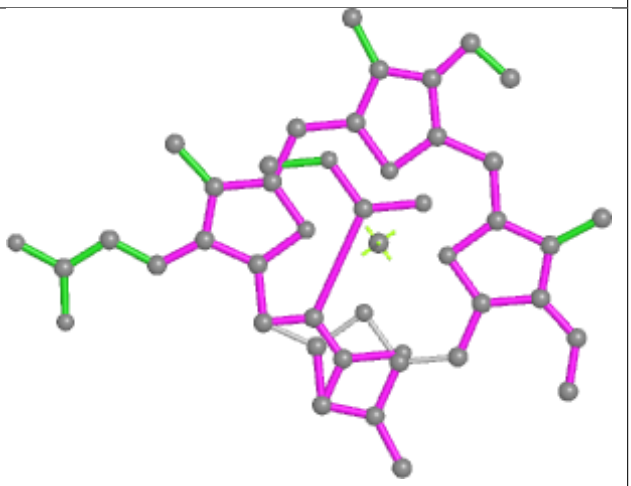

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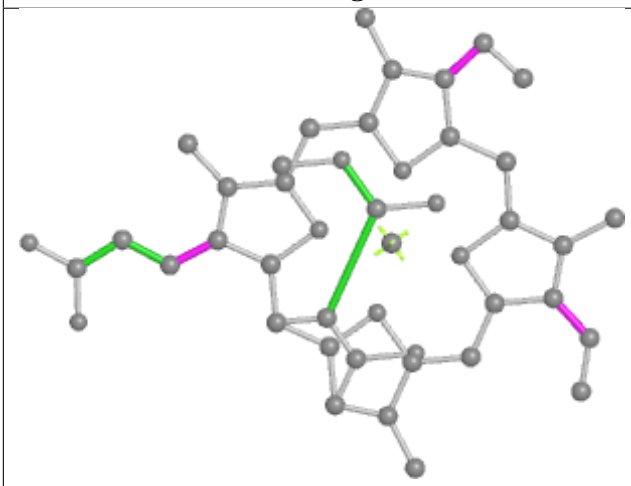

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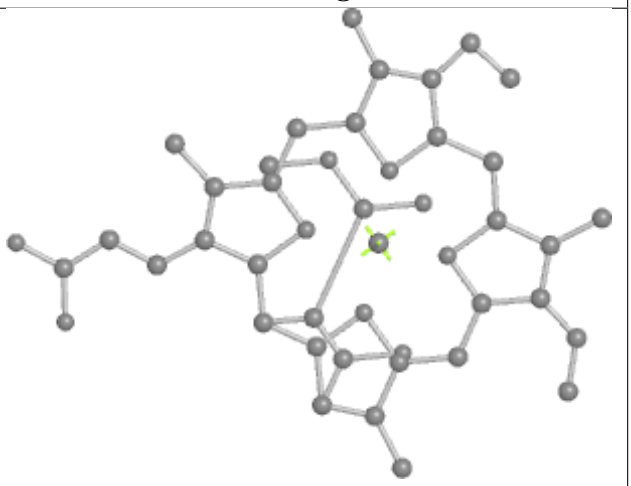
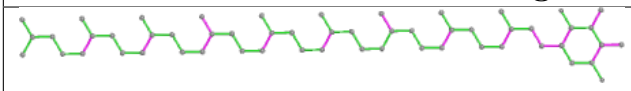


Rings

Ligand PL9 d 406



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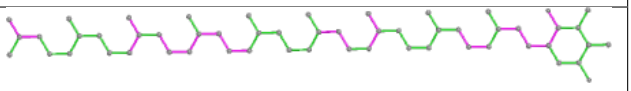

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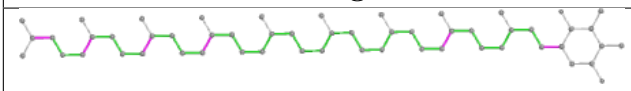

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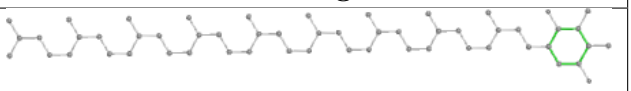
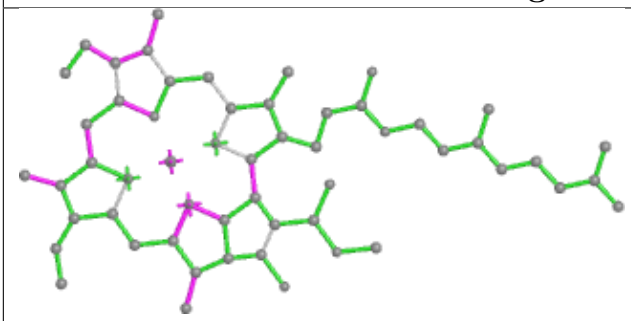


Rings

Ligand CLA 8 312



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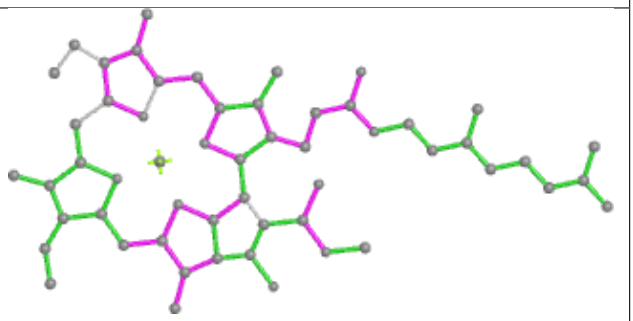

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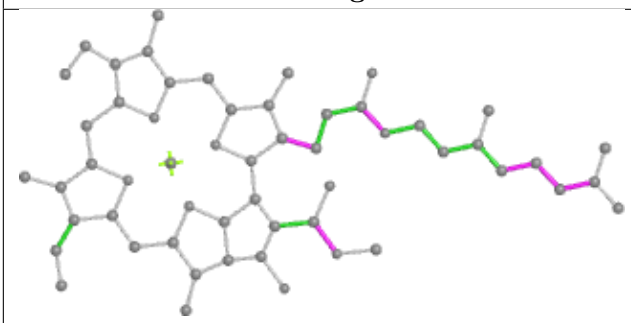

