Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 01:21 AM JST

PDB ID	:	6JLU / pdb_00006jlu
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:

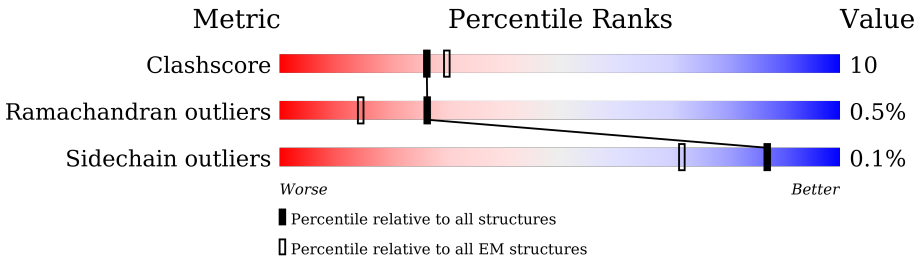
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

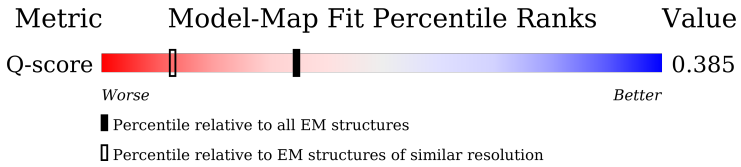
1 Overall quality at a glance

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

The reported resolution of this entry is 3.02 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	70% 23% 7%
1	a	359	71% 22% 7%
2	B	509	5% 76% 23%
2	b	509	5% 77% 21%

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Mol	Chain	Length	Quality of chain
3	C	450	77% 23%
3	c	450	76% 24%
4	D	341	74% 26%
4	d	341	74% 26%
5	E	79	13% 78% 22%
5	e	79	11% 81% 19%
6	F	32	22% 97%
6	f	32	16% 84% 16%
7	G	179	56% 54% 15% 32%
7	g	179	58% 55% 13% 32%
8	H	65	6% 83% 17%
8	h	65	6% 85% 15%
9	I	34	79% 21%
9	i	34	88% 12%
10	J	34	24% 74% 24%
10	j	34	15% 82% 15%
11	K	37	5% 57% 41%
11	k	37	54% 43%
12	L	38	63% 34%
12	l	38	63% 34%
13	M	41	7% 80% 20%
13	m	41	12% 73% 27%
14	N	30	7% 93% 7%
14	n	30	7% 93% 7%
15	O	249	6% 75% 25%

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Mol	Chain	Length	Quality of chain
15	o	249	6% 74% 26%
16	P	226	12% 88% 12%
16	p	226	12% 87% 13%
17	Q	211	10% 58% 11% 30%
17	q	211	11% 60% 10% 30%
18	R	73	29% 99%
18	r	73	29% 99%
19	T	31	10% 84% 13%
19	t	31	6% 81% 16%
20	U	93	5% 77% 23%
20	u	93	5% 77% 23%
21	V	137	77% 23%
21	v	137	77% 23%
22	W	51	27% 86% 12%
22	w	51	25% 86% 12%
23	X	35	40% 89% 11%
23	x	35	37% 89% 11%
24	Y	33	27% 64% 36%
24	y	33	21% 64% 36%
25	Z	61	87% 13%
25	z	61	85% 15%
26	0	178	19% 75% 22%
26	10	178	17% 80% 19%
27	1	172	62% 72% 25%
27	11	172	66% 70% 28%

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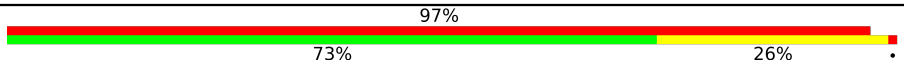
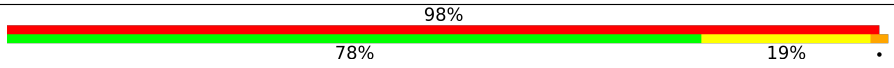
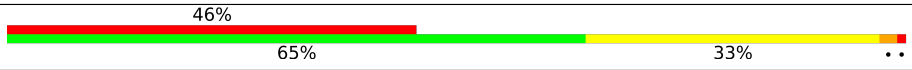
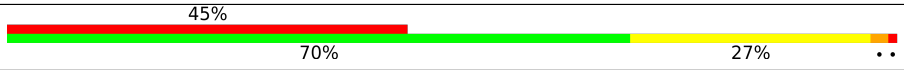
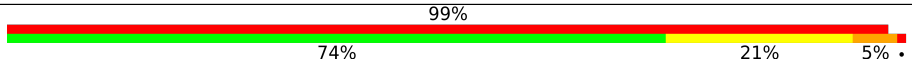
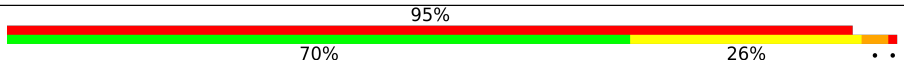
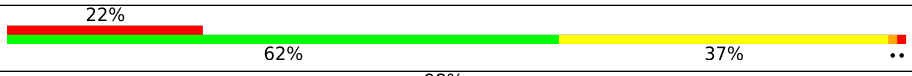
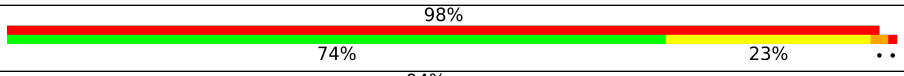
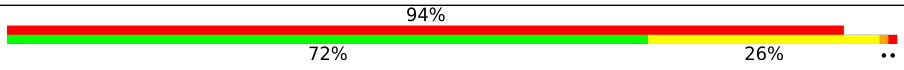
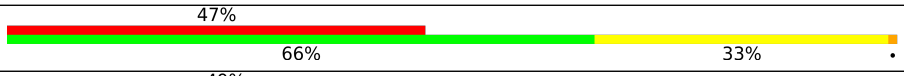
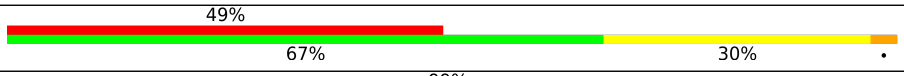
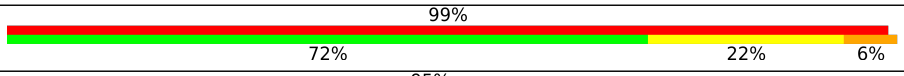
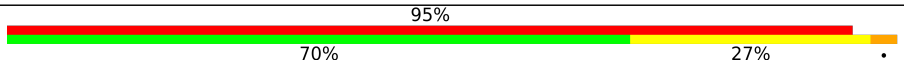
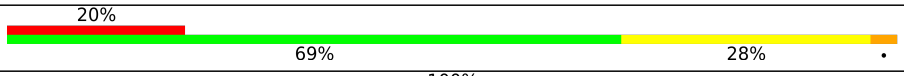
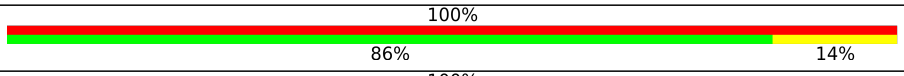
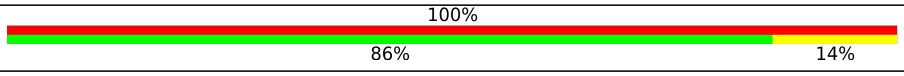
Mol	Chain	Length	Quality of chain
27	12	172	
27	13	172	
27	14	172	
27	15	172	
27	16	172	
27	17	172	
27	18	172	
27	2	172	
27	3	172	
27	4	172	
27	5	172	
27	6	172	
27	7	172	
27	8	172	
28	19	166	
28	9	166	

2 Entry composition (i)

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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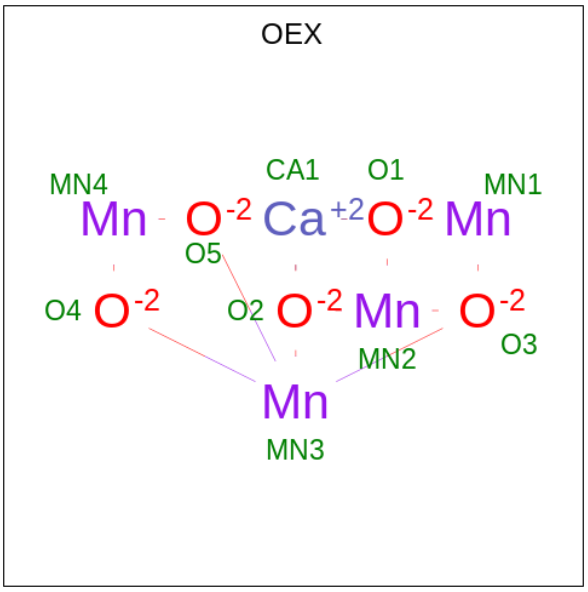
Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	3	172	Total	C	N	O	S	0	0
			1340	874	218	243	5		
27	4	172	Total	C	N	O	S	0	0
			1313	855	212	241	5		
27	5	172	Total	C	N	O	S	0	0
			1280	826	207	242	5		
27	6	172	Total	C	N	O	S	0	0
			1335	871	216	243	5		
27	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 (CCD ID: OEX) (formula: $CaMn_4O_5$).

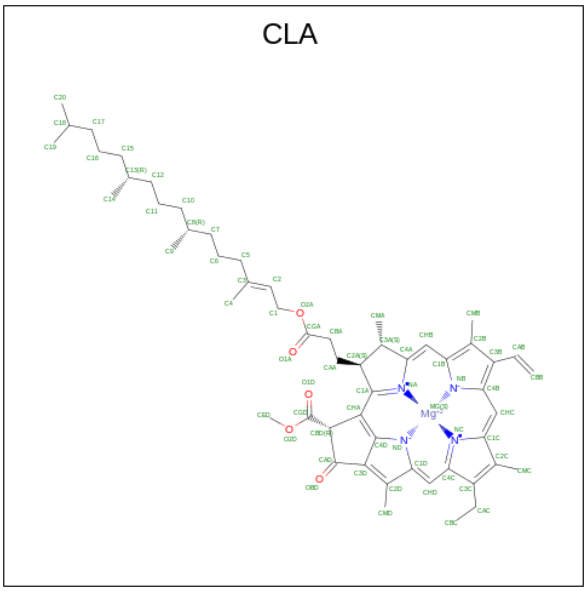


Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

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

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

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



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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
			65	55	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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	z	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	10	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	10	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	10	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	11	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	12	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	12	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	12	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	13	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	13	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
31	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	14	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	14	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	15	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	15	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	15	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	15	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	16	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	16	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	16	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	16	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	16	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	17	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	17	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	17	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	17	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	17	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	18	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	18	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	18	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	18	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	18	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	18	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	19	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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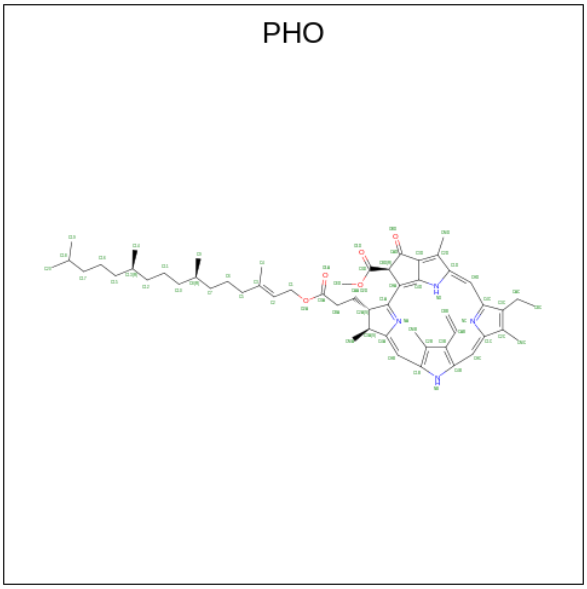
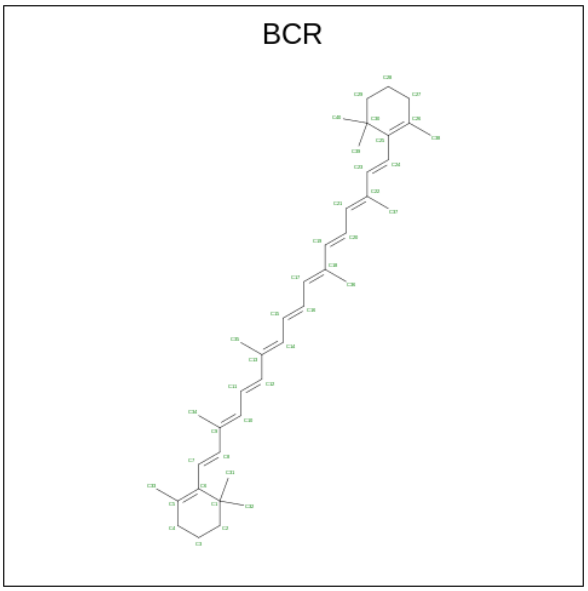
Mol	Chain	Residues	Atoms					AltConf
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	19	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 32 is PHEOPHYTIN A (CCD ID: 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 (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	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 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0

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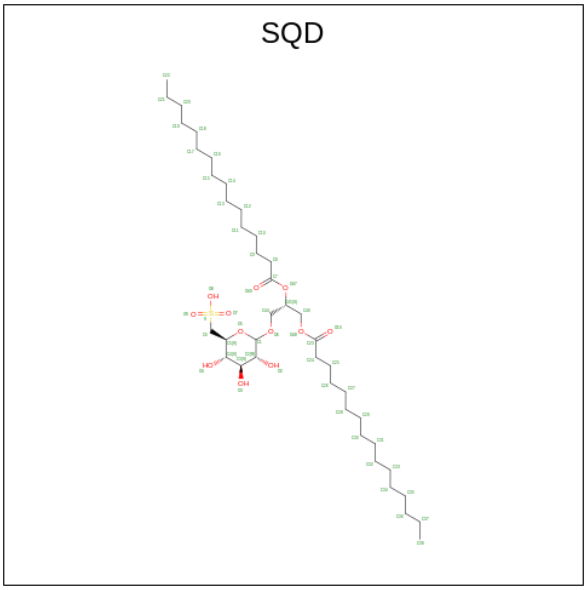
Mol	Chain	Residues	Atoms	AltConf
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	f	1	Total C 40 40	0
33	h	1	Total C 40 40	0
33	y	1	Total C 40 40	0

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C O S 54 41 12 1	0
34	A	1	Total C O S 40 27 12 1	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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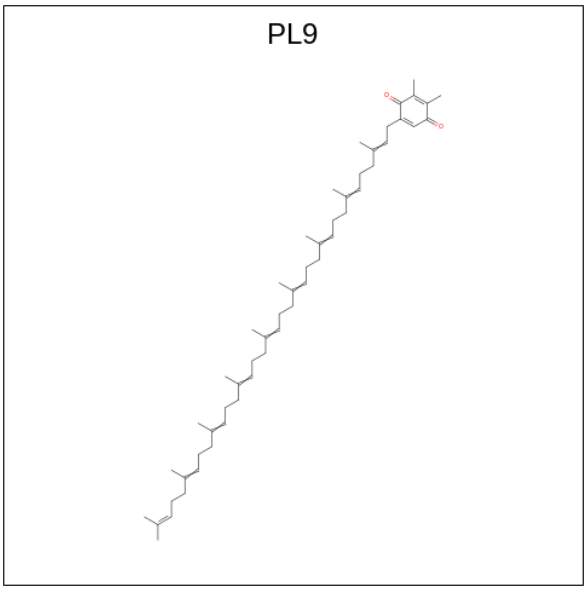
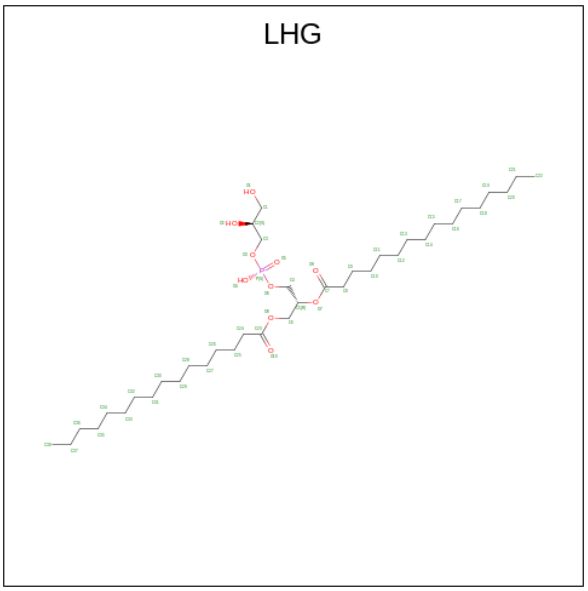
Mol	Chain	Residues	Atoms				AltConf
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	i	1	Total	C	O	S	0
			40	27	12	1	
34	l	1	Total	C	O	S	0
			54	41	12	1	
34	8	1	Total	C	O	S	0
			41	28	12	1	
34	10	1	Total	C	O	S	0
			41	28	12	1	

- 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 (CCD ID: 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 (CCD ID: 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	
36	z	1	Total	C	O	P	0
			25	14	10	1	

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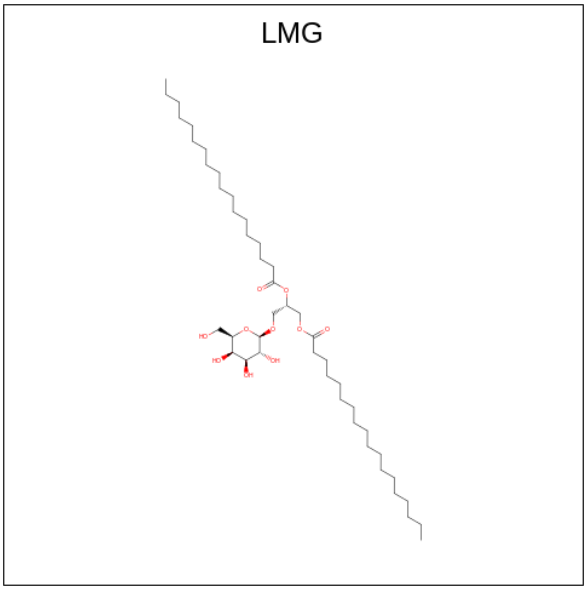
Mol	Chain	Residues	Atoms				AltConf
36	4	1	Total 35	C 24	O 10	P 1	0
36	5	1	Total 25	C 14	O 10	P 1	0
36	8	1	Total 39	C 28	O 10	P 1	0
36	8	1	Total 31	C 20	O 10	P 1	0
36	14	1	Total 35	C 24	O 10	P 1	0
36	15	1	Total 25	C 14	O 10	P 1	0
36	18	1	Total 39	C 28	O 10	P 1	0
36	18	1	Total 31	C 20	O 10	P 1	0

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total 51	C 41	O 10	0
37	C	1	Total 51	C 41	O 10	0
37	D	1	Total 40	C 30	O 10	0

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Mol	Chain	Residues	Atoms	AltConf
37	D	1	Total C O 37 27 10	0
37	F	1	Total C O 46 36 10	0
37	J	1	Total C O 50 40 10	0
37	K	1	Total C O 46 36 10	0
37	M	1	Total C O 40 30 10	0
37	N	1	Total C O 28 18 10	0
37	P	1	Total C O 31 21 10	0
37	W	1	Total C O 48 38 10	0
37	Z	1	Total C O 31 21 10	0
37	b	1	Total C O 51 41 10	0
37	c	1	Total C O 51 41 10	0
37	c	1	Total C O 31 21 10	0
37	d	1	Total C O 40 30 10	0
37	d	1	Total C O 37 27 10	0
37	f	1	Total C O 46 36 10	0
37	j	1	Total C O 50 40 10	0
37	k	1	Total C O 46 36 10	0
37	m	1	Total C O 40 30 10	0
37	n	1	Total C O 28 18 10	0
37	p	1	Total C O 31 21 10	0
37	w	1	Total C O 48 38 10	0

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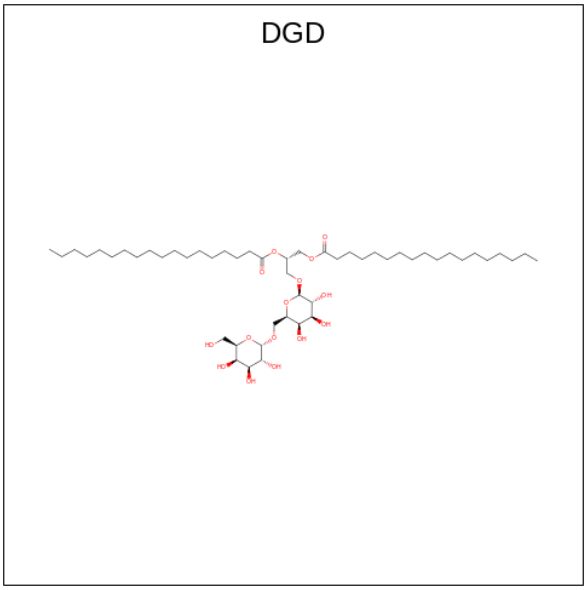
Mol	Chain	Residues	Atoms			AltConf
37	0	1	Total 31	C 21	O 10	0
37	1	1	Total 36	C 26	O 10	0
37	1	1	Total 45	C 35	O 10	0
37	4	1	Total 49	C 39	O 10	0
37	5	1	Total 37	C 27	O 10	0
37	5	1	Total 36	C 26	O 10	0
37	10	1	Total 31	C 21	O 10	0
37	11	1	Total 36	C 26	O 10	0
37	11	1	Total 45	C 35	O 10	0
37	14	1	Total 49	C 39	O 10	0
37	15	1	Total 37	C 27	O 10	0
37	15	1	Total 36	C 26	O 10	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