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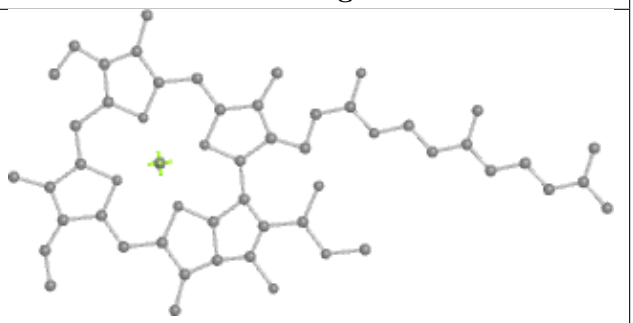
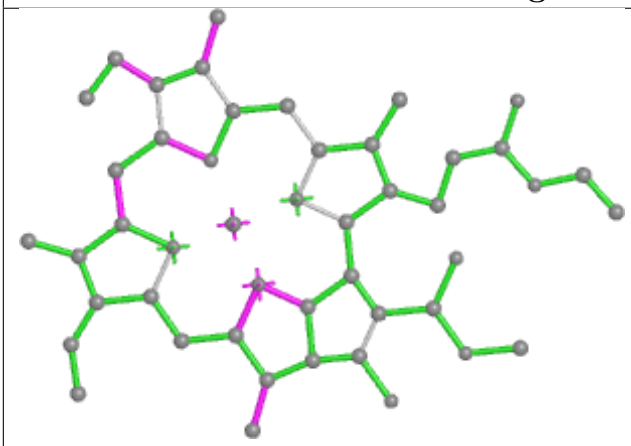


Rings

Ligand CLA 6 313



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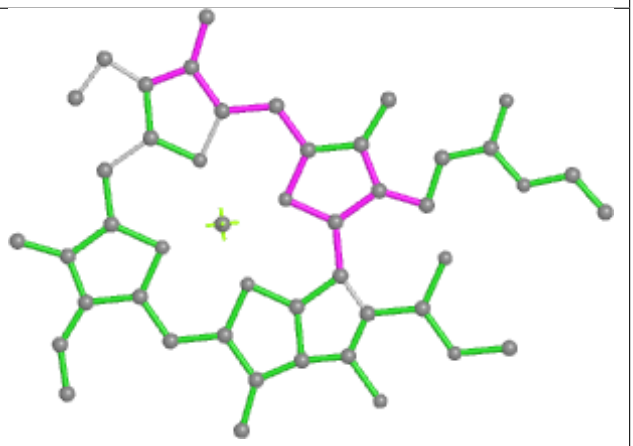

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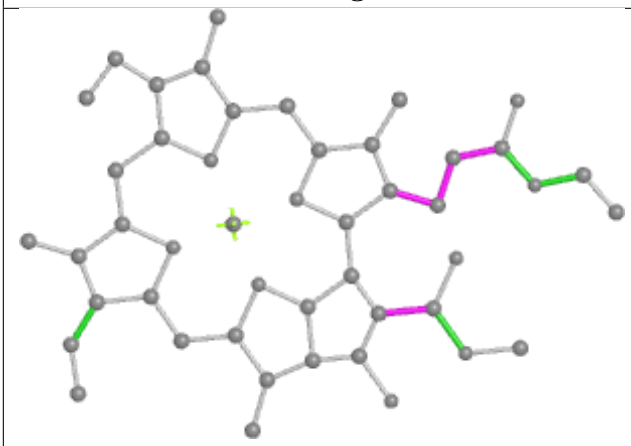

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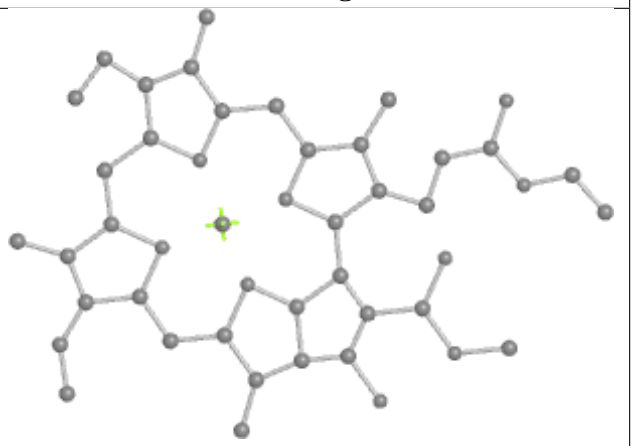
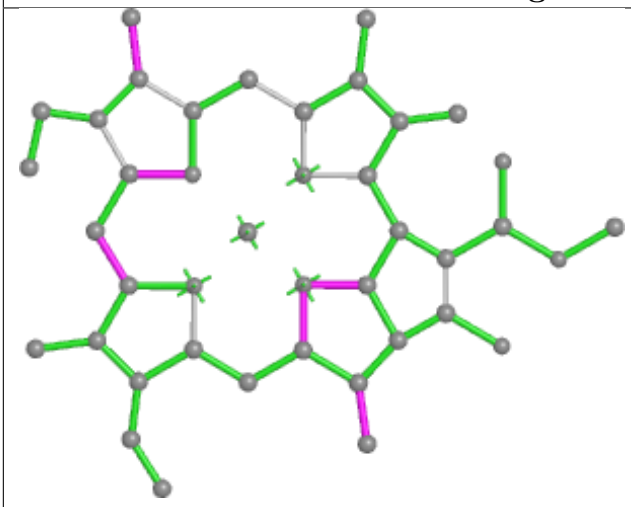


Rings

Ligand CLA 1 315



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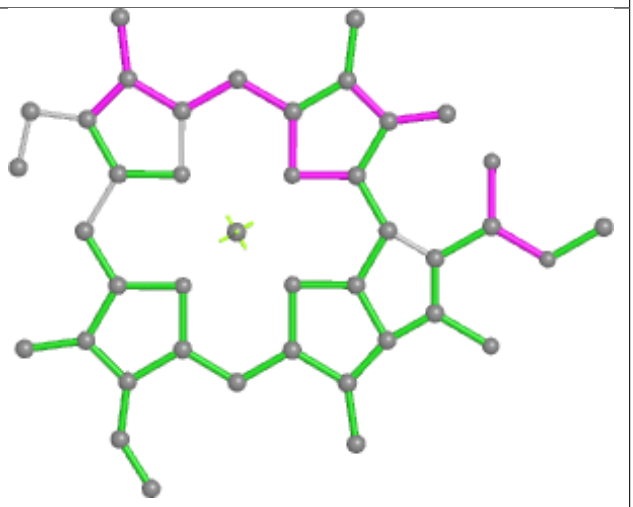

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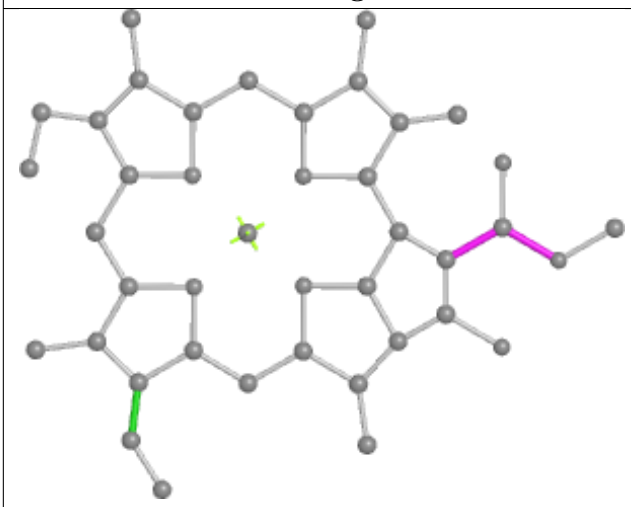

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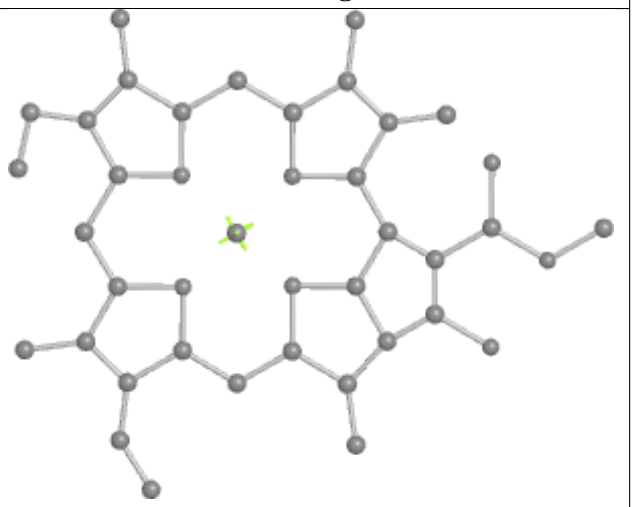
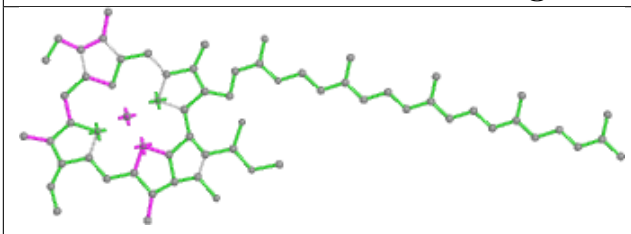


Rings

Ligand CLA 6 309



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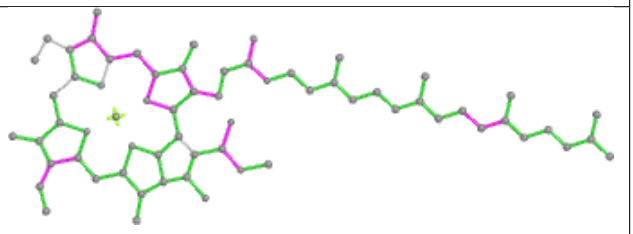
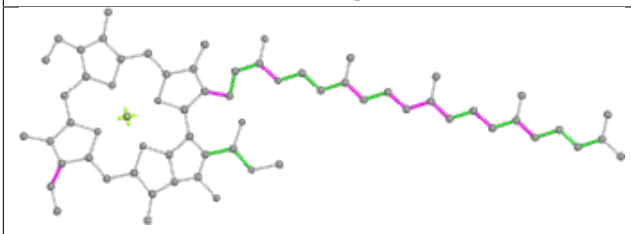


Bond angles



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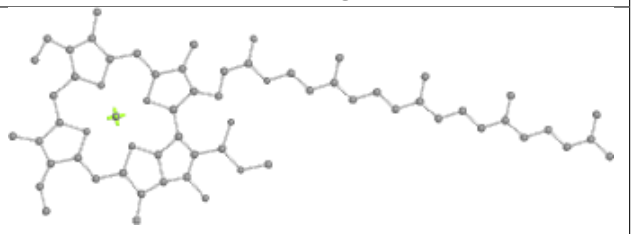
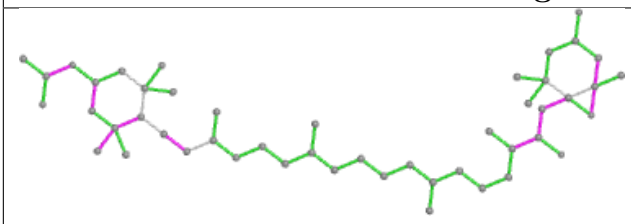