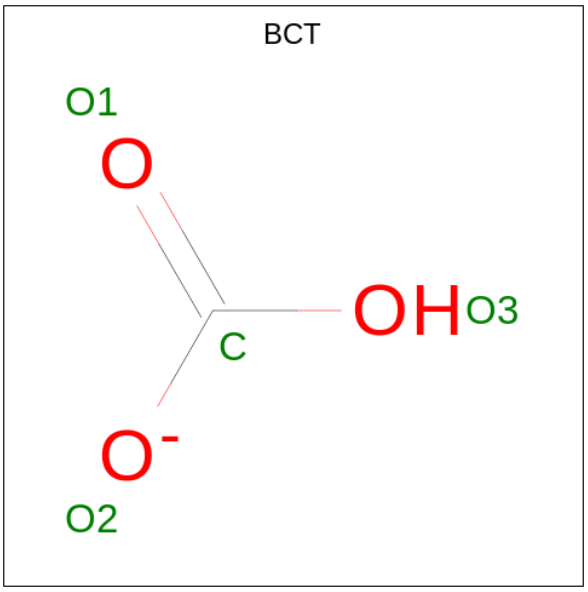


Mol	Chain	Residues	Atoms	AltConf
38	B	1	Total C O 54 39 15	0
38	C	1	Total C O 55 40 15	0
38	C	1	Total C O 62 47 15	0
38	C	1	Total C O 62 47 15	0
38	H	1	Total C O 62 47 15	0
38	W	1	Total C O 56 41 15	0
38	b	1	Total C O 55 40 15	0
38	c	1	Total C O 55 40 15	0
38	c	1	Total C O 62 47 15	0
38	c	1	Total C O 62 47 15	0
38	h	1	Total C O 62 47 15	0
38	w	1	Total C O 56 41 15	0
38	1	1	Total C O 54 39 15	0
38	11	1	Total C O 60 45 15	0

- Molecule 39 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

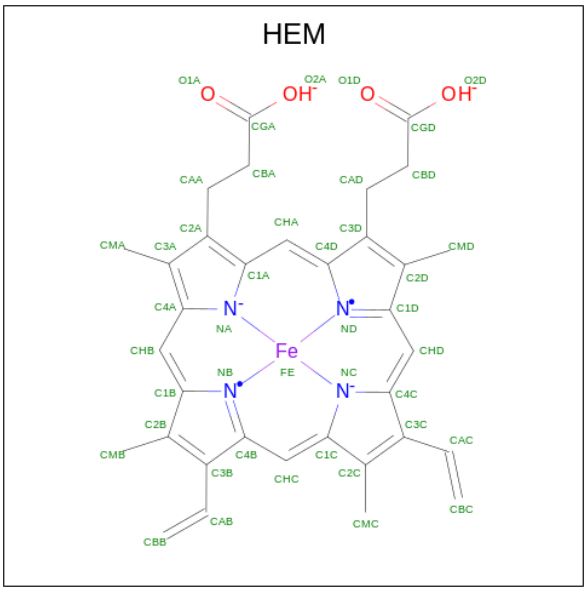
Mol	Chain	Residues	Atoms	AltConf
39	C	1	Total Cl 1 1	0
39	c	1	Total Cl 1 1	0

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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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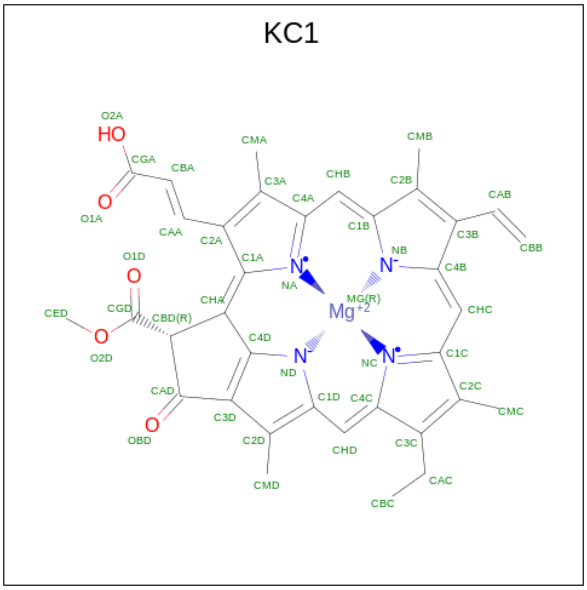
Mol	Chain	Residues	Atoms					AltConf
41	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is Chlorophyll c1 (CCD ID: 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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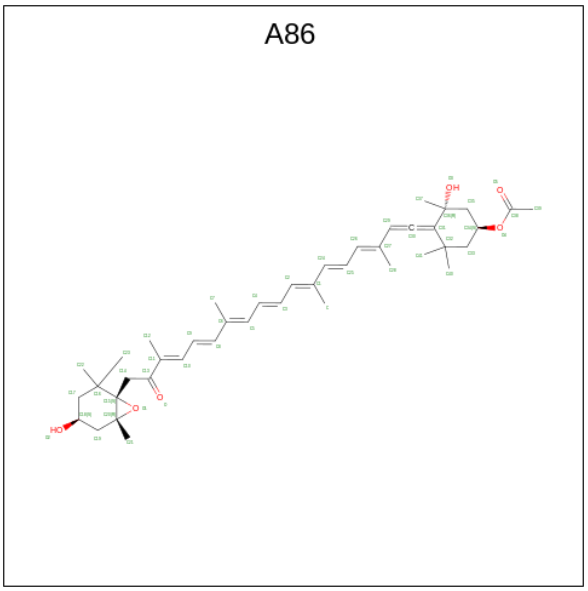
Mol	Chain	Residues	Atoms					AltConf
42	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	12	1	Total	C	Mg	N	O	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	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
42	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
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 (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms	AltConf
43	P	1	Total C O 48 42 6	0
43	P	1	Total C O 48 42 6	0
43	p	1	Total C O 48 42 6	0
43	p	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	0	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
43	1	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0
43	1	1	Total C O 48 42 6	0
43	2	1	Total C O 48 42 6	0
43	2	1	Total C O 48 42 6	0
43	2	1	Total C O 48 42 6	0
43	2	1	Total C O 48 42 6	0
43	2	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	3	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	4	1	Total C O 48 42 6	0
43	5	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	5	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	6	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	7	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	
43	8	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms	AltConf
43	8	1	Total C O 48 42 6	0
43	8	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	9	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	10	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0
43	11	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms			AltConf
43	11	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	12	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	13	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	14	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
43	15	1	Total	C	O	0
			48	42	6	
43	15	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	16	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	17	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	18	1	Total	C	O	0
			48	42	6	
43	19	1	Total	C	O	0
			48	42	6	

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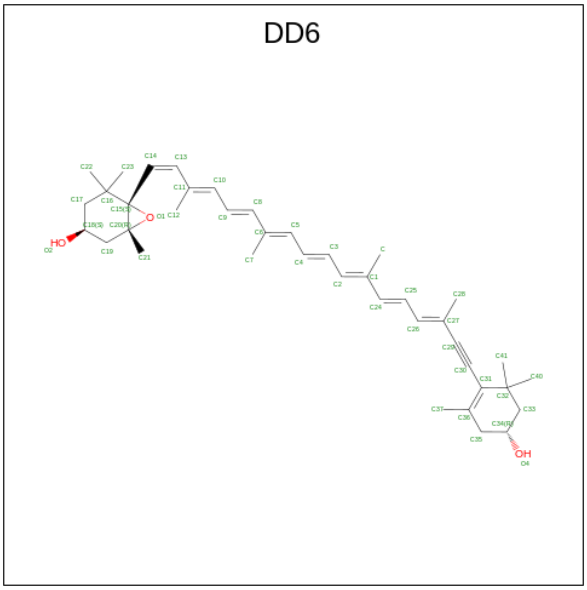
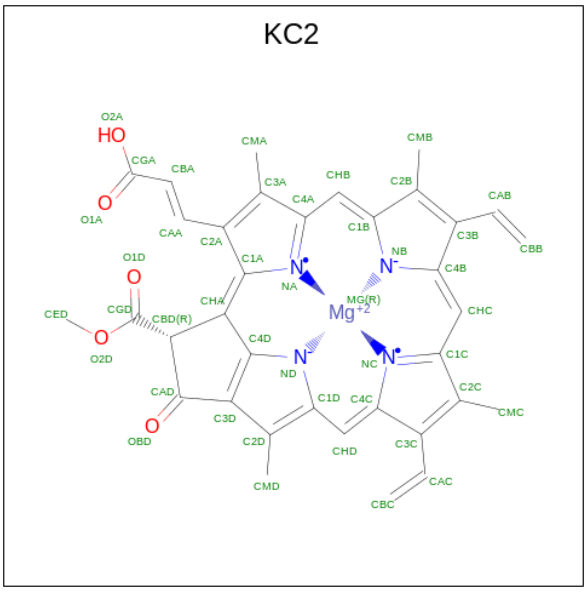
Mol	Chain	Residues	Atoms	AltConf
43	19	1	Total C O 48 42 6	0
43	19	1	Total C O 48 42 6	0
43	19	1	Total C O 48 42 6	0
43	19	1	Total C O 48 42 6	0
43	19	1	Total C O 48 42 6	0

- Molecule 44 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



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

- Molecule 45 is Chlorophyll c2 (CCD ID: 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
			45	35	1	4	5	
45	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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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	

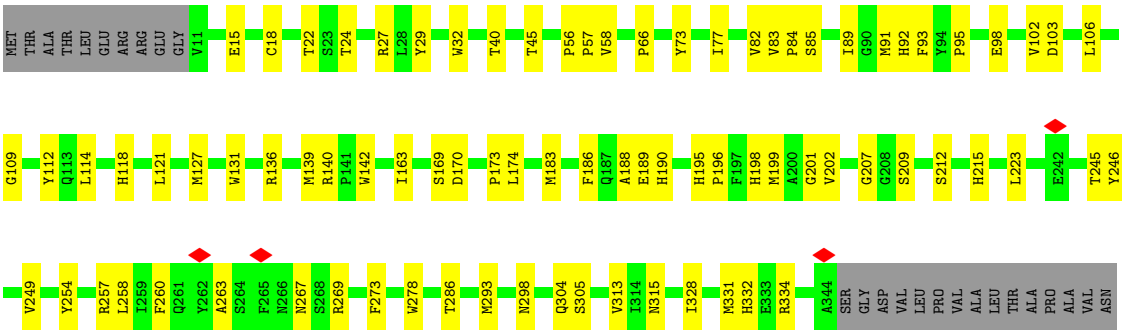
3 Residue-property plots (i)

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:

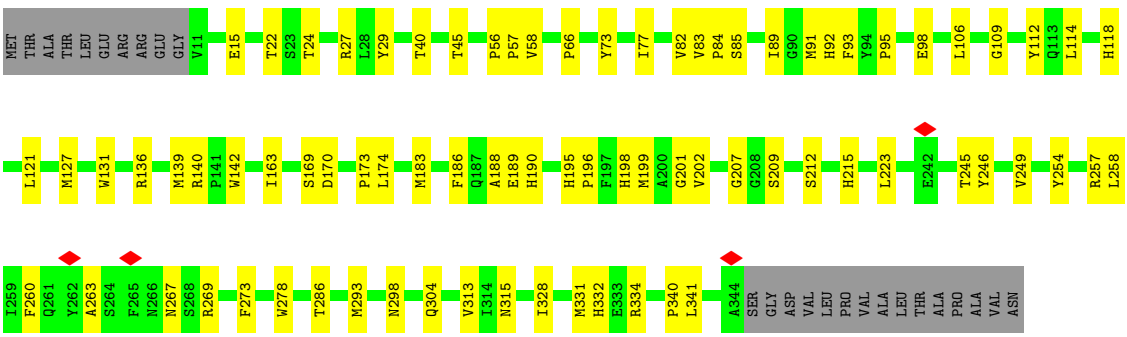




• Molecule 1: PsbA

Chain a:

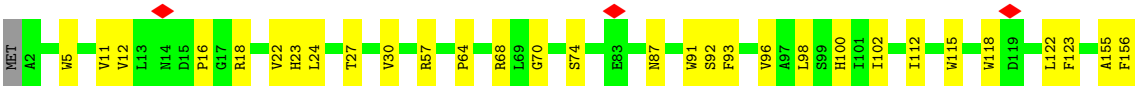


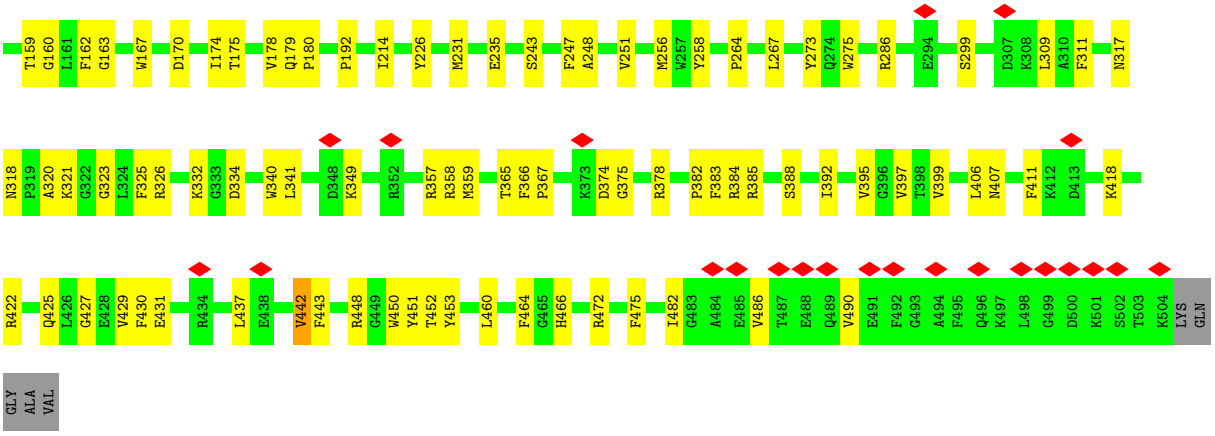


• Molecule 2: PsbB

Chain B:



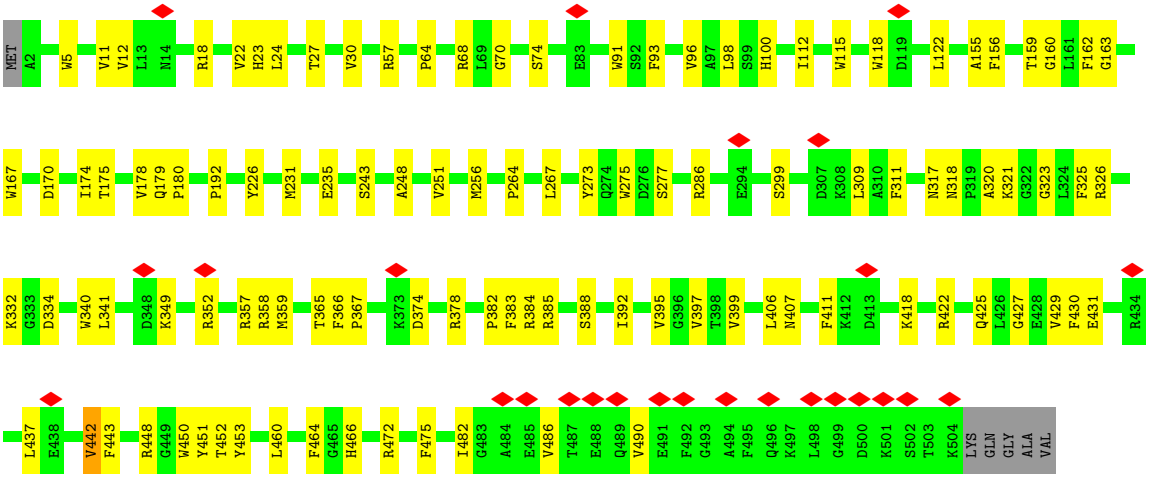




• Molecule 2: PsbB

Chain b:

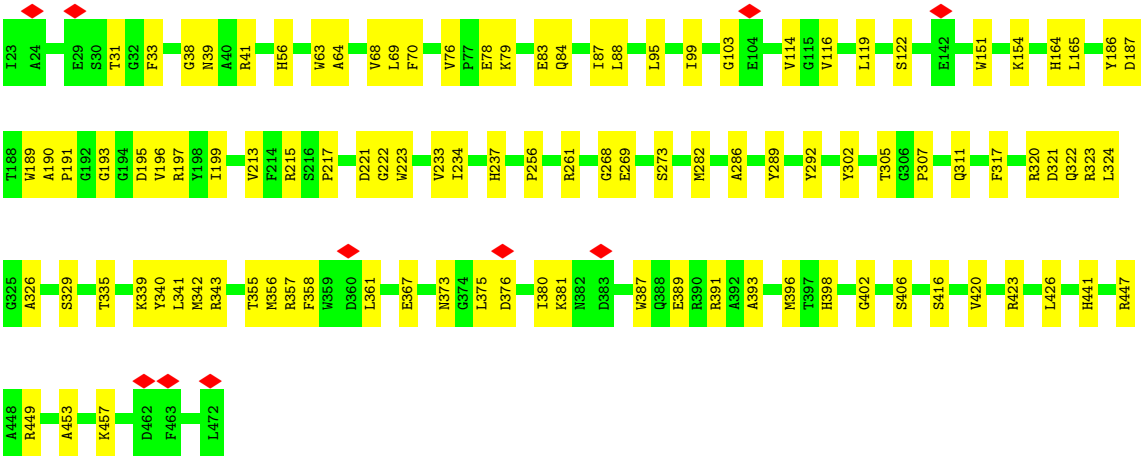




• Molecule 3: PsbC

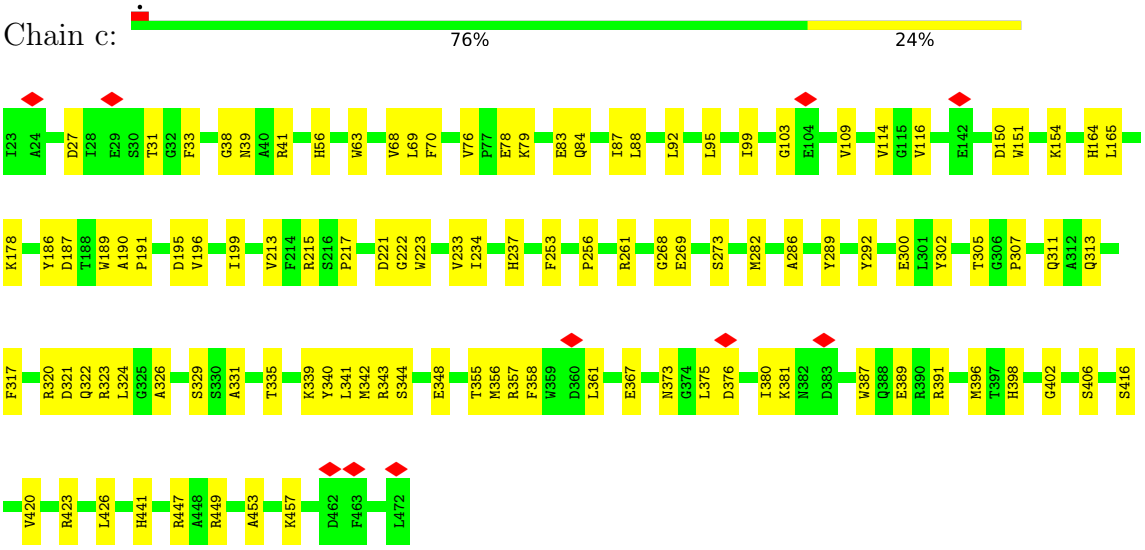
Chain C:





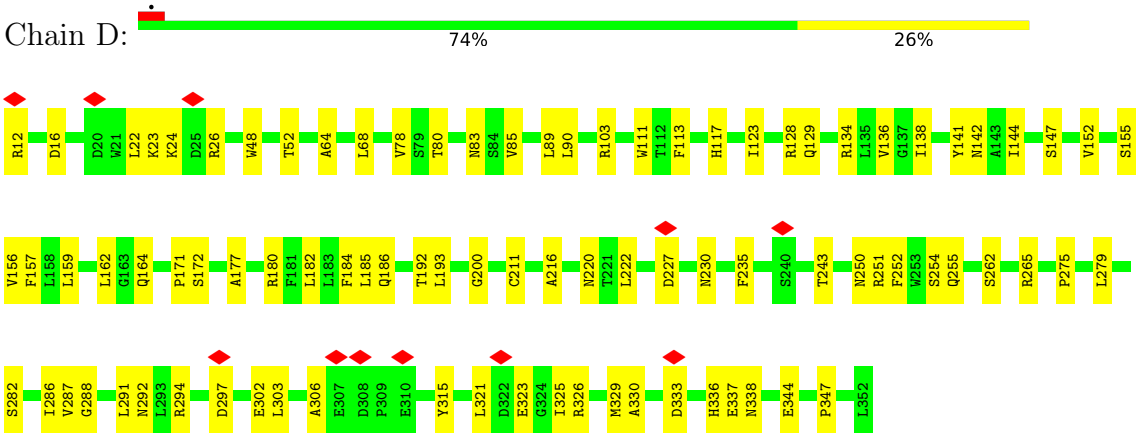
• Molecule 3: PsbC

Chain c:



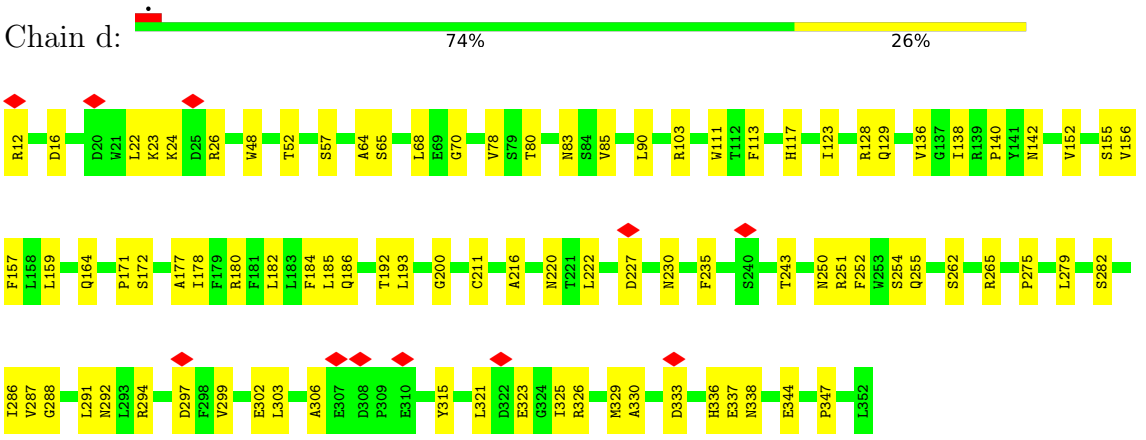
• Molecule 4: PsbD

Chain D:



• Molecule 4: PsbD

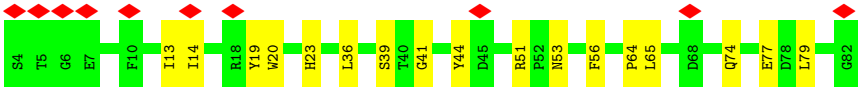
Chain d:



• Molecule 5: PsbE

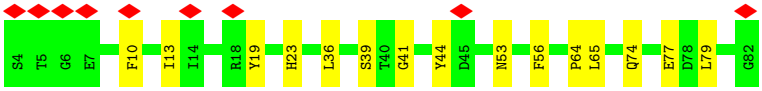
Chain E:



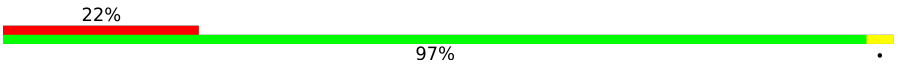


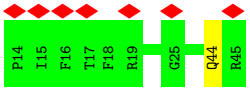
• Molecule 5: PsbE





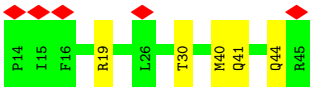
• Molecule 6: PsbF





• Molecule 6: PsbF

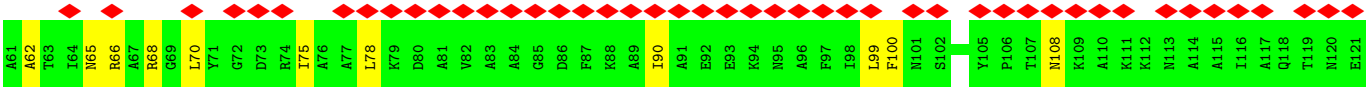


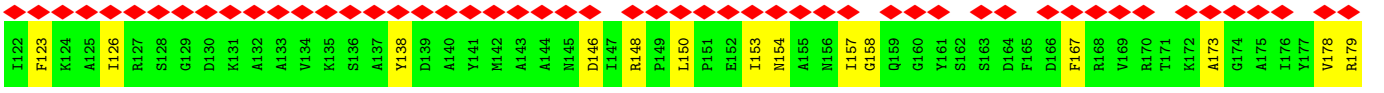


• Molecule 7: Psb31





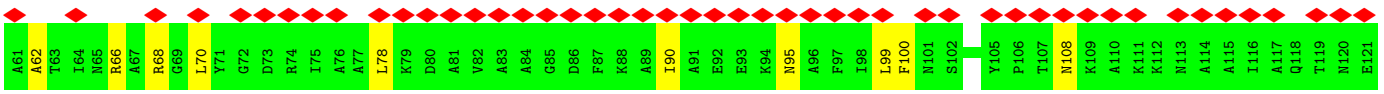


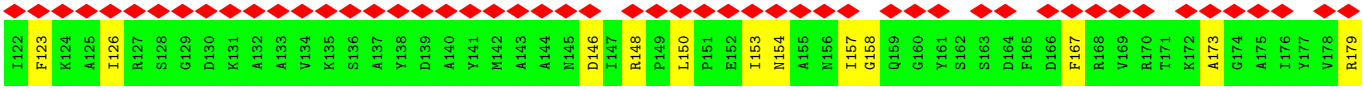


• Molecule 7: Psb31

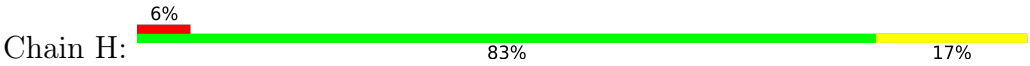


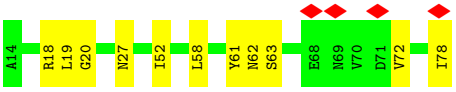




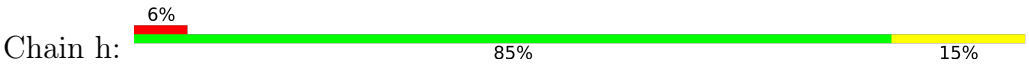


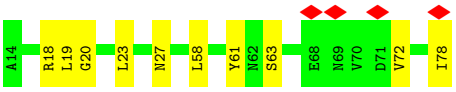
• Molecule 8: Photosystem II reaction center protein H



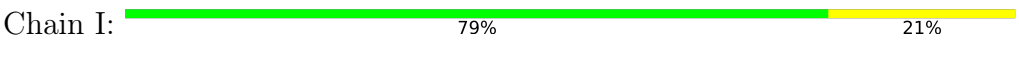


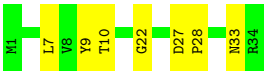
• Molecule 8: Photosystem II reaction center protein H



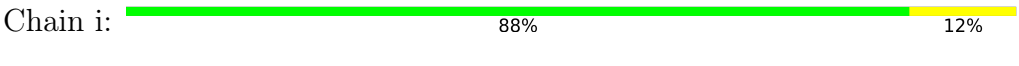


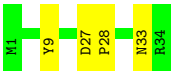
• Molecule 9: PsbI





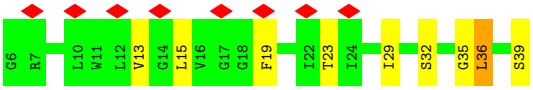
• Molecule 9: PsbI



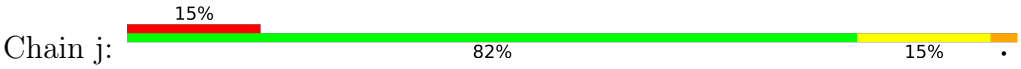


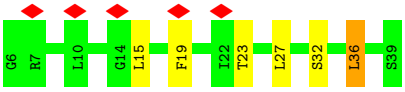
• Molecule 10: PsbJ





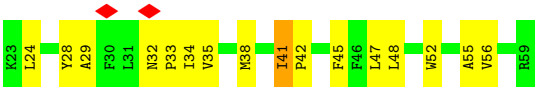
• Molecule 10: PsbJ





• Molecule 11: PsbK

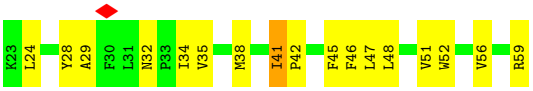




• Molecule 11: PsbK

Chain k:

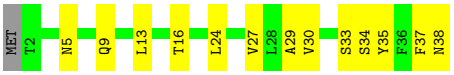




• Molecule 12: PsbL

Chain L:

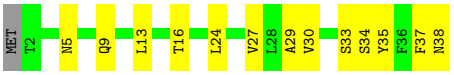




• Molecule 12: PsbL

Chain l:

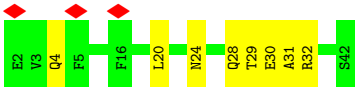




• Molecule 13: PsbM

Chain M:

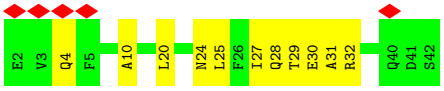




• Molecule 13: PsbM

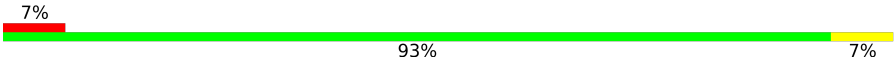
Chain m:

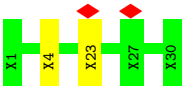




• Molecule 14: Psb34

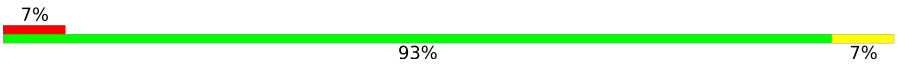
Chain N:

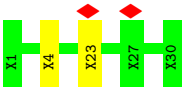




• Molecule 14: Psb34

Chain n:

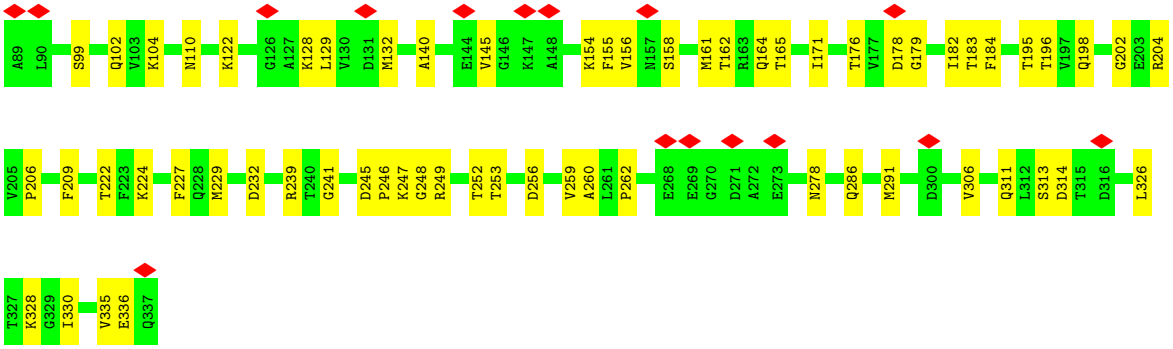




• Molecule 15: Extrinsic protein in photosystem II

Chain O:

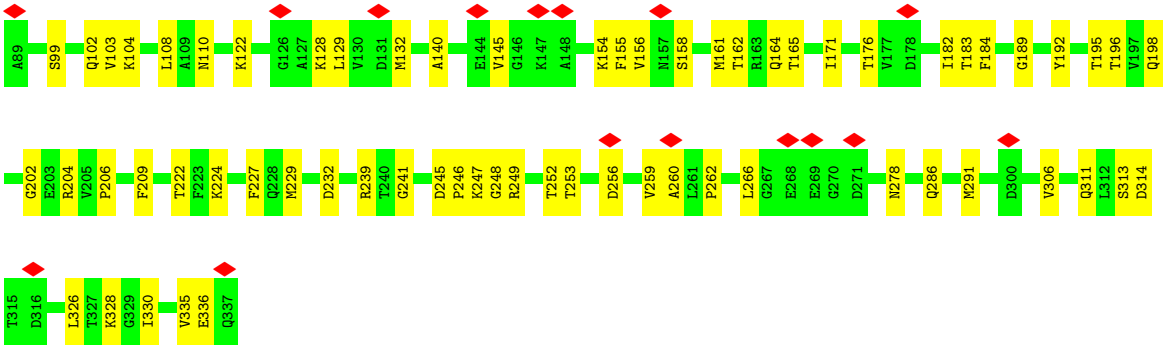




• Molecule 15: Extrinsic protein in photosystem II

Chain o:

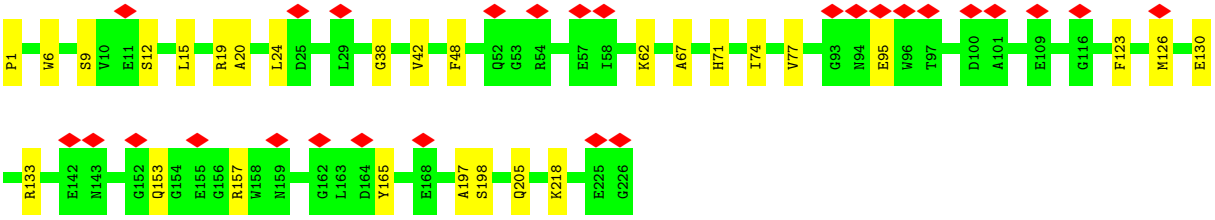




• Molecule 16: FCP-D

Chain P:

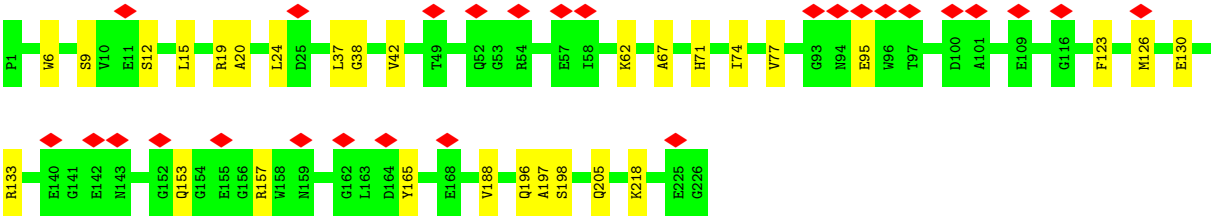




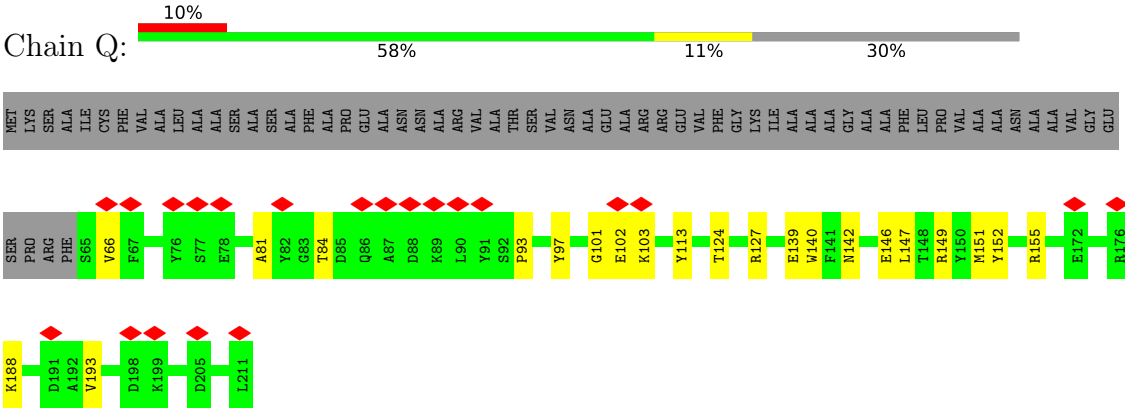
• Molecule 16: FCP-D

Chain p:

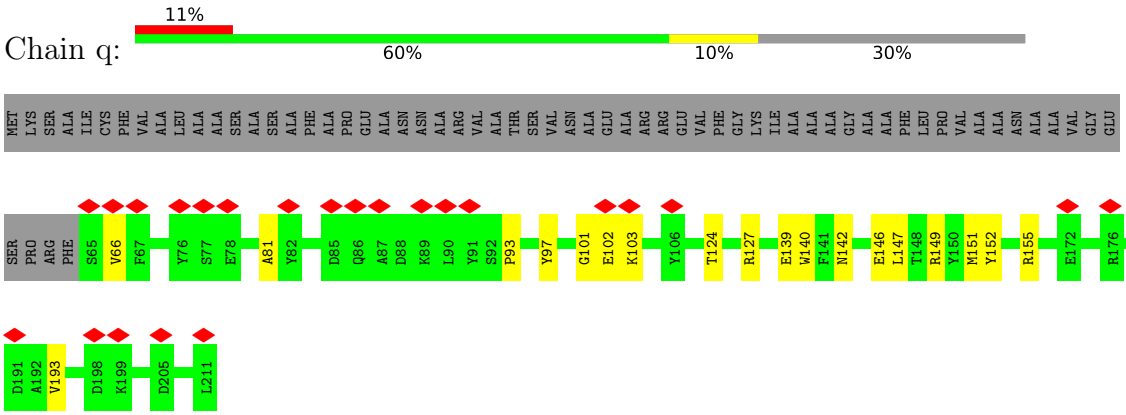




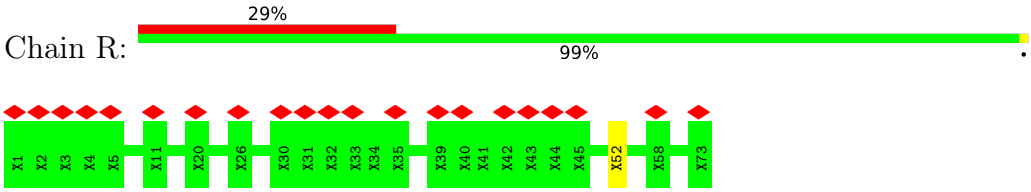
• Molecule 17: Extrinsic protein in photosystem II



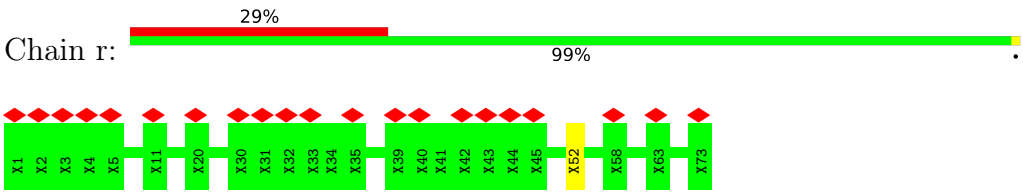
• Molecule 17: Extrinsic protein in photosystem II



• Molecule 18: PsbG

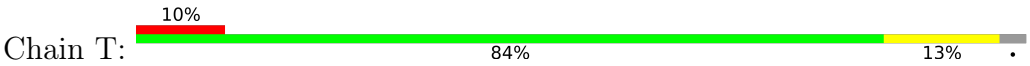


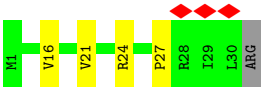
• Molecule 18: PsbG



• Molecule 19: PsbT

Chain T:





• Molecule 19: PsbT

Chain t:

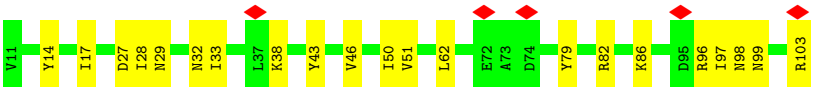




• Molecule 20: Extrinsic protein in photosystem II

Chain U:

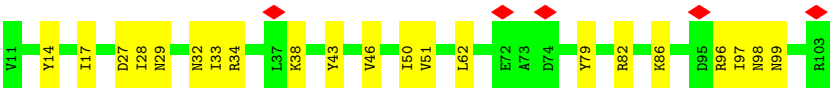




• Molecule 20: Extrinsic protein in photosystem II

Chain u:

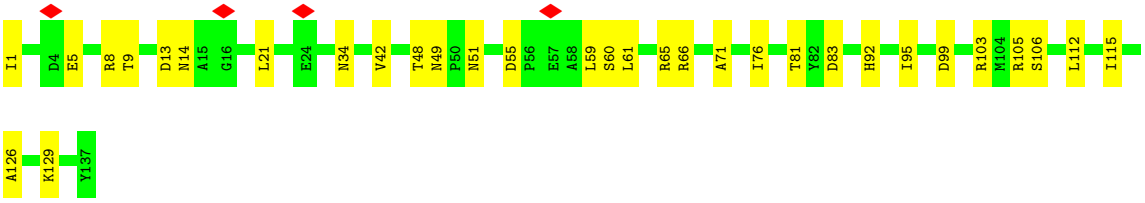




• Molecule 21: Cytochrome c-550

Chain V:

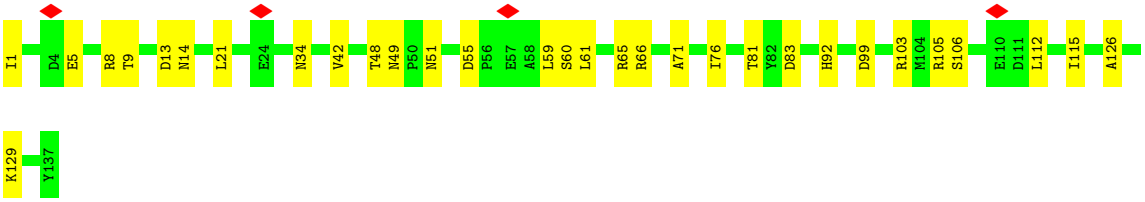




• Molecule 21: Cytochrome c-550

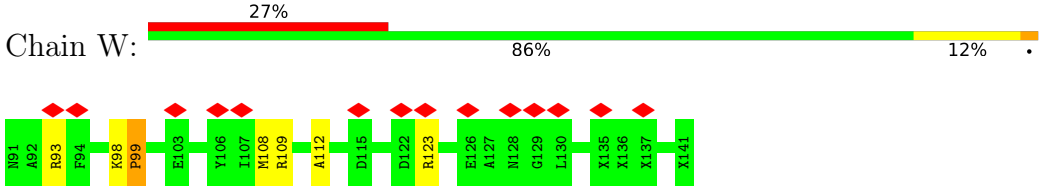
Chain v:





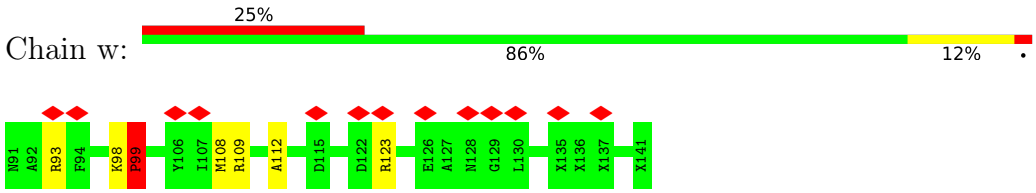
• Molecule 22: PsbW

Chain W:



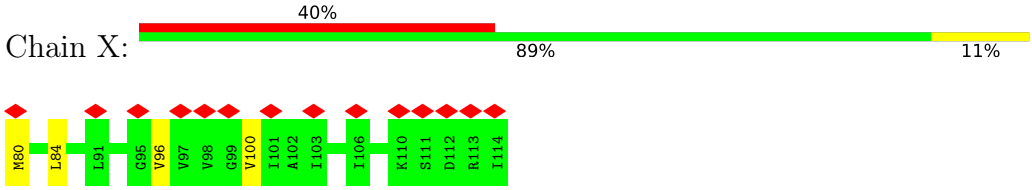
• Molecule 22: PsbW

Chain w:



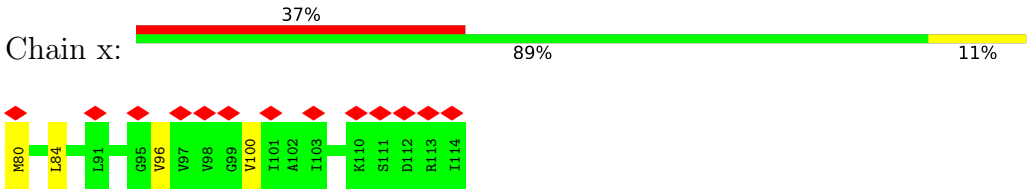
• Molecule 23: Photosystem II reaction center X protein

Chain X:



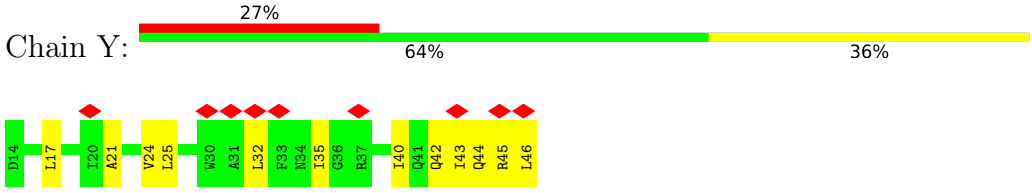
• Molecule 23: Photosystem II reaction center X protein

Chain x:



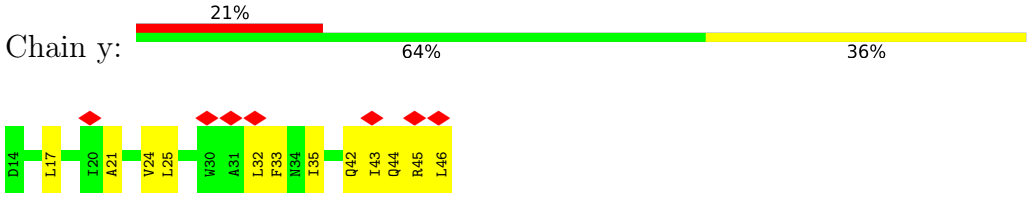
• Molecule 24: PsbY

Chain Y:



• Molecule 24: PsbY

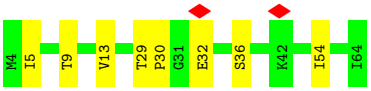
Chain y:



• Molecule 25: PsbZ

Chain Z:

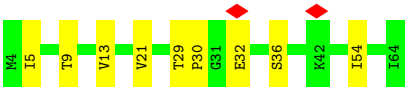




• Molecule 25: PsbZ

Chain z:

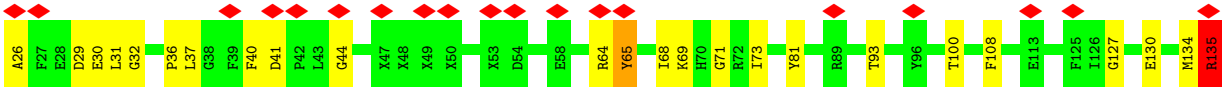


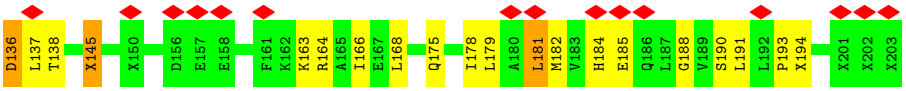


• Molecule 26: FCP-E

Chain 0:



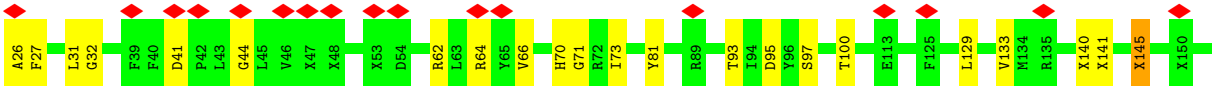


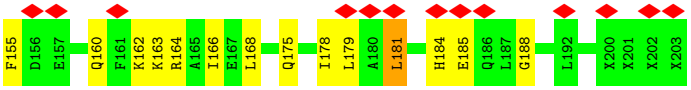


• Molecule 26: FCP-E

Chain 10:



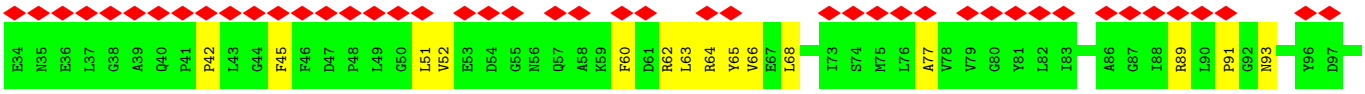




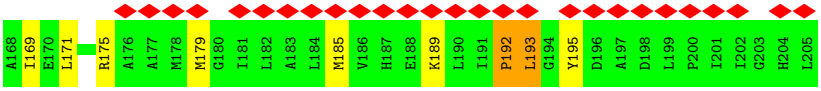
• Molecule 27: FCP-A

Chain 1:



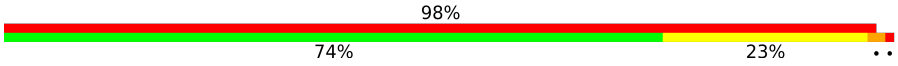


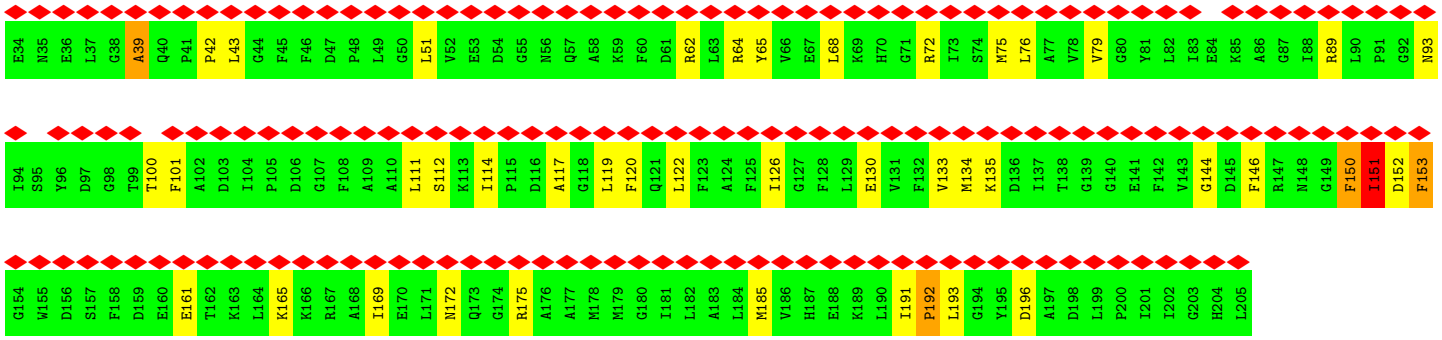




• Molecule 27: FCP-A

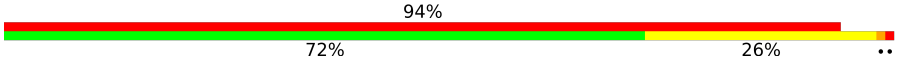
Chain 2:

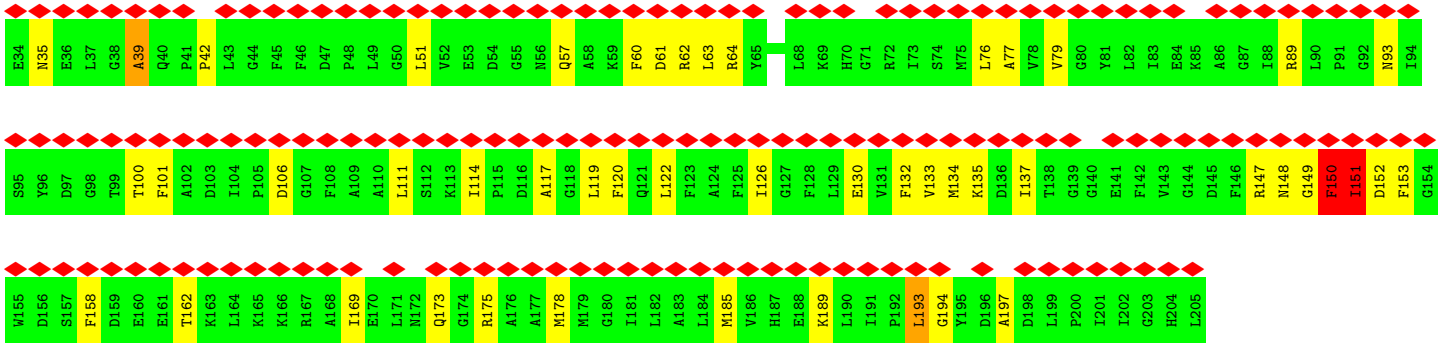




• Molecule 27: FCP-A

Chain 3:





• Molecule 27: FCP-A

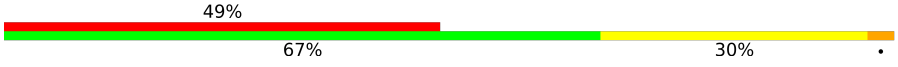
Chain 4:

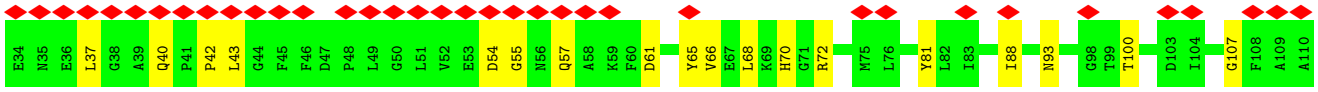


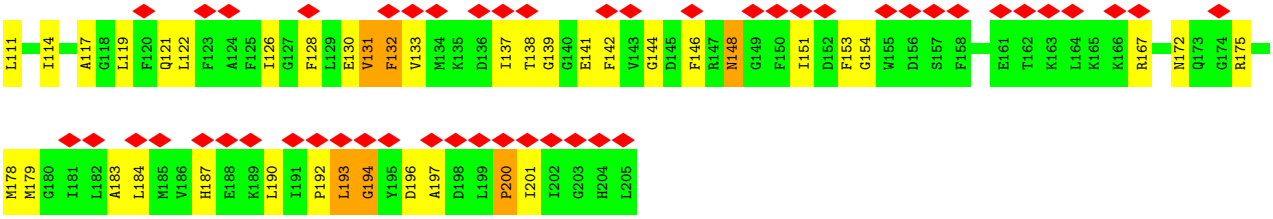


• Molecule 27: FCP-A

Chain 5:

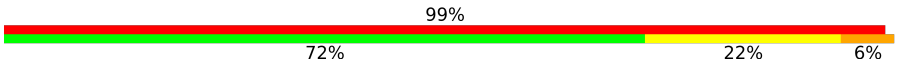


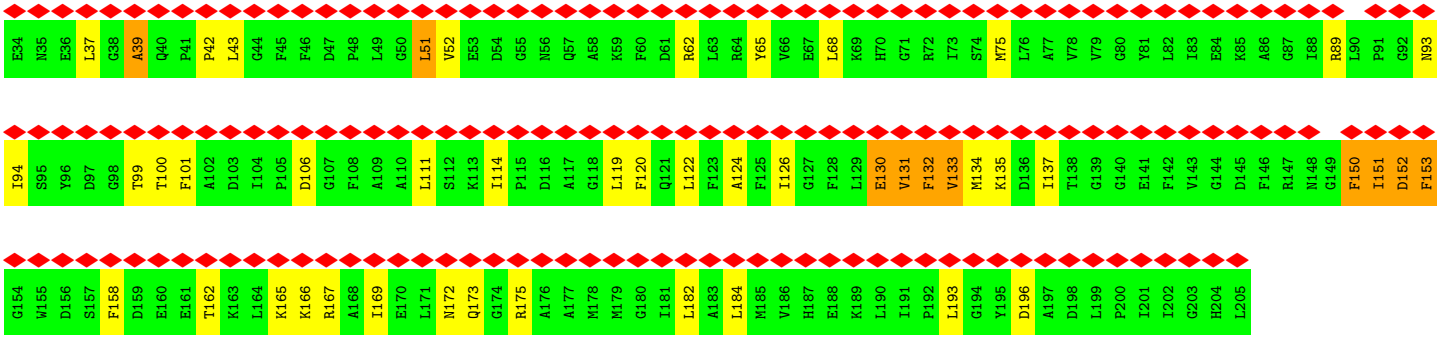




• Molecule 27: FCP-A

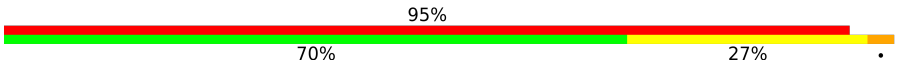
Chain 6:

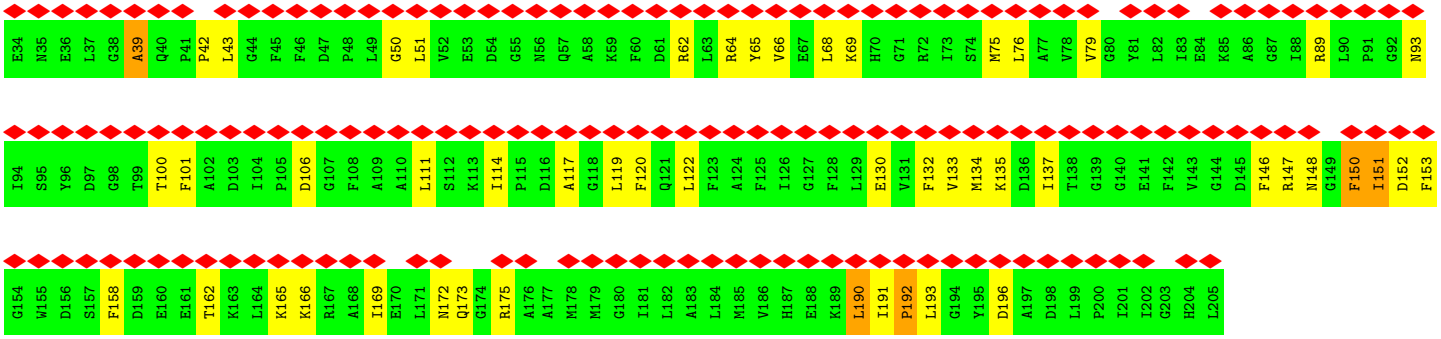




• Molecule 27: FCP-A

Chain 7:

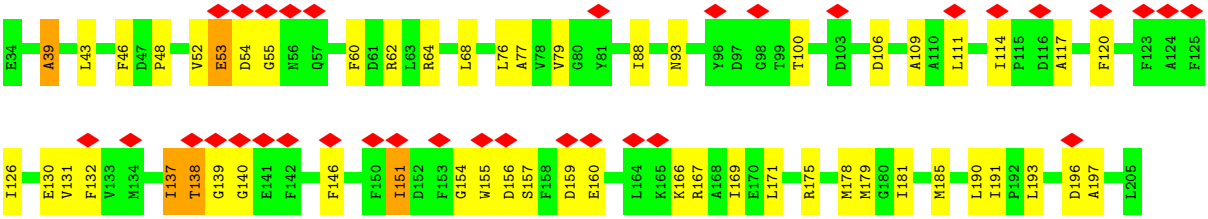




• Molecule 27: FCP-A

Chain 8:

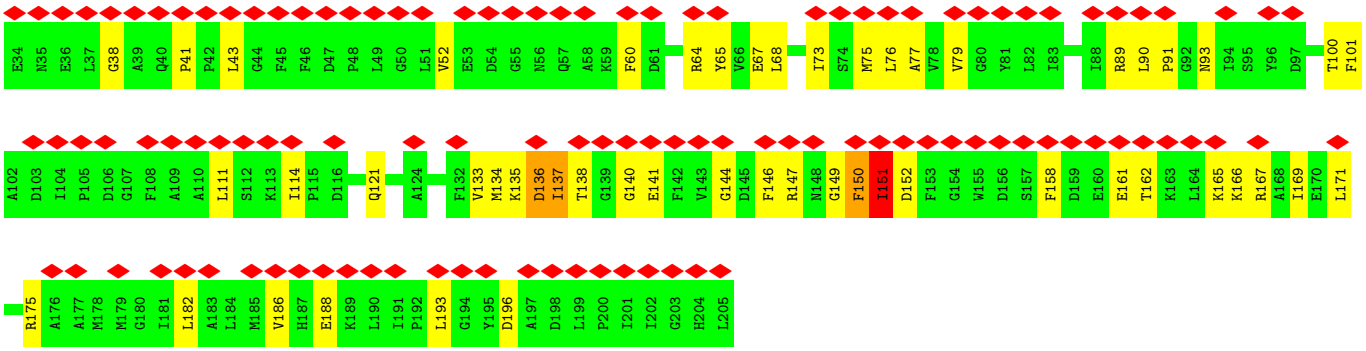




• Molecule 27: FCP-A

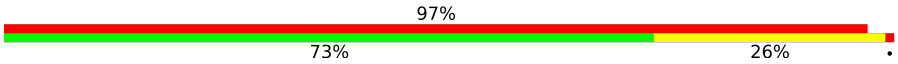
Chain 11:

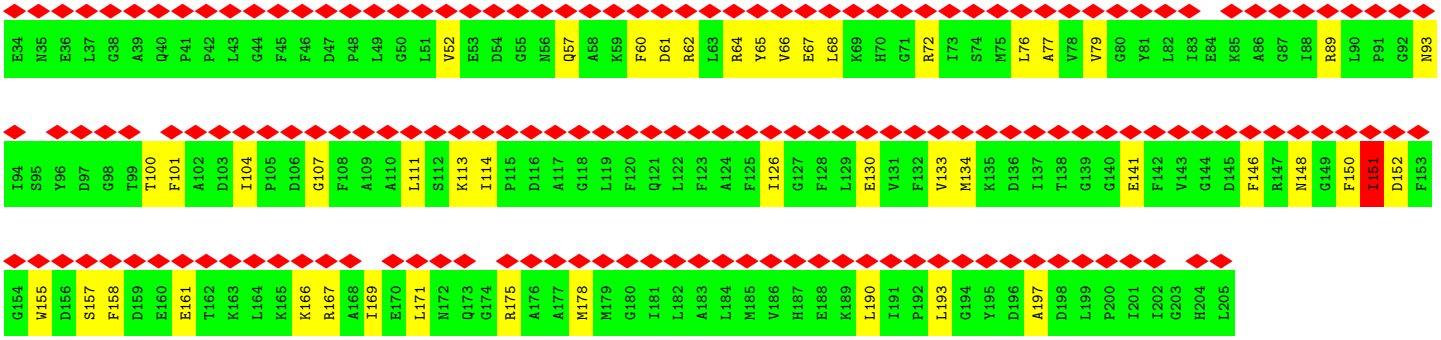




- Molecule 27: FCP-A

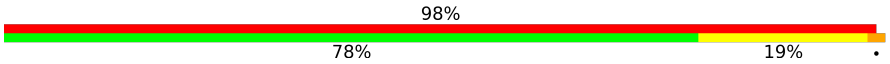
Chain 12:

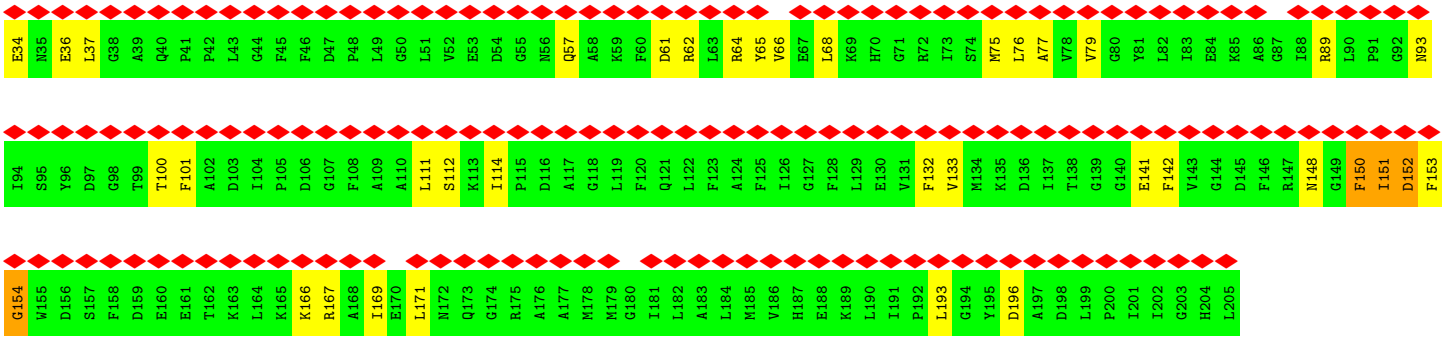




- Molecule 27: FCP-A

Chain 13:

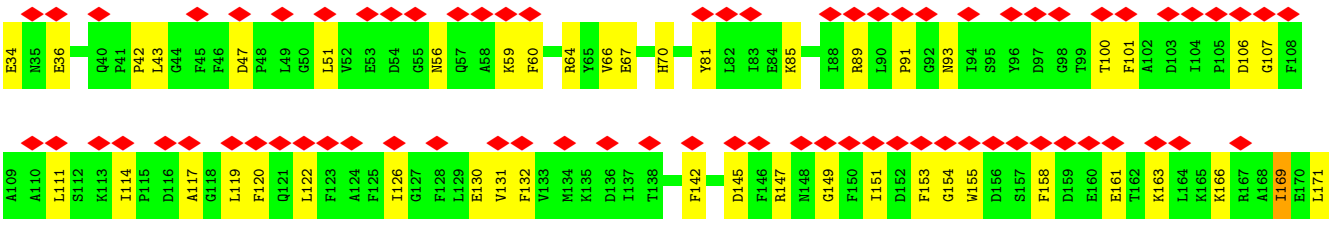


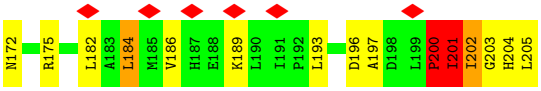


- Molecule 27: FCP-A

Chain 14:



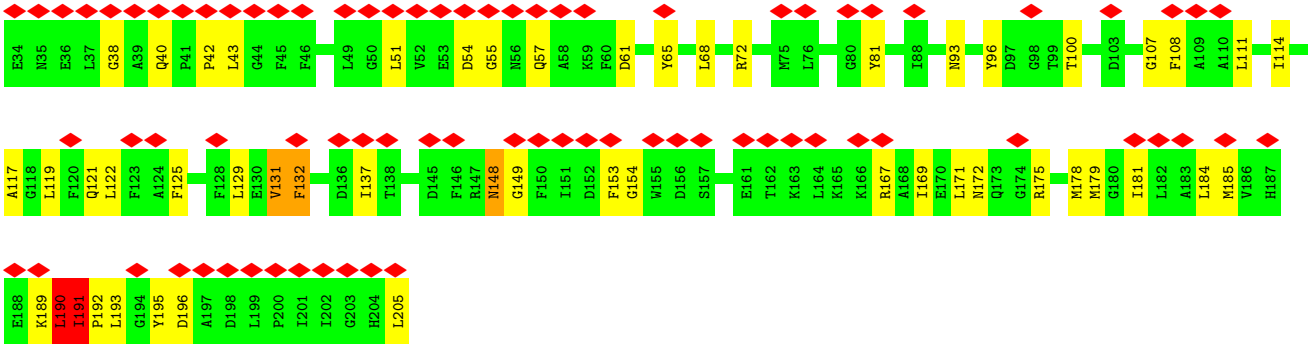




• Molecule 27: FCP-A

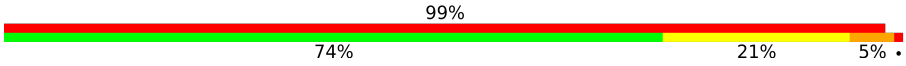
Chain 15:

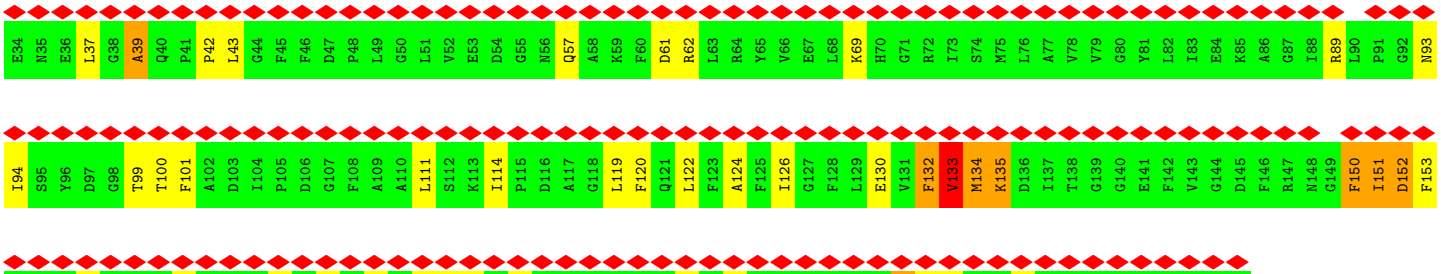




• Molecule 27: FCP-A

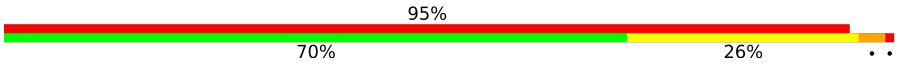
Chain 16:

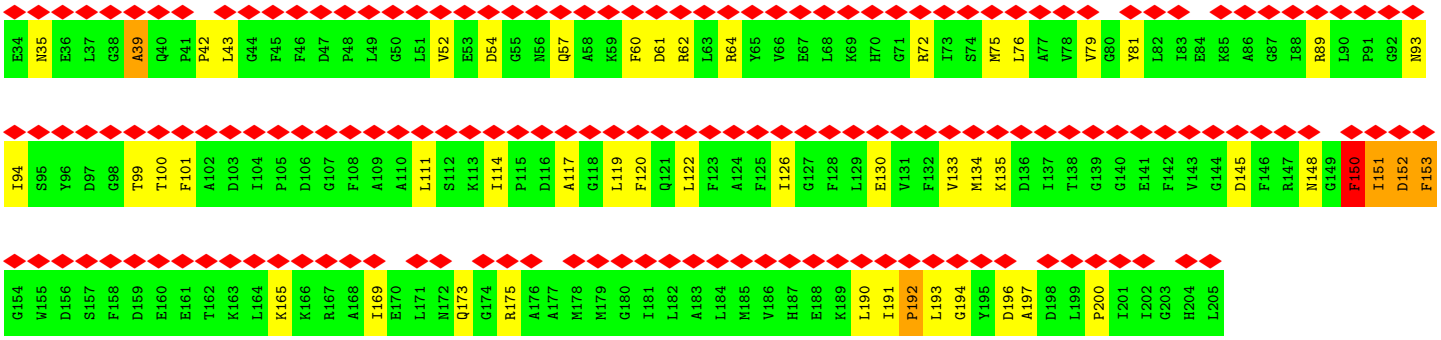




• Molecule 27: FCP-A

Chain 17:

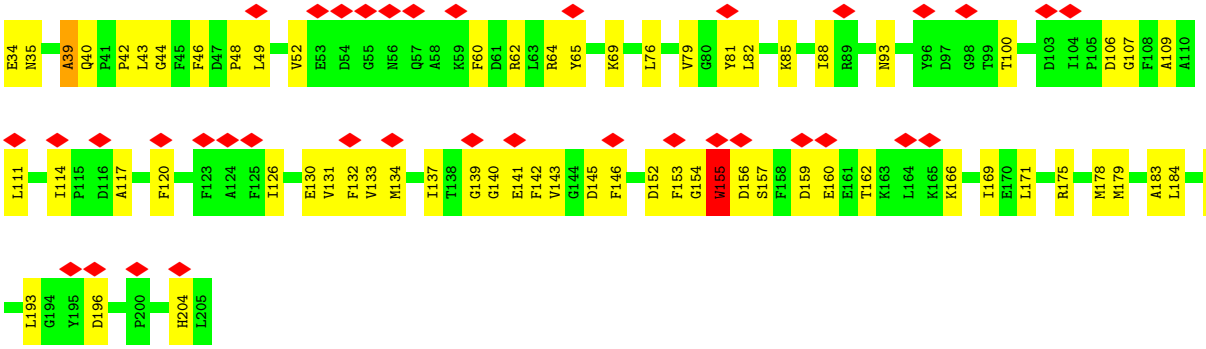




• Molecule 27: FCP-A

Chain 18:

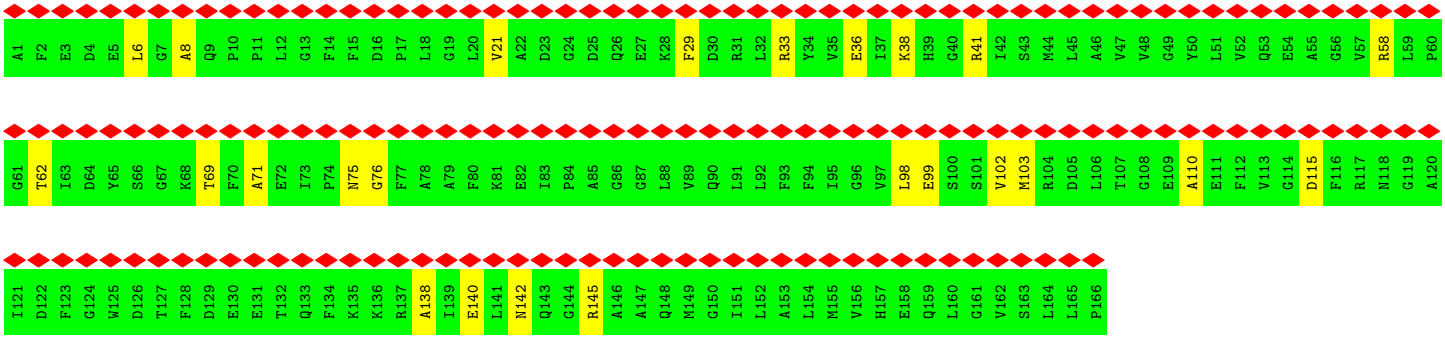




• Molecule 28: FCP-F

Chain 9:

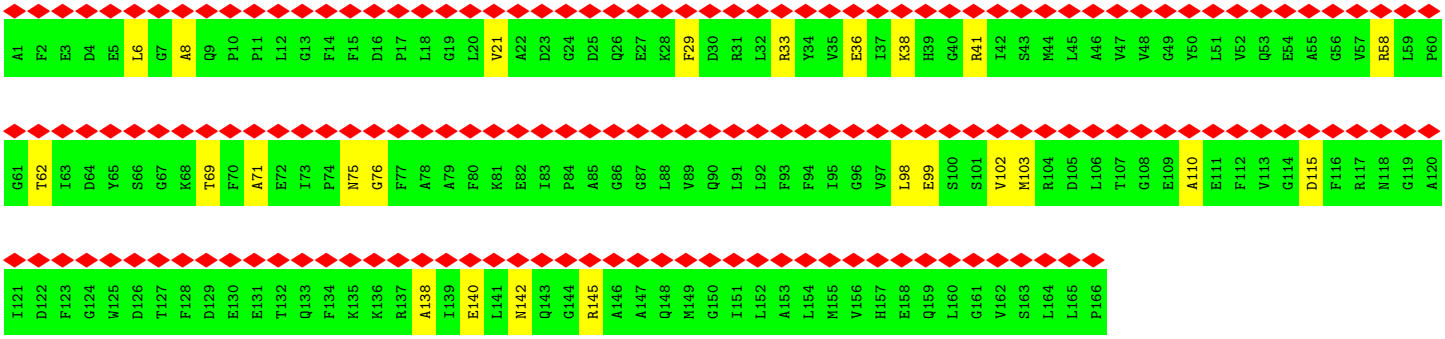




• Molecule 28: FCP-F

Chain 19:





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: LHG, SQD, LMG, FE2, PHO, HEM, KC1, BCR, PL9, A86, OEX, BCT, CLA, CL, DGD, KC2, DD6

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	0.62	0/2700	0.70	0/3681
1	a	0.62	0/2700	0.70	0/3681
2	B	0.61	0/4092	0.71	0/5562
2	b	0.61	0/4092	0.71	0/5562
3	C	0.60	0/3613	0.74	5/4926 (0.1%)
3	c	0.60	0/3613	0.74	7/4926 (0.1%)
4	D	0.63	0/2788	0.72	2/3803 (0.1%)
4	d	0.63	0/2788	0.72	2/3803 (0.1%)
5	E	0.42	0/660	0.61	0/899
5	e	0.42	0/660	0.61	0/899
6	F	0.48	0/268	0.85	0/363
6	f	0.47	0/268	0.85	0/363
7	G	0.36	0/936	0.65	0/1261
7	g	0.36	0/936	0.65	0/1261
8	H	0.47	0/516	0.78	0/704
8	h	0.47	0/516	0.78	0/704
9	I	0.61	0/285	0.76	0/386
9	i	0.61	0/285	0.76	0/386
10	J	0.46	0/253	0.77	0/344
10	j	0.46	0/253	0.77	0/344
11	K	0.56	0/311	0.89	2/427 (0.5%)
11	k	0.56	0/311	0.89	2/427 (0.5%)
12	L	0.59	0/310	0.66	0/423
12	l	0.59	0/310	0.66	0/423
13	M	0.54	0/313	0.65	0/422
13	m	0.54	0/313	0.65	0/422
15	O	0.46	0/1911	0.75	0/2576
15	o	0.46	0/1911	0.75	0/2576
16	P	0.46	0/1795	0.75	0/2441
16	p	0.46	0/1795	0.75	0/2441
17	Q	0.40	0/1164	0.71	0/1569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	q	0.40	0/1164	0.71	0/1569
19	T	0.46	0/256	0.69	0/346
19	t	0.46	0/256	0.69	0/346
20	U	0.41	0/726	0.74	1/986 (0.1%)
20	u	0.41	0/726	0.74	1/986 (0.1%)
21	V	0.45	0/1062	0.66	0/1444
21	v	0.45	0/1062	0.66	0/1444
22	W	0.60	0/368	1.05	1/491 (0.2%)
22	w	0.60	0/368	1.05	1/491 (0.2%)
23	X	0.25	0/244	0.62	0/330
23	x	0.25	0/244	0.62	0/330
24	Y	0.56	0/259	0.99	0/353
24	y	0.56	0/259	0.99	0/353
25	Z	0.41	0/460	0.61	0/633
25	z	0.41	0/460	0.61	0/633
26	0	0.62	0/1151	0.97	6/1550 (0.4%)
26	10	0.56	0/1151	0.81	1/1550 (0.1%)
27	1	0.56	0/1371	1.03	8/1849 (0.4%)
27	11	0.59	0/1365	1.02	4/1841 (0.2%)
27	12	0.53	0/1358	0.92	3/1834 (0.2%)
27	13	0.49	0/1362	0.91	3/1838 (0.2%)
27	14	0.60	0/1342	1.06	7/1813 (0.4%)
27	15	0.65	0/1306	1.20	11/1769 (0.6%)
27	16	0.49	0/1371	1.10	10/1849 (0.5%)
27	17	0.48	0/1371	1.00	4/1849 (0.2%)
27	18	0.66	0/1330	1.11	7/1797 (0.4%)
27	2	0.55	0/1371	1.02	6/1849 (0.3%)
27	3	0.49	0/1371	1.03	5/1849 (0.3%)
27	4	0.61	0/1342	1.05	4/1813 (0.2%)
27	5	0.63	1/1306 (0.1%)	1.04	4/1769 (0.2%)
27	6	0.52	0/1365	1.06	6/1841 (0.3%)
27	7	0.53	0/1365	1.07	2/1841 (0.1%)
27	8	0.65	0/1316	1.15	2/1781 (0.1%)
28	19	0.32	0/1313	0.54	0/1771
28	9	0.32	0/1313	0.54	0/1771
All	All	0.55	1/77120 (0.0%)	0.83	117/104564 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	132	PHE	CD1-CE1	-6.18	1.20	1.38

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	191	ILE	CG1-CB-CG2	-8.83	84.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	12	152	ASP	N-CA-C	8.53	123.73	113.16
27	14	200	PRO	CA-C-N	8.01	136.40	121.97
27	14	200	PRO	C-N-CA	8.01	136.40	121.97
4	D	138	ILE	CA-C-N	7.53	130.86	120.39
4	D	138	ILE	C-N-CA	7.53	130.86	120.39
4	d	138	ILE	CA-C-N	7.51	130.83	120.39
4	d	138	ILE	C-N-CA	7.51	130.83	120.39
26	0	65	TYR	CA-CB-CG	-7.47	100.44	113.90
27	6	51	LEU	N-CA-C	-7.46	106.12	114.62
27	15	191	ILE	O-C-N	-7.38	112.69	121.10
27	12	151	ILE	N-CA-C	7.28	124.48	109.34
27	2	151	ILE	N-CA-C	7.26	124.44	109.34
27	4	52	VAL	CB-CA-C	7.12	120.38	112.19
26	0	137	LEU	N-CA-C	-6.93	105.45	114.04
27	4	52	VAL	N-CA-CB	-6.89	104.33	112.39
27	11	147	ARG	CG-CD-NE	-6.83	96.98	112.00
27	16	134	MET	CG-SD-CE	-6.78	85.99	100.90
27	15	190	LEU	CA-C-N	6.72	134.57	122.13
27	15	190	LEU	C-N-CA	6.72	134.57	122.13
27	16	135	LYS	CD-CE-NZ	-6.72	90.38	111.90
27	15	148	ASN	N-CA-C	6.72	125.11	110.80
27	15	132	PHE	N-CA-CB	-6.61	99.32	110.49
27	4	165	LYS	CD-CE-NZ	-6.57	90.86	111.90
27	15	191	ILE	N-CA-CB	-6.51	102.09	111.21
26	0	135	ARG	CA-C-N	6.49	133.93	121.54
26	0	135	ARG	C-N-CA	6.49	133.93	121.54
27	18	139	GLY	CA-C-N	-6.47	117.25	121.65
27	18	139	GLY	C-N-CA	-6.47	117.25	121.65
27	3	193	LEU	CB-CG-CD1	-6.46	91.33	110.70
27	1	155	TRP	N-CA-C	-6.37	99.19	107.73
27	3	150	PHE	CB-CA-C	-6.37	103.28	111.50
27	15	191	ILE	CA-CB-CG2	6.30	121.21	110.50
27	15	191	ILE	CG1-CB-CG2	-6.21	92.08	110.70
27	18	155	TRP	CA-C-N	6.20	133.38	121.54
27	18	155	TRP	C-N-CA	6.20	133.38	121.54
11	K	56	VAL	N-CA-CB	-6.12	101.13	111.23
11	k	56	VAL	N-CA-CB	-6.10	101.16	111.23
27	1	153	PHE	N-CA-C	6.00	118.21	110.65
27	17	151	ILE	N-CA-C	5.96	121.73	109.34
27	16	132	PHE	CA-C-N	5.91	132.60	121.97
27	16	132	PHE	C-N-CA	5.91	132.60	121.97
27	7	51	LEU	CA-CB-CG	5.89	136.90	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	148	ASN	N-CA-C	5.88	123.32	110.80
27	6	52	VAL	N-CA-CB	-5.87	104.25	112.35
27	13	151	ILE	N-CA-C	5.87	121.55	109.34
27	3	151	ILE	N-CA-C	5.84	121.49	109.34
20	u	46	VAL	N-CA-C	-5.83	106.00	111.48
20	U	46	VAL	N-CA-C	-5.82	106.01	111.48
27	14	201	ILE	N-CA-C	5.80	121.42	109.34
27	14	149	GLY	CA-C-N	-5.80	115.53	122.44
27	14	149	GLY	C-N-CA	-5.80	115.53	122.44
27	6	151	ILE	N-CA-CB	-5.74	101.76	111.23
27	3	193	LEU	CA-CB-CG	5.73	136.35	116.30
27	1	151	ILE	N-CA-C	5.70	121.20	109.34
22	W	99	PRO	N-CA-C	5.70	120.03	111.14
3	C	373	ASN	CA-C-N	5.69	132.57	121.41
3	C	373	ASN	C-N-CA	5.69	132.57	121.41
22	w	99	PRO	N-CA-C	5.68	120.00	111.14
27	1	150	PHE	CB-CA-C	-5.67	103.67	112.07
3	c	373	ASN	CA-C-N	5.67	132.53	121.41
3	c	373	ASN	C-N-CA	5.67	132.53	121.41
27	11	151	ILE	N-CA-CB	-5.67	101.88	111.23
27	11	151	ILE	N-CA-C	5.66	121.12	109.34
27	5	193	LEU	CA-CB-CG	5.64	136.06	116.30
27	1	151	ILE	N-CA-CB	-5.61	101.97	111.23
26	0	191	LEU	CA-CB-CG	5.60	135.90	116.30
27	18	184	LEU	CA-CB-CG	5.59	135.88	116.30
27	12	157	SER	N-CA-C	-5.55	106.56	113.55
27	6	151	ILE	CA-CB-CG2	5.54	119.91	110.50
3	C	76	VAL	CB-CA-C	5.46	115.42	110.13
27	17	150	PHE	CA-C-N	5.44	131.77	121.97
27	17	150	PHE	C-N-CA	5.44	131.77	121.97
27	18	153	PHE	N-CA-CB	-5.44	101.29	110.49
27	3	51	LEU	CA-CB-CG	5.43	135.31	116.30
27	16	133	VAL	N-CA-C	5.38	120.53	109.34
27	16	151	ILE	N-CA-C	5.38	120.53	109.34
27	15	191	ILE	CB-CA-C	5.38	121.15	111.36
27	6	151	ILE	N-CA-C	5.36	120.50	109.34
3	c	76	VAL	CB-CA-C	5.36	115.33	110.13
27	5	200	PRO	CA-C-N	5.35	127.88	120.49
27	5	200	PRO	C-N-CA	5.35	127.88	120.49
26	0	181	LEU	CB-CG-CD2	-5.34	94.67	110.70
27	2	51	LEU	CA-CB-CG	5.30	134.85	116.30
27	11	140	GLY	N-CA-C	-5.26	106.13	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	151	ILE	CA-C-N	5.25	131.57	121.54
27	2	151	ILE	C-N-CA	5.25	131.57	121.54
11	k	56	VAL	CB-CA-C	5.23	119.87	111.29
11	K	56	VAL	CB-CA-C	5.21	119.84	111.29
27	1	192	PRO	CA-C-O	-5.21	115.52	121.56
27	17	151	ILE	N-CA-CB	-5.20	102.65	111.23
27	1	192	PRO	CA-C-N	5.19	131.46	121.54
27	1	192	PRO	C-N-CA	5.19	131.46	121.54
26	10	181	LEU	CB-CG-CD2	-5.17	95.21	110.70
27	16	134	MET	CB-CG-SD	5.15	128.16	112.70
27	14	184	LEU	CB-CG-CD1	-5.14	95.29	110.70
27	6	184	LEU	CA-CB-CG	5.13	134.27	116.30
27	8	156	ASP	CA-C-N	5.13	129.17	120.81
27	8	156	ASP	C-N-CA	5.13	129.17	120.81
27	18	142	PHE	CA-C-O	-5.12	116.91	121.67
3	c	398	HIS	CA-C-N	5.11	128.42	120.60
3	c	398	HIS	C-N-CA	5.11	128.42	120.60
27	7	50	GLY	CA-C-O	-5.11	116.65	122.78
27	16	133	VAL	N-CA-CB	-5.11	102.80	111.23
3	C	398	HIS	CA-C-N	5.10	128.41	120.60
3	C	398	HIS	C-N-CA	5.10	128.41	120.60
27	16	184	LEU	CA-CB-CG	5.10	134.14	116.30
27	2	150	PHE	CA-C-N	5.07	131.10	121.97
27	2	150	PHE	C-N-CA	5.07	131.10	121.97
27	14	202	ILE	N-CA-C	5.06	119.87	109.34
27	13	151	ILE	CA-C-N	5.03	131.14	121.54
27	13	151	ILE	C-N-CA	5.03	131.14	121.54
3	c	150	ASP	CA-C-N	5.02	131.13	121.54
3	c	150	ASP	C-N-CA	5.02	131.13	121.54
27	15	96	TYR	CA-C-N	5.02	128.71	120.63
27	15	96	TYR	C-N-CA	5.02	128.71	120.63
27	16	191	ILE	CA-CB-CG2	5.01	119.02	110.50