Rings

Ligand A86 6 305



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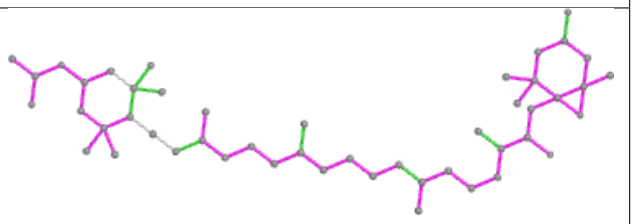
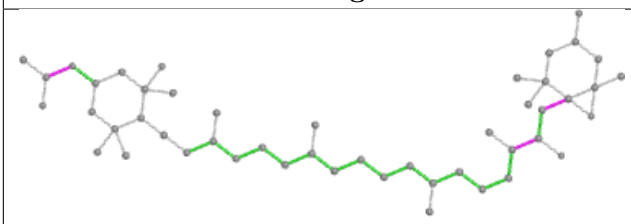
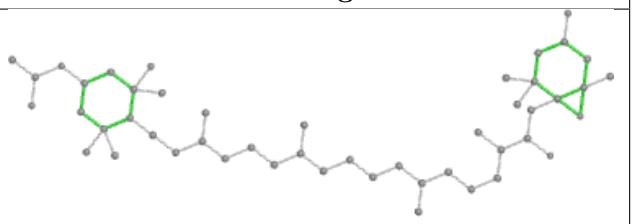


Bond angles

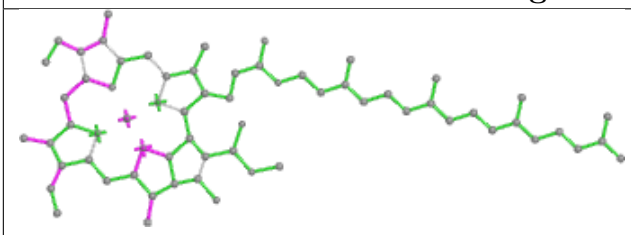


Torsions

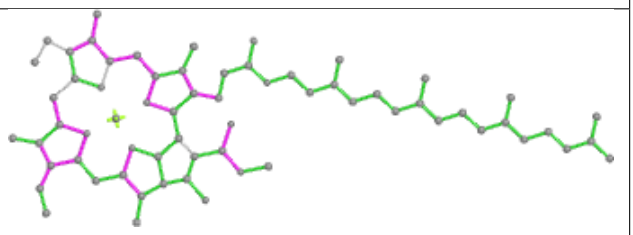


Rings

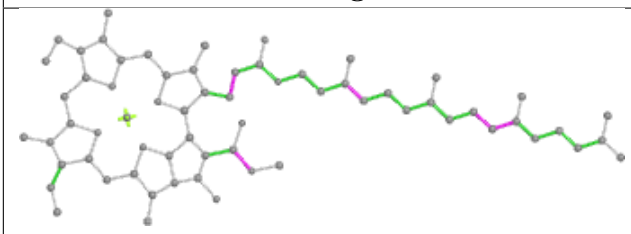
Ligand CLA c 505



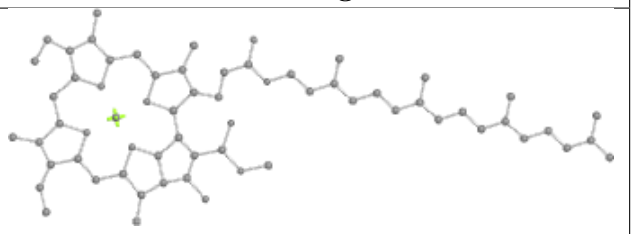
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

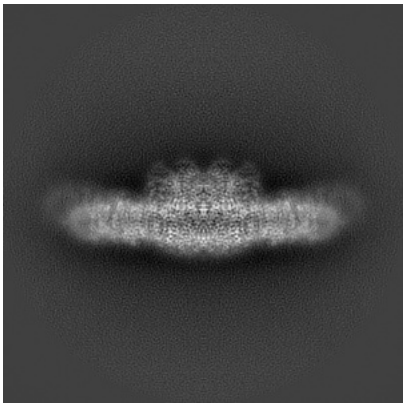
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9839. These allow visual inspection of the internal detail of the map and identification of artifacts.

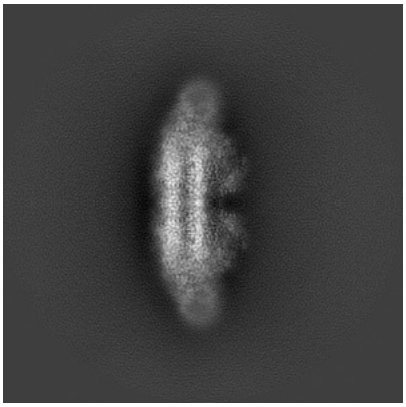
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

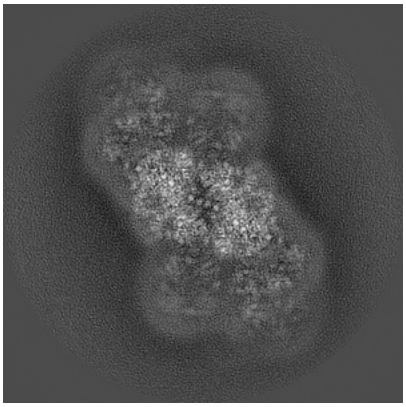
6.1.1 Primary map



X



Y

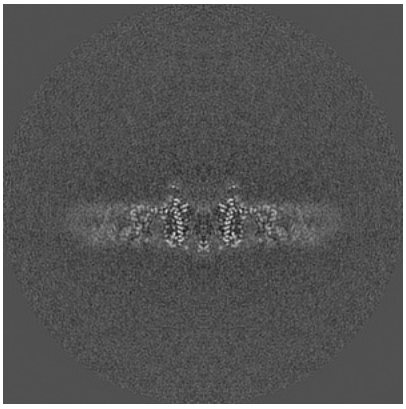


Z

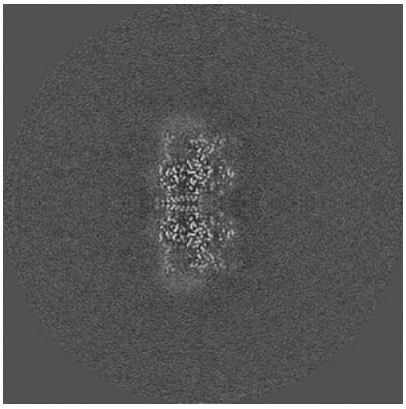
The images above show the map projected in three orthogonal directions.

6.2 Central slices

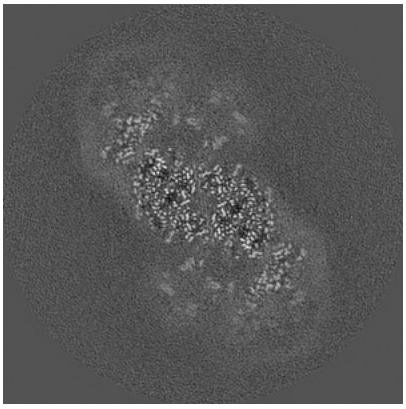
6.2.1 Primary map



X Index: 170



Y Index: 170

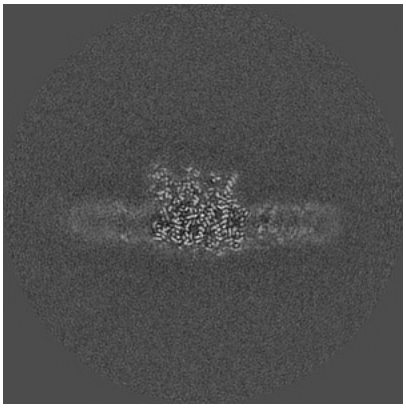


Z Index: 170

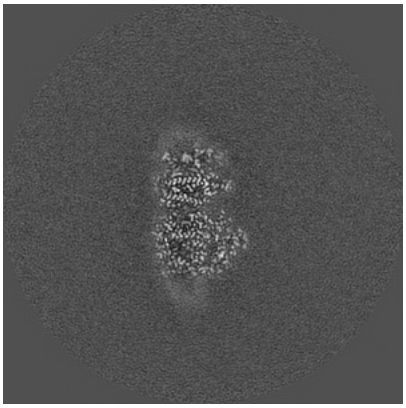
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

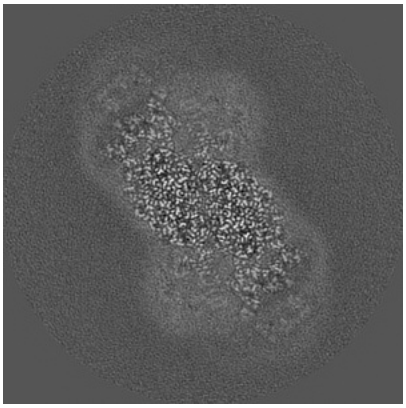
6.3.1 Primary map



X Index: 191



Y Index: 187



Z Index: 165

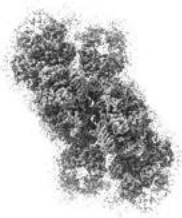
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

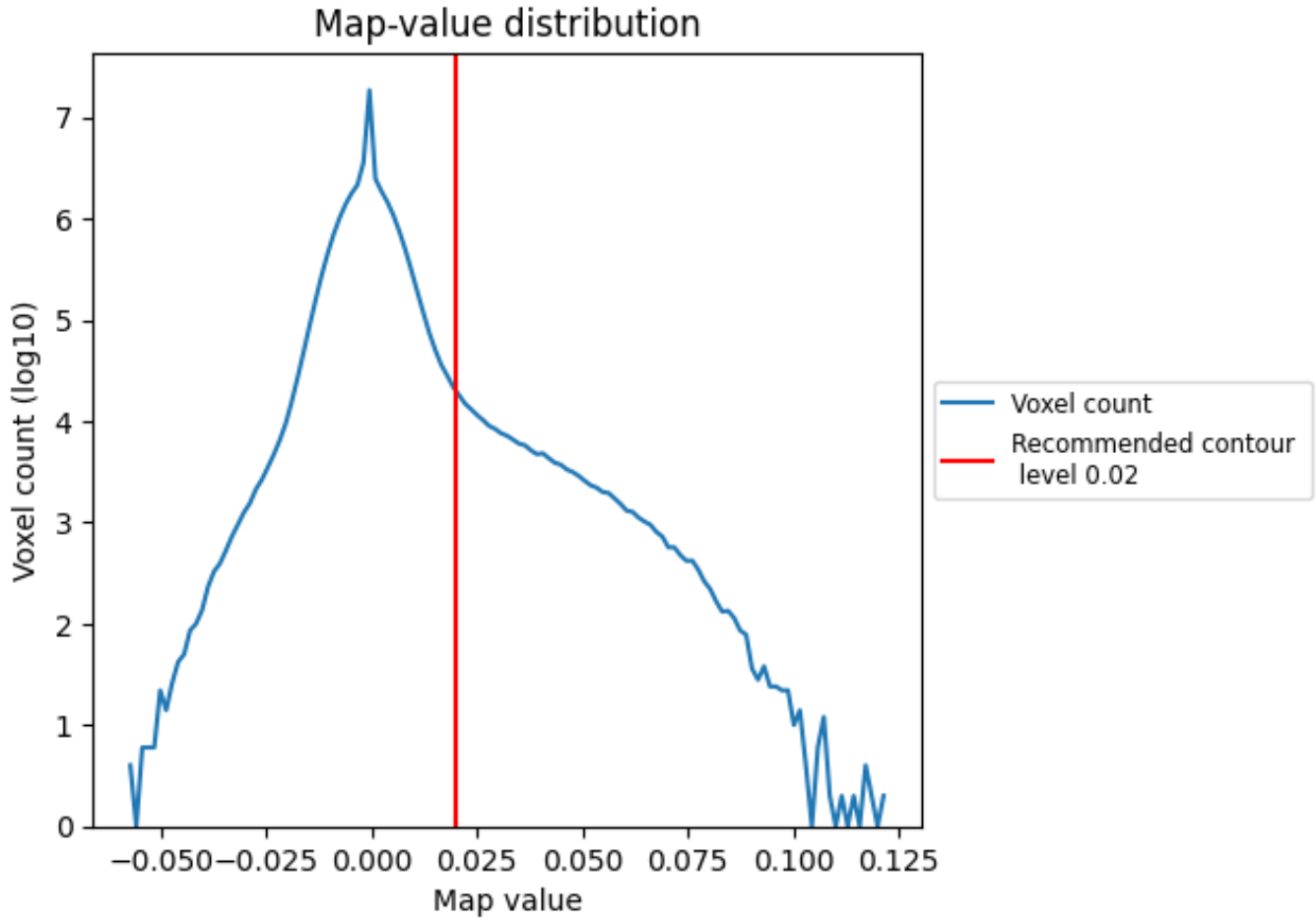
6.5 Mask visualisation (i)