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2517	79	0
1	a	2617	0	2517	75	0
2	B	3960	0	3838	95	0
2	b	3960	0	3838	92	0
3	C	3496	0	3402	80	0
3	c	3496	0	3402	86	0
4	D	2696	0	2593	76	0
4	d	2696	0	2595	81	0
5	E	642	0	623	17	0
5	e	642	0	623	16	0
6	F	259	0	267	2	0
6	f	259	0	267	7	0
7	G	922	0	924	22	0
7	g	922	0	924	22	0
8	H	506	0	532	12	0
8	h	506	0	532	11	0
9	I	278	0	293	9	0
9	i	278	0	293	6	0
10	J	247	0	256	10	0
10	j	247	0	256	7	0
11	K	300	0	311	13	0
11	k	300	0	311	13	0
12	L	301	0	301	13	0
12	l	301	0	301	16	0
13	M	308	0	315	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	308	0	315	9	0
14	N	150	0	32	1	0
14	n	150	0	32	1	0
15	O	1881	0	1881	45	0
15	o	1881	0	1881	45	0
16	P	1745	0	1691	21	0
16	p	1745	0	1691	21	0
17	Q	1143	0	1130	24	0
17	q	1143	0	1130	17	0
18	R	365	0	80	1	0
18	r	365	0	80	1	0
19	T	250	0	268	4	0
19	t	250	0	268	6	0
20	U	711	0	713	16	0
20	u	711	0	713	15	0
21	V	1043	0	1044	24	0
21	v	1043	0	1044	23	0
22	W	394	0	346	8	0
22	w	394	0	346	6	0
23	X	244	0	274	2	0
23	x	244	0	274	2	0
24	Y	256	0	280	11	0
24	y	256	0	280	10	0
25	Z	452	0	479	7	0
25	z	452	0	479	8	0
26	0	1291	0	1165	31	0
26	10	1291	0	1166	35	0
27	1	1340	0	1332	49	0
27	11	1335	0	1325	49	0
27	12	1328	0	1309	42	0
27	13	1332	0	1318	24	0
27	14	1313	0	1294	43	0
27	15	1280	0	1222	33	0
27	16	1340	0	1330	29	0
27	17	1340	0	1330	31	0
27	18	1304	0	1281	46	0
27	2	1340	0	1330	43	0
27	3	1340	0	1330	36	0
27	4	1313	0	1294	47	0
27	5	1280	0	1223	44	0
27	6	1335	0	1325	32	0
27	7	1335	0	1325	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	8	1291	0	1259	44	0
28	19	1286	0	1267	17	0
28	9	1286	0	1267	17	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	0	394	0	313	7	0
31	1	413	0	369	24	0
31	10	442	0	349	8	0
31	11	351	0	304	15	0
31	12	330	0	267	8	0
31	13	345	0	303	10	0
31	14	374	0	345	10	0
31	15	295	0	249	15	0
31	16	280	0	231	8	0
31	17	265	0	194	7	0
31	18	307	0	255	12	0
31	19	408	0	407	9	0
31	2	330	0	265	17	0
31	3	345	0	303	13	0
31	4	313	0	284	8	0
31	5	295	0	249	12	0
31	6	280	0	231	12	0
31	7	265	0	194	12	0
31	8	307	0	256	11	0
31	9	408	0	408	7	0
31	A	174	0	170	9	0
31	B	1040	0	1152	42	0
31	C	829	0	900	32	0
31	D	195	0	216	14	0
31	P	447	0	382	10	0
31	R	47	0	35	1	0
31	W	65	0	72	3	0
31	Z	51	0	41	1	0
31	a	174	0	170	9	0
31	b	1040	0	1152	44	0
31	c	829	0	900	37	0
31	d	195	0	216	14	0
31	p	447	0	382	10	0
31	r	47	0	35	0	0
31	w	65	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	z	99	0	77	3	0
32	A	64	0	74	4	0
32	D	64	0	74	2	0
32	a	64	0	74	4	0
32	d	64	0	74	3	0
33	A	40	0	56	3	0
33	B	120	0	168	10	0
33	C	120	0	168	3	0
33	F	40	0	56	2	0
33	H	40	0	56	3	0
33	Y	40	0	56	6	0
33	a	40	0	56	2	0
33	b	120	0	168	7	0
33	c	120	0	168	5	0
33	f	40	0	56	3	0
33	h	40	0	56	4	0
33	y	40	0	56	5	0
34	10	41	0	45	1	0
34	8	41	0	45	2	0
34	A	94	0	118	5	0
34	B	54	0	77	7	0
34	L	54	0	77	4	0
34	a	54	0	74	3	0
34	b	54	0	76	9	0
34	i	40	0	44	2	0
34	l	54	0	77	6	0
35	A	33	0	42	1	0
35	D	55	0	80	4	0
35	a	33	0	42	2	0
35	d	55	0	80	5	0
36	14	35	0	43	2	0
36	15	25	0	20	0	0
36	18	70	0	80	4	0
36	4	35	0	43	3	0
36	5	25	0	20	0	0
36	8	70	0	80	2	0
36	A	37	0	44	1	0
36	B	43	0	59	1	0
36	C	40	0	50	1	0
36	D	49	0	74	5	0
36	L	49	0	74	5	0
36	P	27	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	Z	25	0	20	0	0
36	a	37	0	44	1	0
36	b	43	0	59	0	0
36	d	49	0	74	5	0
36	l	49	0	74	5	0
36	p	27	0	24	1	0
36	w	40	0	50	1	0
36	z	25	0	20	0	0
37	0	31	0	32	2	0
37	1	81	0	102	4	0
37	10	31	0	32	2	0
37	11	81	0	102	5	0
37	14	49	0	68	5	0
37	15	73	0	86	4	0
37	4	49	0	68	5	0
37	5	73	0	86	5	0
37	B	51	0	72	3	0
37	C	51	0	72	3	0
37	D	77	0	93	1	0
37	F	46	0	61	4	0
37	J	50	0	73	6	0
37	K	46	0	62	6	0
37	M	40	0	50	6	0
37	N	28	0	25	1	0
37	P	31	0	32	1	0
37	W	48	0	66	3	0
37	Z	31	0	32	0	0
37	b	51	0	72	2	0
37	c	82	0	104	2	0
37	d	77	0	93	3	0
37	f	46	0	61	5	0
37	j	50	0	73	4	0
37	k	46	0	62	4	0
37	m	40	0	50	3	0
37	n	28	0	25	1	0
37	p	31	0	32	2	0
37	w	48	0	66	4	0
38	1	54	0	66	2	0
38	11	60	0	81	2	0
38	B	54	0	66	6	0
38	C	179	0	228	8	0
38	H	62	0	82	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	56	0	70	0	0
38	b	55	0	68	12	0
38	c	179	0	229	6	0
38	h	62	0	82	4	0
38	w	56	0	70	0	0
39	C	1	0	0	0	0
39	c	1	0	0	0	0
40	D	4	0	1	1	0
40	d	4	0	1	1	0
41	E	43	0	30	2	0
41	V	43	0	30	4	0
41	e	43	0	30	2	0
41	v	43	0	30	3	0
42	0	45	0	0	0	0
42	1	45	0	0	0	0
42	10	45	0	0	0	0
42	11	45	0	0	0	0
42	12	45	0	0	0	0
42	13	45	0	0	0	0
42	14	45	0	0	0	0
42	15	45	0	0	0	0
42	16	45	0	0	0	0
42	17	45	0	0	0	0
42	18	45	0	0	0	0
42	19	45	0	0	0	0
42	2	45	0	0	0	0
42	3	45	0	0	0	0
42	4	45	0	0	1	0
42	5	45	0	0	0	0
42	6	45	0	0	0	0
42	7	45	0	0	0	0
42	8	45	0	0	1	0
42	9	45	0	0	0	0
42	P	45	0	0	0	0
42	p	45	0	0	0	0
43	0	288	0	0	1	0
43	1	336	0	0	2	0
43	10	336	0	0	1	0
43	11	336	0	0	1	0
43	12	288	0	0	0	0
43	13	288	0	0	2	0
43	14	240	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	15	240	0	0	4	0
43	16	288	0	0	1	0
43	17	336	0	0	2	0
43	18	240	0	0	10	0
43	19	288	0	0	2	0
43	2	240	0	0	0	0
43	3	288	0	0	0	0
43	4	288	0	0	3	0
43	5	288	0	0	5	0
43	6	336	0	0	1	0
43	7	288	0	0	1	0
43	8	240	0	0	0	0
43	9	288	0	0	2	0
43	P	96	0	0	1	0
43	p	96	0	0	1	0
44	P	43	0	0	1	0
44	p	43	0	0	3	0
45	0	45	0	0	0	0
45	1	90	0	0	0	0
45	10	45	0	0	1	0
45	11	90	0	0	0	0
45	12	90	0	0	0	0
45	13	90	0	0	0	0
45	14	90	0	0	0	0
45	15	90	0	0	1	0
45	16	90	0	0	1	0
45	17	90	0	0	1	0
45	18	90	0	0	1	0
45	19	45	0	0	1	0
45	2	90	0	0	1	0
45	3	90	0	0	1	0
45	4	90	0	0	1	0
45	5	90	0	0	1	0
45	6	90	0	0	1	0
45	7	90	0	0	1	0
45	8	90	0	0	1	0
45	9	45	0	0	1	0
46	Z	1	0	0	0	0
All	All	102777	0	92507	1968	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1968) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:153:PHE:CZ	27:2:151:ILE:CG2	1.77	1.65
26:10:155:PHE:CZ	26:10:163:LYS:HE3	1.51	1.43
27:11:150:PHE:CD2	27:12:151:ILE:CD1	2.01	1.42
27:11:150:PHE:CE2	27:12:151:ILE:HD11	1.53	1.41
27:1:153:PHE:HZ	27:2:151:ILE:CG2	1.16	1.35
27:1:153:PHE:CZ	27:2:151:ILE:HG21	1.46	1.30
27:1:153:PHE:CE2	27:2:151:ILE:HG21	1.67	1.28
27:11:150:PHE:CE2	27:12:151:ILE:CD1	2.12	1.28
26:10:155:PHE:CE1	26:10:163:LYS:HE3	1.68	1.27
27:11:150:PHE:CD2	27:12:151:ILE:HD12	1.66	1.20
26:0:135:ARG:HB2	26:0:138:THR:OG1	1.41	1.19
27:1:153:PHE:CZ	27:2:151:ILE:HG22	1.56	1.12
16:P:95:GLU:OE1	43:P:613:A86:C41	2.01	1.08
16:p:95:GLU:OE1	43:p:613:A86:C41	2.01	1.08
26:10:155:PHE:CZ	26:10:163:LYS:CE	2.46	0.99
26:10:155:PHE:CE1	26:10:163:LYS:CE	2.50	0.95
27:11:150:PHE:HE2	27:12:151:ILE:HD11	1.26	0.93
27:1:153:PHE:HZ	27:2:151:ILE:HG23	1.33	0.92
31:P:602:CLA:H161	44:P:612:DD6:C12	2.00	0.91
26:10:155:PHE:CE1	31:10:317:CLA:C3	2.55	0.89
27:16:153:PHE:HE2	31:16:313:CLA:H3A	1.36	0.88
27:11:150:PHE:CD2	27:12:151:ILE:HD13	2.09	0.86
27:2:151:ILE:HG22	27:2:151:ILE:O	1.75	0.85
31:p:602:CLA:H161	44:p:612:DD6:C12	2.06	0.84
27:1:153:PHE:CE1	27:2:151:ILE:HG22	2.13	0.84
15:O:104:LYS:HG2	22:W:93:ARG:HH12	1.46	0.81
3:c:165:LEU:HD21	31:c:507:CLA:HAB	1.62	0.81
27:1:153:PHE:HZ	27:2:151:ILE:HG22	1.00	0.80
3:C:165:LEU:HD21	31:C:507:CLA:HAB	1.62	0.80
27:11:150:PHE:HD2	27:12:151:ILE:CD1	1.88	0.78
31:11:313:CLA:H12	31:11:313:CLA:H3A	1.66	0.78
26:0:135:ARG:CB	26:0:138:THR:OG1	2.28	0.78
27:11:151:ILE:HD13	27:14:166:LYS:HZ1	1.50	0.76
27:15:193:LEU:HD12	27:15:195:TYR:H	1.50	0.76
3:c:305:THR:HG22	3:c:423:ARG:HH12	1.51	0.75
3:C:305:THR:HG22	3:C:423:ARG:HH12	1.51	0.75
27:12:133:VAL:HG12	27:12:134:MET:HG3	1.69	0.75
31:P:606:CLA:HAA1	27:5:132:PHE:CE2	2.22	0.74
27:4:158:PHE:HB3	27:4:161:GLU:HB3	1.70	0.74
31:1:313:CLA:H12	31:1:313:CLA:H3A	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:11:310:CLA:HED2	31:11:310:CLA:H2A	1.70	0.73
37:K:101:LMG:HC62	17:Q:97:TYR:HD1	1.53	0.73
31:1:321:CLA:O1D	27:4:172:ASN:ND2	2.22	0.73
27:14:186:VAL:HA	27:14:189:LYS:HG2	1.71	0.72
3:c:307:PRO:HB2	3:c:361:LEU:HD12	1.71	0.72
27:2:151:ILE:CG2	27:2:151:ILE:O	2.38	0.71
27:5:172:ASN:ND2	31:5:306:CLA:O1D	2.22	0.71
9:I:9:TYR:HB3	22:W:109:ARG:HH12	1.56	0.71
3:C:307:PRO:HB2	3:C:361:LEU:HD12	1.71	0.71
27:12:161:GLU:OE2	27:13:148:ASN:ND2	2.23	0.71
1:A:56:PRO:HB2	15:O:204:ARG:HH22	1.56	0.70
31:C:505:CLA:NB	38:C:519:DGD:HB62	2.07	0.70
4:d:329:MET:HG2	4:d:333:ASP:HB2	1.73	0.70
15:o:132:MET:HB3	15:o:171:ILE:HB	1.73	0.70
17:q:124:THR:HA	17:q:151:MET:HE1	1.73	0.70
35:d:407:PL9:H201	36:l:102:LHG:H191	1.73	0.70
27:7:75:MET:HE1	31:7:313:CLA:HBB1	1.74	0.70
4:D:329:MET:HG2	4:D:333:ASP:HB2	1.73	0.70
17:Q:124:THR:HA	17:Q:151:MET:HE1	1.73	0.69
4:d:180:ARG:NH1	4:d:333:ASP:OD1	2.25	0.69
4:d:83:ASN:O	7:g:58:SER:N	2.25	0.69
27:13:77:ALA:HA	31:13:310:CLA:HAB	1.75	0.69
31:c:505:CLA:NB	38:c:519:DGD:HB62	2.07	0.69
4:d:23:LYS:NZ	37:d:404:LMG:O10	2.26	0.69
27:15:131:VAL:HA	27:15:137:ILE:HD11	1.72	0.69
4:D:180:ARG:NH1	4:D:333:ASP:OD1	2.25	0.69
27:17:133:VAL:HG12	27:17:134:MET:HG3	1.73	0.69
3:C:322:GLN:HE22	3:C:381:LYS:HA	1.58	0.69
1:a:56:PRO:HB2	15:o:204:ARG:HH22	1.58	0.69
11:K:41:ILE:HG23	33:Y:101:BCR:H352	1.74	0.68
31:c:504:CLA:H72	31:c:504:CLA:H142	1.75	0.68
1:A:15:GLU:HA	22:W:123:ARG:HH21	1.57	0.68
11:K:52:TRP:HE1	24:Y:46:LEU:HB3	1.57	0.68
15:O:132:MET:HB3	15:O:171:ILE:HB	1.73	0.68
20:u:32:ASN:HD22	20:u:99:ASN:HB2	1.58	0.68
3:C:154:LYS:HE2	3:C:261:ARG:HG3	1.76	0.68
2:B:374:ASP:HB3	7:G:148:ARG:HH21	1.59	0.68
27:12:65:TYR:HB2	27:12:141:GLU:HG3	1.75	0.68
3:c:322:GLN:HE22	3:c:381:LYS:HA	1.58	0.68
2:B:320:ALA:HB1	4:D:292:ASN:HD22	1.59	0.68
27:4:42:PRO:HG2	27:4:43:LEU:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:18:ARG:HE	14:n:4:UNK:HA	1.59	0.67
20:U:32:ASN:HD22	20:U:99:ASN:HB2	1.58	0.67
3:c:154:LYS:HE2	3:c:261:ARG:HG3	1.76	0.67
27:18:133:VAL:HG12	27:18:134:MET:HG2	1.76	0.67
26:10:162:LYS:HG2	26:10:166:ILE:HD11	1.76	0.67
4:D:323:GLU:HB3	4:D:326:ARG:HH21	1.60	0.67
10:J:15:LEU:HD12	33:Y:101:BCR:H383	1.77	0.67
4:d:323:GLU:HB3	4:d:326:ARG:HH21	1.60	0.67
27:5:193:LEU:H	27:5:196:ASP:HB3	1.59	0.67
27:6:165:LYS:HZ2	27:7:146:PHE:HB3	1.60	0.67
31:B:614:CLA:H101	34:l:101:SQD:H241	1.76	0.67
31:C:504:CLA:H72	31:C:504:CLA:H142	1.75	0.66
11:k:41:ILE:HG23	33:y:101:BCR:H352	1.77	0.66
26:10:26:ALA:O	26:10:164:ARG:NH1	2.28	0.66
27:14:155:TRP:HE1	27:14:163:LYS:HD3	1.60	0.66
8:H:18:ARG:HE	14:N:4:UNK:HA	1.61	0.66
26:0:37:LEU:HD21	26:0:40:PHE:HB2	1.76	0.66
27:8:185:MET:HE2	34:8:301:SQD:H112	1.77	0.66
31:1:310:CLA:HED2	31:1:310:CLA:H2A	1.76	0.66
27:18:204:HIS:HB2	36:18:316:LHG:H172	1.77	0.66
15:O:102:GLN:HA	16:p:218:LYS:HD3	1.76	0.65
27:15:42:PRO:HG2	27:15:43:LEU:HD12	1.77	0.65
4:D:68:LEU:HD21	5:E:44:TYR:HE1	1.61	0.65
3:c:326:ALA:HB2	20:u:97:ILE:HG21	1.79	0.65
26:0:93:THR:HG22	26:0:100:THR:HG22	1.79	0.65
26:10:32:GLY:HA3	26:10:168:LEU:HD23	1.78	0.65
2:b:320:ALA:HB1	4:d:292:ASN:HD22	1.60	0.65
2:b:374:ASP:HB3	7:g:148:ARG:HH21	1.60	0.65
15:o:209:PHE:HA	15:o:311:GLN:HE22	1.61	0.65
27:15:185:MET:HG3	27:15:189:LYS:HE2	1.79	0.65
27:13:66:VAL:HG22	31:13:312:CLA:HED3	1.79	0.64
12:L:27:VAL:HG11	36:L:101:LHG:H201	1.80	0.64
15:O:209:PHE:HA	15:O:311:GLN:HE22	1.61	0.64
2:b:256:MET:O	2:b:448:ARG:NH1	2.30	0.64
15:o:104:LYS:HG2	22:w:93:ARG:HH12	1.63	0.64
31:7:313:CLA:H12	31:7:313:CLA:H3A	1.79	0.64
27:13:166:LYS:HA	27:13:169:ILE:HG12	1.79	0.64
27:4:191:ILE:HG22	27:4:192:PRO:HD2	1.79	0.64
27:12:166:LYS:HA	27:12:169:ILE:HG12	1.78	0.64
2:b:122:LEU:HD12	8:h:20:GLY:HA2	1.79	0.64
26:10:26:ALA:O	26:10:164:ARG:CZ	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:11:133:VAL:HG12	27:11:134:MET:HG3	1.79	0.64
27:6:93:ASN:O	43:6:303:A86:O3	2.16	0.64
21:v:8:ARG:NH1	21:v:21:LEU:O	2.31	0.64
12:l:27:VAL:HG11	36:l:102:LHG:H201	1.80	0.63
1:a:84:PRO:HD3	1:a:173:PRO:HB3	1.80	0.63
26:10:93:THR:HG22	26:10:100:THR:HG22	1.79	0.63
31:17:313:CLA:H12	31:17:313:CLA:H3A	1.79	0.63
3:C:213:VAL:O	3:C:223:TRP:NE1	2.31	0.63
3:C:38:GLY:HA3	31:C:512:CLA:HMD2	1.81	0.63