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

7 Map analysis

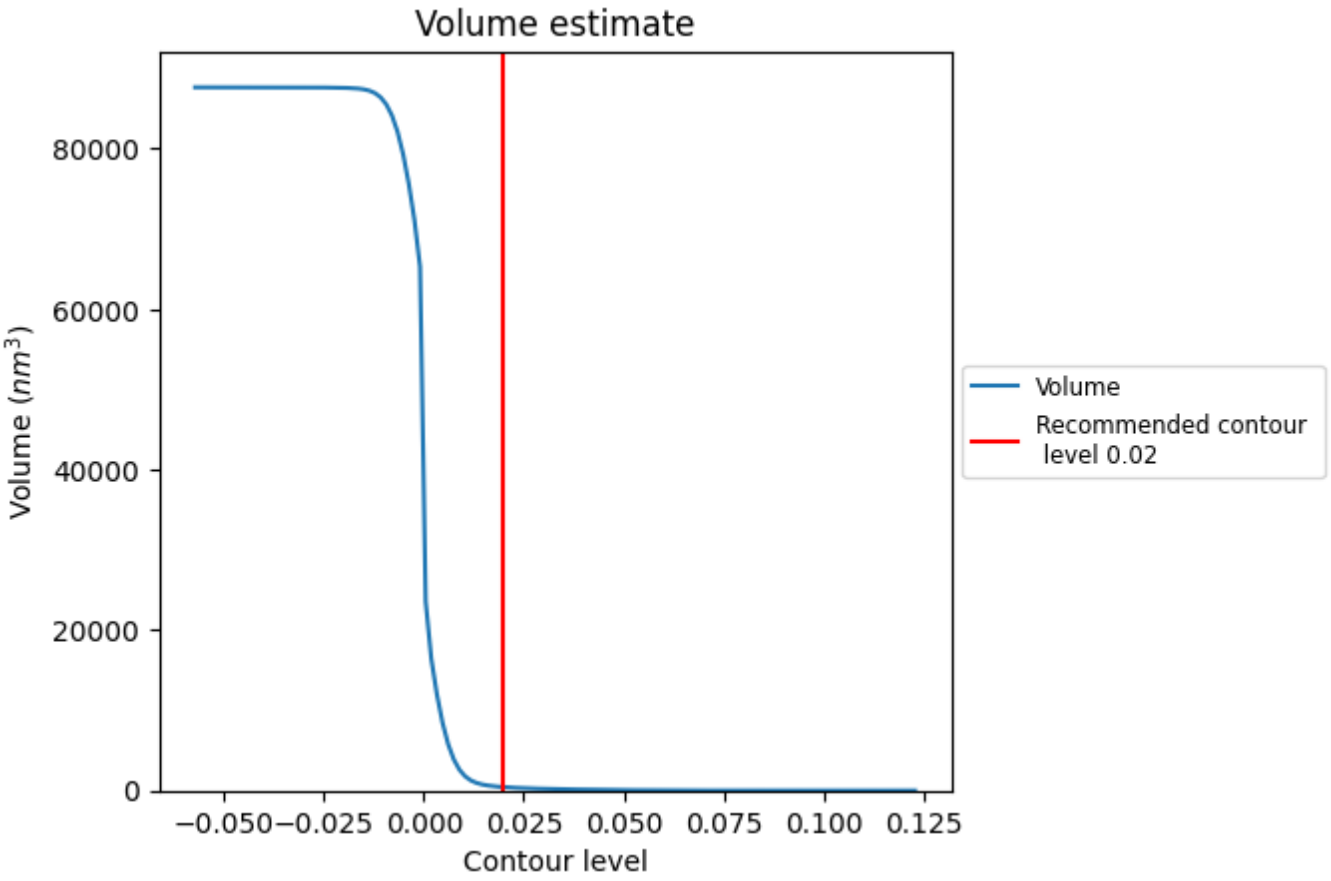
This section contains the results of statistical analysis of the map.

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.

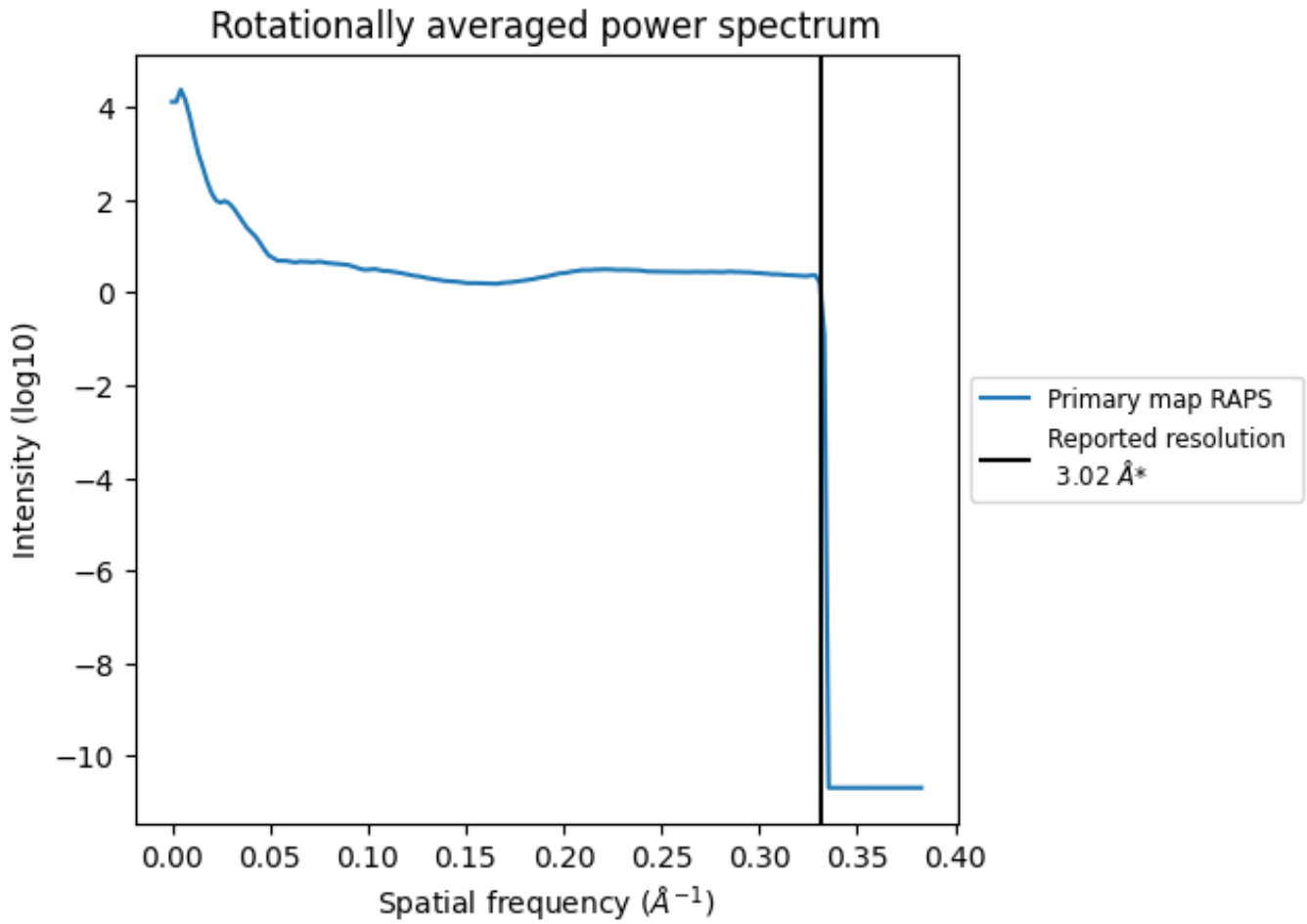
7.2 Volume estimate



The volume at the recommended contour level is 428 nm^3; this corresponds to an approximate mass of 387 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 0.331 Å^{-1}

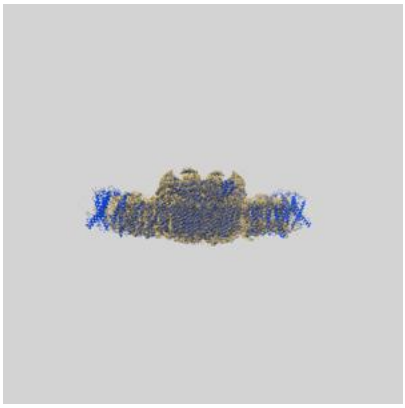
8 Fourier-Shell correlation

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

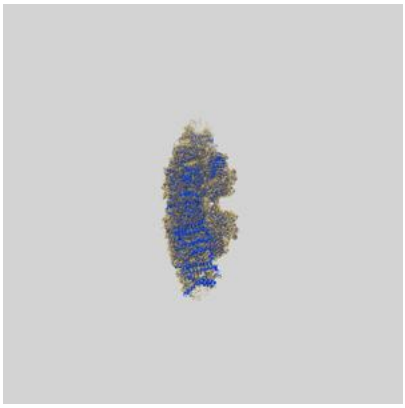
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9839 and PDB model 6JLU. Per-residue inclusion information can be found in section 3 on page 52.

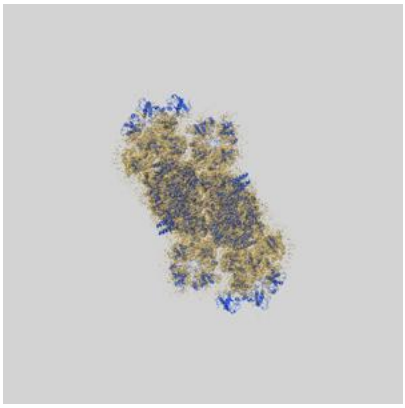
9.1 Map-model overlay



X



Y



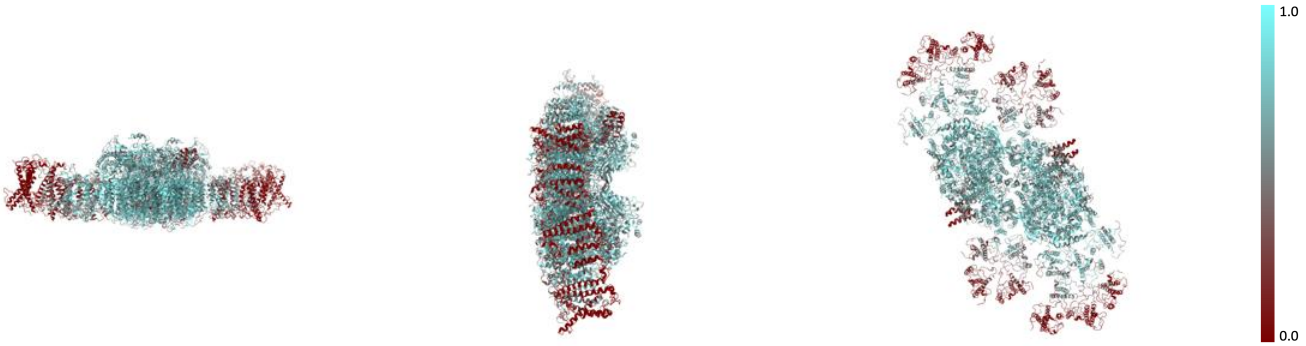
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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

This section was not generated.