2:B:256:MET:O	2:B:448:ARG:NH1	2.30	0.63
4:D:83:ASN:O	7:G:58:SER:N	2.31	0.63
3:c:38:GLY:HA3	31:c:512:CLA:HMD2	1.81	0.63
27:1:68:LEU:HD21	27:1:167:ARG:HH22	1.64	0.63
3:C:326:ALA:HB2	20:U:97:ILE:HG21	1.81	0.63
3:c:449:ARG:NH1	9:i:27:ASP:OD2	2.31	0.63
34:L:102:SQD:H241	31:b:615:CLA:H101	1.80	0.63
11:k:52:TRP:HE1	24:y:46:LEU:HB3	1.64	0.63
27:15:190:LEU:HD11	27:15:205:LEU:HD23	1.80	0.63
1:A:84:PRO:HD3	1:A:173:PRO:HB3	1.80	0.62
2:B:122:LEU:HD12	8:H:20:GLY:HA2	1.80	0.62
15:O:140:ALA:HB1	15:O:155:PHE:HB3	1.81	0.62
17:Q:113:TYR:OH	21:V:95:ILE:O	2.14	0.62
21:V:8:ARG:NH1	21:V:21:LEU:O	2.31	0.62
4:d:68:LEU:HD21	5:e:44:TYR:HE1	1.63	0.62
4:D:302:GLU:OE2	15:O:247:LYS:NZ	2.32	0.62
26:10:160:GLN:HG2	26:10:164:ARG:NE	2.13	0.62
27:14:175:ARG:HB2	43:14:301:A86:C23	2.30	0.62
5:E:51:ARG:HH11	17:Q:66:VAL:HG22	1.63	0.62
27:11:77:ALA:HA	31:11:310:CLA:HAB	1.80	0.62
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.33	0.62
2:B:311:PHE:HD1	2:B:430:PHE:HE2	1.45	0.62
9:i:9:TYR:HB3	22:w:109:ARG:HH12	1.63	0.62
15:o:140:ALA:HB1	15:o:155:PHE:HB3	1.81	0.62
27:1:150:PHE:CD2	27:2:151:ILE:HD12	2.35	0.62
11:K:47:LEU:HB3	33:Y:101:BCR:H21C	1.80	0.62
4:d:186:GLN:HB2	31:d:405:CLA:HBC1	1.81	0.62
27:12:66:VAL:HG22	31:12:312:CLA:HED3	1.81	0.62
27:12:107:GLY:HA3	27:12:193:LEU:HD22	1.80	0.62
27:15:40:GLN:NE2	31:15:306:CLA:O1D	2.33	0.62
3:C:391:ARG:NH2	17:Q:152:TYR:OH	2.32	0.62
20:U:50:ILE:HG12	20:U:62:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:334:ARG:NH2	15:o:245:ASP:O	2.33	0.62
34:a:408:SQD:O9	4:d:230:ASN:ND2	2.30	0.62
27:14:205:LEU:HD13	36:14:317:LHG:HC32	1.82	0.62
1:A:170:ASP:OD2	3:C:357:ARG:NH1	2.33	0.62
3:C:323:ARG:NH2	3:C:389:GLU:OE1	2.33	0.62
15:O:110:ASN:HD21	15:O:164:GLN:HB3	1.65	0.62
2:B:30:VAL:HG11	31:B:612:CLA:H112	1.81	0.61
35:D:407:PL9:H201	36:L:101:LHG:H191	1.82	0.61
1:a:170:ASP:OD2	3:c:357:ARG:NH1	2.32	0.61
3:c:416:SER:HB3	21:v:42:VAL:HG23	1.80	0.61
20:u:50:ILE:HG12	20:u:62:LEU:HD11	1.82	0.61
27:2:133:VAL:HG12	27:2:134:MET:HG3	1.83	0.61
27:12:89:ARG:NH1	27:12:101:PHE:O	2.33	0.61
4:D:186:GLN:HB2	31:D:405:CLA:HBC1	1.81	0.61
16:P:198:SER:OG	16:P:205:GLN:NE2	2.33	0.61
2:b:30:VAL:HG11	31:b:613:CLA:H112	1.81	0.61
5:e:19:TYR:O	5:e:23:HIS:ND1	2.31	0.61
1:A:334:ARG:NH2	15:O:245:ASP:O	2.31	0.61
2:b:311:PHE:HD1	2:b:430:PHE:HE2	1.45	0.61
27:12:68:LEU:HD21	27:12:167:ARG:HH22	1.64	0.61
1:a:27:ARG:NH2	19:t:21:VAL:O	2.34	0.61
26:0:93:THR:HA	26:0:100:THR:HA	1.82	0.61
1:A:209:SER:HB2	4:D:275:PRO:HB3	1.83	0.61
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.34	0.61
27:4:119:LEU:HD23	27:4:122:LEU:HD12	1.82	0.61
2:b:235:GLU:OE1	2:b:472:ARG:NH1	2.33	0.61
5:e:53:ASN:O	21:v:1:ILE:N	2.33	0.61
26:10:93:THR:HA	26:10:100:THR:HA	1.82	0.61
2:b:460:LEU:HD11	4:d:287:VAL:HG21	1.82	0.61
27:14:42:PRO:HG2	27:14:43:LEU:HD12	1.83	0.61
2:b:18:ARG:HE	2:b:118:TRP:HB3	1.66	0.61
27:11:150:PHE:HD2	27:12:151:ILE:HD13	1.52	0.61
2:B:460:LEU:HD11	4:D:287:VAL:HG21	1.81	0.61
31:B:602:CLA:H171	38:H:102:DGD:HAW1	1.81	0.61
3:c:343:ARG:HD2	15:o:165:THR:HA	1.82	0.61
15:o:110:ASN:HD21	15:o:164:GLN:HB3	1.65	0.61
27:1:150:PHE:CE2	27:2:151:ILE:HD12	2.36	0.61
27:14:119:LEU:HD23	27:14:122:LEU:HD12	1.81	0.61
3:c:213:VAL:O	3:c:223:TRP:NE1	2.31	0.60
27:5:42:PRO:HG2	27:5:43:LEU:HD12	1.83	0.60
1:A:139:MET:HE1	4:D:252:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:14:56:ASN:HB3	27:14:59:LYS:HB3	1.83	0.60
17:Q:102:GLU:HG2	17:Q:103:LYS:H	1.67	0.60
36:d:408:LHG:HC32	12:l:16:THR:HG21	1.83	0.60
27:1:166:LYS:HA	27:1:169:ILE:HG12	1.84	0.60
2:B:422:ARG:NH1	15:O:256:ASP:OD2	2.35	0.60
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.34	0.60
2:B:365:THR:HG21	15:O:259:VAL:HG13	1.84	0.60
2:B:357:ARG:NH2	4:D:337:GLU:O	2.35	0.60
16:P:130:GLU:OE2	16:P:133:ARG:NH2	2.35	0.60
3:c:79:LYS:HD2	3:c:84:GLN:HB3	1.84	0.60
11:k:47:LEU:HB3	33:y:101:BCR:H21C	1.82	0.60
27:14:91:PRO:HD2	37:14:316:LMG:H291	1.82	0.60
2:B:325:PHE:O	12:L:38:ASN:ND2	2.34	0.60
5:E:19:TYR:O	5:E:23:HIS:ND1	2.31	0.60
10:J:15:LEU:O	10:J:19:PHE:N	2.29	0.60
16:p:130:GLU:OE2	16:p:133:ARG:NH2	2.35	0.60
16:p:198:SER:OG	16:p:205:GLN:NE2	2.34	0.60
27:2:112:SER:HA	31:2:315:CLA:HBC3	1.83	0.60
3:C:449:ARG:NH1	9:I:27:ASP:OD2	2.35	0.60
27:14:66:VAL:O	27:14:70:HIS:ND1	2.28	0.60
31:B:602:CLA:H2	31:B:602:CLA:HBD	1.84	0.60
3:c:311:GLN:NE2	3:c:355:THR:OG1	2.35	0.60
17:q:102:GLU:HG2	17:q:103:LYS:H	1.67	0.60
27:11:68:LEU:HD21	27:11:167:ARG:HH22	1.67	0.60
27:13:152:ASP:HB3	27:14:151:ILE:HD11	1.84	0.60
28:19:62:THR:HA	28:19:69:THR:HA	1.84	0.60
5:E:14:ILE:HG13	10:J:13:VAL:HG11	1.83	0.59
13:M:20:LEU:O	13:M:24:ASN:ND2	2.35	0.59
13:m:20:LEU:O	13:m:24:ASN:ND2	2.35	0.59
26:0:135:ARG:HG2	26:0:136:ASP:H	1.66	0.59
27:1:77:ALA:HA	31:1:310:CLA:HAB	1.84	0.59
28:9:36:GLU:OE2	28:9:145:ARG:NE	2.30	0.59
1:a:139:MET:HE1	4:d:252:PHE:HB2	1.83	0.59
1:a:209:SER:HB2	4:d:275:PRO:HB3	1.83	0.59
31:b:603:CLA:HBD	31:b:603:CLA:H2	1.84	0.59
3:c:269:GLU:OE1	3:c:447:ARG:NH1	2.34	0.59
27:18:39:ALA:HB2	27:18:175:ARG:HH12	1.67	0.59
16:P:67:ALA:O	16:P:71:HIS:ND1	2.28	0.59
2:b:286:ARG:NH2	7:g:108:ASN:OD1	2.35	0.59
4:d:180:ARG:O	4:d:184:PHE:N	2.34	0.59
27:4:56:ASN:HB3	27:4:59:LYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:323:ARG:NH2	3:c:389:GLU:OE1	2.33	0.59
2:B:286:ARG:NH2	7:G:108:ASN:OD1	2.35	0.59
1:a:15:GLU:HA	22:w:123:ARG:HH21	1.68	0.59
1:a:56:PRO:HA	1:a:73:TYR:HE2	1.67	0.59
4:d:254:SER:HB2	19:t:24:ARG:HH22	1.68	0.59
27:2:42:PRO:HG3	31:2:306:CLA:HAB	1.84	0.59
1:A:56:PRO:HA	1:A:73:TYR:HE2	1.67	0.59
11:K:34:ILE:HA	24:Y:24:VAL:HG11	1.85	0.59
2:b:357:ARG:NH2	4:d:337:GLU:O	2.35	0.59
3:c:39:ASN:ND2	31:c:511:CLA:O1A	2.36	0.59
27:5:121:GLN:NE2	37:5:316:LMG:O8	2.35	0.59
27:8:88:ILE:HG12	36:8:316:LHG:H171	1.84	0.59
27:12:64:ARG:HH21	27:12:171:LEU:HD11	1.68	0.59
3:C:39:ASN:ND2	31:C:511:CLA:O1A	2.36	0.59
20:u:29:ASN:ND2	20:u:86:LYS:O	2.35	0.59
20:U:38:LYS:HA	21:V:61:LEU:HD13	1.85	0.59
1:a:163:ILE:O	3:c:292:TYR:OH	2.19	0.59
5:E:53:ASN:O	21:V:1:ILE:N	2.36	0.59
31:P:606:CLA:HAA1	27:5:132:PHE:CZ	2.38	0.59
27:4:51:LEU:O	27:4:56:ASN:ND2	2.36	0.59
27:12:161:GLU:HG2	27:12:166:LYS:HE2	1.85	0.59
4:D:129:GLN:NE2	32:D:403:PHO:OBD	2.36	0.58
24:y:44:GLN:HG3	25:z:29:THR:HG23	1.84	0.58
27:4:193:LEU:HD12	27:4:196:ASP:H	1.66	0.58
27:14:93:ASN:HA	27:14:100:THR:HA	1.85	0.58
27:15:172:ASN:ND2	31:15:306:CLA:O1D	2.35	0.58
1:A:163:ILE:O	3:C:292:TYR:OH	2.21	0.58
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.85	0.58
2:B:18:ARG:HE	2:B:118:TRP:HB3	1.67	0.58
15:O:249:ARG:NH1	15:O:278:ASN:OD1	2.34	0.58
31:b:603:CLA:H171	38:h:102:DGD:HAW1	1.83	0.58
3:c:87:ILE:HG23	3:c:88:LEU:HG	1.85	0.58
1:A:136:ARG:NH2	9:I:27:ASP:OD1	2.36	0.58
3:C:87:ILE:HG23	3:C:88:LEU:HG	1.85	0.58
31:C:504:CLA:H172	31:C:511:CLA:HBB2	1.85	0.58
4:D:180:ARG:O	4:D:184:PHE:N	2.34	0.58
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.85	0.58
3:c:70:PHE:HZ	37:k:101:LMG:HC92	1.68	0.58
31:c:511:CLA:HMA2	31:c:511:CLA:H2	1.85	0.58
26:10:178:ILE:HD12	26:10:181:LEU:HD23	1.84	0.58
27:11:150:PHE:CG	27:12:151:ILE:HD12	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:17:93:ASN:HA	27:17:100:THR:HA	1.86	0.58
1:A:57:PRO:HD2	15:O:204:ARG:HH12	1.68	0.58
3:C:311:GLN:NE2	3:C:355:THR:OG1	2.35	0.58
16:P:197:ALA:HA	36:8:317:LHG:H121	1.84	0.58
27:4:205:LEU:HD13	36:4:317:LHG:HC32	1.85	0.58
31:10:317:CLA:H2A	31:10:317:CLA:HED3	1.85	0.58
34:10:320:SQD:H3	27:18:109:ALA:HB2	1.85	0.58
1:A:254:TYR:HE2	4:D:142:ASN:HD22	1.52	0.58
20:U:29:ASN:ND2	20:U:86:LYS:O	2.35	0.58
4:d:302:GLU:OE2	15:o:247:LYS:NZ	2.36	0.58
27:11:188:GLU:HG2	27:11:193:LEU:HA	1.86	0.58
3:C:311:GLN:HG3	3:C:361:LEU:HD13	1.86	0.58
4:D:192:THR:HG23	31:D:405:CLA:HBC2	1.86	0.58
3:c:311:GLN:HG3	3:c:361:LEU:HD13	1.86	0.58
10:j:15:LEU:O	10:j:19:PHE:N	2.30	0.58
3:C:70:PHE:HZ	37:K:101:LMG:HC92	1.68	0.58
3:C:199:ILE:HG13	3:C:234:ILE:HG13	1.86	0.58
21:V:66:ARG:NH1	21:V:71:ALA:O	2.37	0.58
26:0:31:LEU:HB2	26:0:64:ARG:HH21	1.69	0.58
26:0:178:ILE:HD12	26:0:181:LEU:HD23	1.86	0.58
3:C:269:GLU:OE1	3:C:447:ARG:NH1	2.34	0.57
33:Y:101:BCR:HC21	25:Z:13:VAL:HG13	1.85	0.57
31:c:504:CLA:H172	31:c:511:CLA:HBB2	1.85	0.57
16:p:197:ALA:HA	36:18:316:LHG:H122	1.85	0.57
27:1:93:ASN:HA	27:1:100:THR:HA	1.86	0.57
27:1:153:PHE:CE2	27:2:151:ILE:CG2	2.46	0.57
27:18:65:TYR:HE2	27:18:137:ILE:HG23	1.68	0.57
26:10:155:PHE:HE1	31:10:317:CLA:C3	2.14	0.57
1:A:334:ARG:HH12	15:O:248:GLY:HA2	1.69	0.57
3:C:79:LYS:HD2	3:C:84:GLN:HB3	1.84	0.57
31:C:511:CLA:HMA2	31:C:511:CLA:H2	1.85	0.57
4:D:123:ILE:HD11	38:H:102:DGD:HAH2	1.87	0.57
16:P:12:SER:OG	16:P:15:LEU:O	2.22	0.57
1:a:254:TYR:HE2	4:d:142:ASN:HD22	1.51	0.57
26:10:81:TYR:OH	26:10:185:GLU:OE2	2.21	0.57
27:14:81:TYR:CZ	27:14:184:LEU:HD11	2.39	0.57
27:18:193:LEU:HD12	27:18:196:ASP:H	1.69	0.57
31:B:614:CLA:H143	34:l:101:SQD:H272	1.86	0.57
5:E:20:TRP:HZ2	10:J:13:VAL:HG13	1.70	0.57
2:b:365:THR:HG21	15:o:259:VAL:HG13	1.86	0.57
21:v:66:ARG:NH1	21:v:71:ALA:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:32:LEU:HD12	24:y:35:ILE:HD12	1.86	0.57
27:1:150:PHE:HD2	31:1:313:CLA:H41	1.68	0.57
27:15:121:GLN:NE2	37:15:315:LMG:O8	2.37	0.57
24:Y:32:LEU:HD12	24:Y:35:ILE:HD12	1.86	0.57
3:c:426:LEU:HD22	31:c:503:CLA:HED2	1.87	0.57
27:1:162:THR:HA	27:1:166:LYS:HB2	1.87	0.57
27:8:154:GLY:O	27:8:157:SER:OG	2.23	0.57
27:16:93:ASN:HA	27:16:100:THR:HA	1.86	0.57
27:18:155:TRP:HA	27:18:162:THR:HG21	1.87	0.57
2:B:5:TRP:HE1	36:L:101:LHG:HC5	1.68	0.57
3:c:391:ARG:NH2	17:q:152:TYR:OH	2.38	0.57
26:0:32:GLY:HA3	26:0:168:LEU:HD23	1.87	0.57
27:4:204:HIS:HB3	36:4:317:LHG:H172	1.86	0.57
34:A:408:SQD:O9	4:D:230:ASN:ND2	2.33	0.57
37:J:101:LMG:HO4	37:K:101:LMG:HO5	1.51	0.57
33:y:101:BCR:HC21	25:z:13:VAL:HG13	1.86	0.57
27:3:35:ASN:ND2	27:3:57:GLN:OE1	2.37	0.57
27:4:107:GLY:O	43:4:304:A86:O2	2.23	0.57
27:15:38:GLY:HA3	27:15:171:LEU:HD23	1.85	0.57
27:16:153:PHE:CE2	31:16:313:CLA:H3A	2.28	0.57
27:18:143:VAL:HG12	27:18:145:ASP:H	1.70	0.57
3:C:416:SER:HB3	21:V:42:VAL:HG23	1.85	0.57
34:b:601:SQD:H371	38:b:622:DGD:HBE1	1.86	0.57
28:9:62:THR:HA	28:9:69:THR:HA	1.85	0.57
27:13:68:LEU:HD21	27:13:167:ARG:HH22	1.70	0.57
27:14:193:LEU:O	27:14:197:ALA:N	2.38	0.57
16:p:12:SER:OG	16:p:15:LEU:O	2.22	0.57
27:4:148:ASN:H	31:4:312:CLA:HBA2	1.69	0.57
27:14:175:ARG:CB	43:14:301:A86:C23	2.82	0.57
27:15:119:LEU:HD23	27:15:122:LEU:HD12	1.87	0.57
2:B:68:ARG:HB3	2:B:267:LEU:HD21	1.87	0.57
38:C:520:DGD:O2D	10:J:32:SER:O	2.22	0.57
1:a:140:ARG:HH11	4:d:222:LEU:HD12	1.70	0.57
4:d:192:THR:HG23	31:d:405:CLA:HBC2	1.86	0.57
5:e:65:LEU:HB2	7:g:66:ARG:HH12	1.69	0.57
37:k:101:LMG:HC62	17:q:97:TYR:HD1	1.68	0.57
34:L:102:SQD:H272	31:b:615:CLA:H143	1.87	0.56
1:a:328:ILE:HG23	4:d:321:LEU:HD22	1.85	0.56
15:o:247:LYS:HZ1	15:o:260:ALA:HB2	1.69	0.56
27:4:151:ILE:HG22	27:4:154:GLY:HA2	1.85	0.56
3:C:343:ARG:HD2	15:O:165:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:129:GLN:NE2	32:d:403:PHO:OBD	2.37	0.56
24:y:35:ILE:HD11	25:z:21:VAL:HA	1.87	0.56
27:18:117:ALA:HA	27:18:120:PHE:HD2	1.70	0.56
3:C:191:PRO:HD2	17:Q:179:GLU:HG2	1.87	0.56
1:a:45:THR:HG22	32:a:405:PHO:H71	1.87	0.56
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.88	0.56
33:b:618:BCR:H372	37:m:101:LMG:H332	1.86	0.56
3:c:199:ILE:HG13	3:c:234:ILE:HG13	1.86	0.56
3:c:282:MET:HG2	31:c:502:CLA:H72	1.87	0.56
15:o:128:LYS:H	15:o:336:GLU:HB2	1.70	0.56
31:p:606:CLA:HAA2	27:15:131:VAL:HG11	1.86	0.56
31:z:103:CLA:HED3	31:z:103:CLA:H2A	1.87	0.56
27:14:107:GLY:O	43:14:303:A86:O2	2.22	0.56
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.88	0.56
2:b:325:PHE:O	12:l:38:ASN:ND2	2.38	0.56
37:f:102:LMG:O4	37:f:102:LMG:O5	2.21	0.56
27:8:117:ALA:HA	27:8:120:PHE:HD2	1.71	0.56