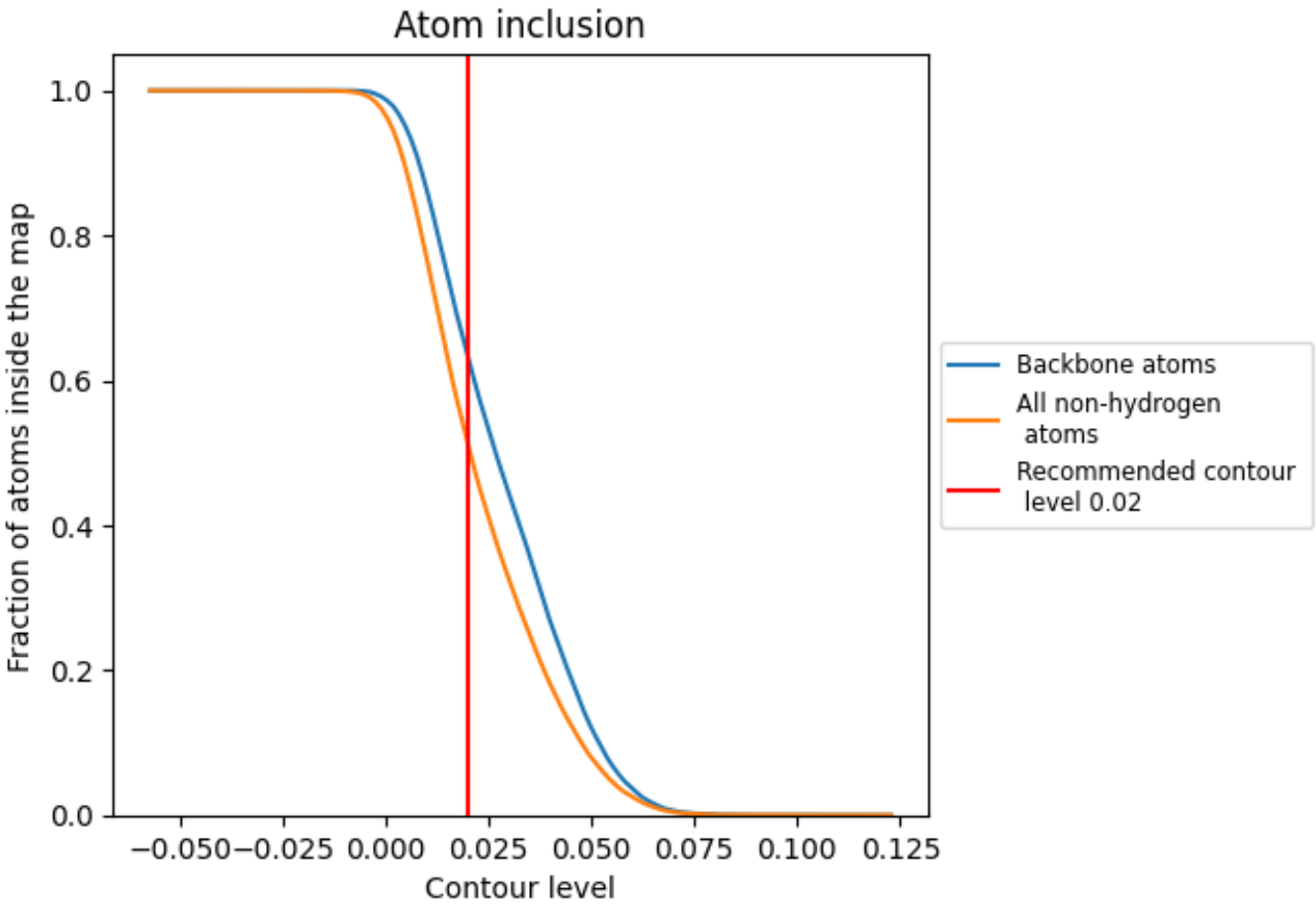
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 51% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5130
0	0.5861
1	0.3471
10	0.5903
11	0.3311
12	0.0900
13	0.0838
14	0.4275
15	0.4054
16	0.0473
17	0.0836
18	0.5776
19	0.0060
2	0.0906
3	0.0878
4	0.4241
5	0.3995
6	0.0355
7	0.0818
8	0.5894
9	0.0050
A	0.7632
B	0.7292
C	0.7558
D	0.7545
E	0.6502
F	0.5794
G	0.2400
H	0.7274
I	0.7473
J	0.5514
K	0.6550
L	0.6266
M	0.5942
N	0.7584

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
O	0.6794
P	0.6384
Q	0.6193
R	0.6275
T	0.6531
U	0.6902
V	0.7304
W	0.5476
X	0.4669
Y	0.5190
Z	0.6112
a	0.7698
b	0.7286
c	0.7564
d	0.7561
e	0.6532
f	0.5794
g	0.2389
h	0.7291
i	0.6741
j	0.5822
k	0.6550
l	0.6366
m	0.5942
n	0.7809
o	0.6821
p	0.6376
q	0.6229
r	0.6299
t	0.6612
u	0.6945
v	0.7352
w	0.5290
x	0.4835
y	0.5225
z	0.6343