20:U:51:VAL:O	20:U:96:ARG:NH1	2.39	0.56
2:b:179:GLN:HE22	8:h:78:ILE:HA	1.71	0.56
1:a:24:THR:O	4:d:251:ARG:NH2	2.39	0.56
1:A:328:ILE:HG23	4:D:321:LEU:HD22	1.86	0.56
31:b:602:CLA:HAC1	33:h:101:BCR:H383	1.87	0.56
4:d:155:SER:HA	4:d:159:LEU:HB2	1.88	0.56
16:p:38:GLY:HA3	27:18:48:PRO:HB2	1.86	0.56
27:5:131:VAL:HA	27:5:137:ILE:HD11	1.87	0.56
27:5:183:ALA:O	27:5:187:HIS:ND1	2.29	0.56
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.88	0.56
1:A:215:HIS:ND1	35:A:409:PL9:O1	2.34	0.56
3:C:426:LEU:HD22	31:C:503:CLA:HED2	1.87	0.56
3:C:320:ARG:NH1	21:V:49:ASN:OD1	2.39	0.56
22:W:108:MET:HE3	22:W:112:ALA:HB2	1.87	0.56
2:b:326:ARG:HH12	2:b:442:VAL:HG13	1.71	0.56
22:w:108:MET:HE3	22:w:112:ALA:HB2	1.87	0.56
27:3:148:ASN:HB2	27:3:151:ILE:HG23	1.86	0.56
2:B:349:LYS:NZ	2:B:395:VAL:O	2.38	0.56
27:4:66:VAL:O	27:4:70:HIS:ND1	2.28	0.56
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.88	0.55
3:C:191:PRO:HB3	17:Q:147:LEU:HD21	1.88	0.55
2:b:68:ARG:HB3	2:b:267:LEU:HD21	1.87	0.55
27:4:93:ASN:HA	27:4:100:THR:HA	1.87	0.55
27:16:89:ARG:NH1	27:16:101:PHE:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HE3	1:A:298:ASN:HA	1.88	0.55
1:A:331:MET:HE1	4:D:347:PRO:HB2	1.87	0.55
3:C:187:ASP:HB3	3:C:190:ALA:HB2	1.89	0.55
36:D:408:LHG:HC32	12:L:16:THR:HG21	1.87	0.55
1:a:215:HIS:ND1	35:a:409:PL9:O1	2.34	0.55
3:c:233:VAL:O	3:c:237:HIS:ND1	2.37	0.55
1:A:45:THR:HG22	32:A:405:PHO:H71	1.87	0.55
1:A:140:ARG:HH11	4:D:222:LEU:HD12	1.70	0.55
2:B:275:TRP:HB2	2:B:318:ASN:HD21	1.71	0.55
6:F:44:GLN:HG2	10:J:35:GLY:HA2	1.89	0.55
27:4:166:LYS:NZ	42:4:313:KC1:O2A	2.39	0.55
27:6:42:PRO:HG3	31:6:308:CLA:HAB	1.87	0.55
27:14:67:GLU:OE2	27:14:175:ARG:NE	2.32	0.55
1:A:24:THR:O	4:D:251:ARG:NH2	2.40	0.55
4:D:155:SER:HA	4:D:159:LEU:HB2	1.88	0.55
2:b:275:TRP:HB2	2:b:318:ASN:HD21	1.71	0.55
31:c:502:CLA:HBB1	31:c:502:CLA:H71	1.88	0.55
27:3:57:GLN:O	27:3:61:ASP:N	2.38	0.55
27:14:81:TYR:CE1	27:14:85:LYS:HE3	2.42	0.55
15:O:128:LYS:H	15:O:336:GLU:HB2	1.70	0.55
24:Y:45:ARG:HH11	25:Z:30:PRO:HG2	1.72	0.55
27:3:148:ASN:HA	31:3:313:CLA:HBA2	1.87	0.55
2:B:179:GLN:HE22	8:H:78:ILE:HA	1.72	0.55
4:D:254:SER:HB2	19:T:24:ARG:HH22	1.72	0.55
15:O:99:SER:H	15:O:102:GLN:HE21	1.55	0.55
1:a:334:ARG:HH12	15:o:248:GLY:HA2	1.71	0.55
5:e:56:PHE:HB2	21:v:1:ILE:HG21	1.87	0.55
27:4:81:TYR:CZ	27:4:184:LEU:HD11	2.42	0.55
27:17:35:ASN:ND2	27:17:57:GLN:OE1	2.40	0.55
27:18:42:PRO:HG2	27:18:43:LEU:HD12	1.88	0.55
2:b:349:LYS:NZ	2:b:395:VAL:O	2.38	0.55
27:7:93:ASN:HA	27:7:100:THR:HA	1.87	0.55
26:10:31:LEU:HB2	26:10:64:ARG:HH21	1.71	0.55
27:13:111:LEU:HD12	27:13:114:ILE:HD12	1.89	0.55
28:19:36:GLU:OE2	28:19:145:ARG:NE	2.30	0.55
31:A:404:CLA:HED2	31:A:404:CLA:H2A	1.89	0.55
3:C:342:MET:HE1	3:C:356:MET:HB3	1.89	0.55
31:C:504:CLA:H142	31:C:504:CLA:H51	1.89	0.55
27:3:106:ASP:HB3	27:3:193:LEU:HD11	1.88	0.55
27:4:62:ARG:NH2	45:4:308:KC2:O2D	2.36	0.55
11:K:33:PRO:HG3	24:Y:17:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:128:PHE:O	27:5:133:VAL:N	2.38	0.55
2:B:452:THR:HG23	4:D:291:LEU:HD22	1.89	0.55
1:a:293:MET:HE3	1:a:298:ASN:HA	1.88	0.55
3:c:375:LEU:HB3	3:c:380:ILE:HD11	1.89	0.55
31:c:504:CLA:H142	31:c:504:CLA:H51	1.89	0.55
16:P:77:VAL:HG12	31:P:604:CLA:HAB	1.89	0.54
1:a:331:MET:HE1	4:d:347:PRO:HB2	1.89	0.54
15:o:99:SER:H	15:o:102:GLN:HE21	1.55	0.54
16:p:77:VAL:HG12	31:p:604:CLA:HAB	1.88	0.54
27:1:150:PHE:O	27:1:152:ASP:N	2.37	0.54
27:2:193:LEU:HD12	27:2:196:ASP:H	1.72	0.54
27:4:40:GLN:NE2	27:4:172:ASN:HD21	2.06	0.54
43:4:303:A86:C41	43:4:303:A86:C28	2.85	0.54
3:C:78:GLU:OE2	21:V:106:SER:OG	2.21	0.54
3:C:375:LEU:HB3	3:C:380:ILE:HD11	1.89	0.54
2:b:422:ARG:NH1	15:o:256:ASP:OD2	2.40	0.54
20:u:38:LYS:HA	21:v:61:LEU:HD13	1.89	0.54
27:1:111:LEU:HD12	27:1:114:ILE:HD12	1.90	0.54
27:4:67:GLU:HG2	27:4:171:LEU:HD11	1.89	0.54
43:18:305:A86:C12	43:18:305:A86:C22	2.86	0.54
3:C:282:MET:HG2	31:C:502:CLA:H72	1.87	0.54
31:C:502:CLA:HBB1	31:C:502:CLA:H71	1.88	0.54
3:c:187:ASP:HB3	3:c:190:ALA:HB2	1.89	0.54
20:u:51:VAL:O	20:u:96:ARG:NH1	2.39	0.54
3:c:342:MET:HE1	3:c:356:MET:HB3	1.89	0.54
31:w:203:CLA:H152	31:w:203:CLA:H72	1.90	0.54
43:14:301:A86:C19	43:14:301:A86:C22	2.86	0.54
27:17:165:LYS:HZ3	27:18:146:PHE:HD1	1.53	0.54
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.90	0.54
20:U:51:VAL:HG13	20:U:96:ARG:HB3	1.89	0.54
31:p:602:CLA:H52	44:p:612:DD6:C22	2.37	0.54
27:3:89:ARG:NH1	27:3:101:PHE:O	2.40	0.54
43:13:306:A86:C17	43:14:302:A86:O4	2.52	0.54
2:B:490:VAL:HG12	4:D:136:VAL:HG13	1.90	0.54
31:B:601:CLA:HAC1	33:H:101:BCR:H383	1.89	0.54
37:f:102:LMG:H231	37:f:102:LMG:H341	1.90	0.54
27:4:81:TYR:CE1	27:4:85:LYS:HE3	2.43	0.54
27:6:93:ASN:HA	27:6:100:THR:HA	1.87	0.54
27:11:52:VAL:HG11	27:11:60:PHE:HD1	1.73	0.54
3:c:256:PRO:HA	31:c:507:CLA:HED3	1.88	0.54
11:k:29:ALA:O	11:k:32:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:89:ARG:NH1	27:7:101:PHE:O	2.39	0.54
17:Q:139:GLU:OE1	17:Q:142:ASN:ND2	2.41	0.54
3:c:114:VAL:HG22	37:c:521:LMG:H132	1.89	0.54
2:B:11:VAL:HG13	2:B:12:VAL:HG23	1.88	0.54
37:F:102:LMG:H231	37:F:102:LMG:H341	1.90	0.54
15:O:247:LYS:HZ1	15:O:260:ALA:HB2	1.72	0.54
15:O:313:SER:OG	15:O:314:ASP:N	2.40	0.54
31:a:404:CLA:HED2	31:a:404:CLA:H2A	1.89	0.54
26:0:41:ASP:OD1	26:0:44:GLY:N	2.34	0.54
33:A:407:BCR:H401	38:b:622:DGD:HG31	1.91	0.54
38:B:621:DGD:O5E	38:B:621:DGD:O4E	2.24	0.54
3:C:256:PRO:HA	31:C:507:CLA:HED3	1.88	0.54
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.90	0.54
3:c:78:GLU:OE2	21:v:106:SER:OG	2.23	0.54
3:c:402:GLY:HA3	3:c:420:VAL:HG22	1.90	0.54
27:8:52:VAL:HG11	27:8:60:PHE:HD1	1.72	0.54
27:16:93:ASN:O	43:16:303:A86:O3	2.26	0.54
11:K:29:ALA:O	11:K:32:ASN:ND2	2.41	0.53
31:W:202:CLA:H152	31:W:202:CLA:H72	1.90	0.53
27:14:67:GLU:HG2	27:14:171:LEU:HD11	1.91	0.53
27:16:161:GLU:OE1	27:17:148:ASN:ND2	2.41	0.53
27:18:62:ARG:HH12	45:18:308:KC2:CGA	2.20	0.53
27:18:88:ILE:HG12	36:18:315:LHG:H171	1.89	0.53
3:C:233:VAL:O	3:C:237:HIS:ND1	2.37	0.53
4:d:70:GLY:HA2	10:j:36:LEU:HD13	1.88	0.53
20:u:51:VAL:HG13	20:u:96:ARG:HB3	1.89	0.53
27:4:91:PRO:HD2	37:4:316:LMG:H291	1.91	0.53
15:O:161:MET:HB2	15:O:196:THR:HG23	1.90	0.53
2:b:156:PHE:O	2:b:163:GLY:N	2.39	0.53
7:g:68:ARG:HH22	7:g:146:ASP:HB3	1.73	0.53
27:1:193:LEU:HD12	27:1:195:TYR:H	1.73	0.53
27:6:120:PHE:O	27:6:124:ALA:N	2.38	0.53
27:8:193:LEU:HD12	27:8:196:ASP:H	1.73	0.53
27:17:93:ASN:O	43:17:303:A86:O3	2.27	0.53
33:B:617:BCR:H372	37:M:101:LMG:H332	1.90	0.53
3:C:114:VAL:HG22	37:C:522:LMG:H132	1.90	0.53
2:b:11:VAL:HG13	2:b:12:VAL:HG23	1.90	0.53
3:c:191:PRO:HD2	17:q:179:GLU:HG2	1.90	0.53
3:c:449:ARG:HH22	9:i:28:PRO:HG3	1.73	0.53
27:2:89:ARG:NH1	27:2:101:PHE:O	2.38	0.53
27:3:126:ILE:O	27:3:130:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:54:ASP:OD1	27:4:56:ASN:ND2	2.42	0.53
27:18:137:ILE:HG21	31:18:311:CLA:H2A	1.90	0.53
7:G:68:ARG:HH22	7:G:146:ASP:HB3	1.72	0.53
27:4:89:ARG:NH2	27:4:106:ASP:OD1	2.36	0.53
26:10:162:LYS:HG2	26:10:166:ILE:CD1	2.39	0.53
27:16:191:ILE:HG22	27:16:192:PRO:HD2	1.89	0.53
27:5:40:GLN:NE2	27:5:172:ASN:HD21	2.07	0.53
27:8:62:ARG:HH12	45:8:309:KC2:CGA	2.22	0.53
1:A:57:PRO:HB2	1:A:66:PRO:HB2	1.91	0.53
11:K:28:TYR:HE1	25:Z:9:THR:HG21	1.74	0.53
2:b:18:ARG:HD2	2:b:115:TRP:CE3	2.44	0.53
6:f:41:GLN:HG3	10:j:27:LEU:HD23	1.90	0.53
27:3:62:ARG:HH12	45:3:309:KC2:CGA	2.21	0.53
27:7:148:ASN:HA	31:7:313:CLA:HBA2	1.90	0.53
27:16:193:LEU:HD12	27:16:196:ASP:H	1.73	0.53
21:V:81:THR:OG1	21:V:83:ASP:OD1	2.26	0.53
1:a:57:PRO:HD2	15:o:204:ARG:HH12	1.73	0.53
27:5:130:GLU:HG2	31:5:311:CLA:NB	2.24	0.53
27:11:121:GLN:NE2	37:11:301:LMG:O7	2.42	0.53
27:18:60:PHE:HZ	27:18:64:ARG:HH11	1.57	0.53
2:B:122:LEU:O	8:H:27:ASN:ND2	2.38	0.53
15:O:306:VAL:HG22	15:O:330:ILE:HG22	1.91	0.53
27:8:39:ALA:HB2	27:8:175:ARG:HH12	1.72	0.53
26:10:145:UNK:HA	31:10:314:CLA:HAA2	1.91	0.53
27:14:193:LEU:HD12	27:14:196:ASP:H	1.74	0.53
2:B:326:ARG:HH12	2:B:442:VAL:HG13	1.73	0.53
2:b:452:THR:HG23	4:d:291:LEU:HD22	1.89	0.53
2:b:490:VAL:HG12	4:d:136:VAL:HG13	1.90	0.53
15:o:249:ARG:NH1	15:o:278:ASN:OD1	2.34	0.53
27:1:89:ARG:NH1	27:1:101:PHE:O	2.42	0.53
15:o:161:MET:HB2	15:o:196:THR:HG23	1.90	0.52
17:q:139:GLU:OE1	17:q:142:ASN:ND2	2.41	0.52
27:2:119:LEU:HD23	27:2:122:LEU:HD12	1.91	0.52
11:K:42:PRO:HA	11:K:45:PHE:HD2	1.74	0.52
2:b:378:ARG:NH1	7:g:157:ILE:O	2.43	0.52
2:b:453:TYR:HE1	4:d:288:GLY:HA2	1.73	0.52
26:0:163:LYS:HG2	26:0:166:ILE:HD12	1.90	0.52
26:0:190:SER:O	26:0:194:UNK:N	2.43	0.52
27:1:148:ASN:HA	31:1:313:CLA:HBA2	1.91	0.52
27:11:166:LYS:HA	27:11:169:ILE:HG12	1.90	0.52
43:18:302:A86:C39	43:18:302:A86:C35	2.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:PHE:O	2:B:163:GLY:N	2.37	0.52
38:b:622:DGD:O5E	38:b:622:DGD:O4E	2.25	0.52
26:0:71:GLY:N	26:0:175:GLN:HE21	2.07	0.52
27:1:60:PHE:HA	27:1:63:LEU:HD12	1.91	0.52
26:10:31:LEU:HB2	26:10:64:ARG:NH2	2.23	0.52
27:11:175:ARG:NH2	31:11:308:CLA:O1D	2.41	0.52
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.45	0.52
2:B:23:HIS:ND1	31:B:615:CLA:OBD	2.40	0.52
16:p:67:ALA:O	16:p:71:HIS:ND1	2.28	0.52
31:6:308:CLA:C2B	27:7:133:VAL:HG21	2.40	0.52
2:B:443:PHE:HE2	15:O:262:PRO:HG2	1.75	0.52
3:C:449:ARG:HH22	9:I:28:PRO:HG3	1.73	0.52
12:L:34:SER:HA	12:L:37:PHE:HD2	1.74	0.52
16:P:42:VAL:HG11	27:8:46:PHE:HD1	1.74	0.52
1:a:57:PRO:HB2	1:a:66:PRO:HB2	1.91	0.52
2:b:464:PHE:HD2	31:b:612:CLA:HAC2	1.75	0.52
25:z:5:ILE:HG23	25:z:54:ILE:HD11	1.91	0.52
3:c:191:PRO:HB3	17:q:147:LEU:HD21	1.92	0.52
31:3:316:CLA:HBD	31:3:316:CLA:H171	1.91	0.52
43:4:303:A86:C40	43:4:303:A86:C35	2.86	0.52
31:13:310:CLA:HED2	31:13:310:CLA:H2A	1.90	0.52
4:d:123:ILE:HD11	38:h:102:DGD:HAH2	1.92	0.52
15:o:313:SER:OG	15:o:314:ASP:N	2.40	0.52
27:5:40:GLN:HG3	31:5:306:CLA:HED3	1.92	0.52
27:5:119:LEU:HD23	27:5:122:LEU:HD12	1.92	0.52
27:7:106:ASP:HB3	27:7:193:LEU:HD22	1.90	0.52
27:7:172:ASN:ND2	31:7:307:CLA:O1D	2.39	0.52
28:9:142:ASN:ND2	31:9:307:CLA:O1D	2.43	0.52
2:b:482:ILE:HD12	2:b:486:VAL:HG21	1.91	0.52
27:13:89:ARG:NH1	27:13:101:PHE:O	2.42	0.52
43:15:305:A86:O3	45:15:308:KC2:O1A	2.27	0.52
1:A:85:SER:HA	1:A:109:GLY:HA3	1.91	0.52
12:L:33:SER:OG	12:L:34:SER:N	2.42	0.52
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.90	0.52
2:b:5:TRP:HE1	36:l:102:LHG:HC5	1.75	0.52
31:b:609:CLA:HBA1	37:d:409:LMG:H111	1.92	0.52
11:k:42:PRO:HA	11:k:45:PHE:HD2	1.74	0.52
27:1:185:MET:HE2	31:1:316:CLA:HHB	1.92	0.52
27:17:39:ALA:HB2	27:17:175:ARG:HH12	1.75	0.52
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.43	0.52
2:B:482:ILE:HD12	2:B:486:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:5:ILE:HG23	25:Z:54:ILE:HD11	1.91	0.52
2:b:311:PHE:O	2:b:317:ASN:ND2	2.43	0.52
12:l:33:SER:OG	12:l:34:SER:N	2.42	0.52
24:y:45:ARG:HH11	25:z:30:PRO:HG2	1.75	0.52
27:13:75:MET:HE1	31:13:313:CLA:HBB1	1.92	0.52
12:L:9:GLN:O	37:M:101:LMG:O3	2.28	0.51
12:l:34:SER:HA	12:l:37:PHE:HD2	1.74	0.51
18:r:52:UNK:HA	27:11:138:THR:HG21	1.92	0.51
27:5:192:PRO:HB2	27:5:197:ALA:HA	1.91	0.51
27:16:39:ALA:HB2	27:16:175:ARG:HH12	1.75	0.51
27:18:130:GLU:HG2	31:18:311:CLA:NB	2.25	0.51
2:B:102:ILE:HG12	38:B:621:DGD:HBF2	1.92	0.51
2:B:273:TYR:OH	4:D:164:GLN:O	2.23	0.51
2:b:170:ASP:OD2	2:b:175:THR:OG1	2.27	0.51
4:d:22:LEU:HD12	4:d:23:LYS:HG3	1.92	0.51
4:d:193:LEU:O	12:l:35:TYR:OH	2.23	0.51
11:k:35:VAL:HA	11:k:38:MET:HE2	1.92	0.51
15:o:306:VAL:HG22	15:o:330:ILE:HG22	1.91	0.51
27:8:166:LYS:HA	27:8:169:ILE:HG12	1.91	0.51
4:D:22:LEU:HD12	4:D:23:LYS:HG3	1.92	0.51
1:a:85:SER:HA	1:a:109:GLY:HA3	1.91	0.51
27:8:166:LYS:NZ	42:8:314:KC1:O1A	2.43	0.51
1:A:269:ARG:HH21	4:D:243:THR:HB	1.75	0.51
2:B:170:ASP:OD2	2:B:175:THR:OG1	2.27	0.51
31:B:611:CLA:H71	36:L:101:LHG:H292	1.92	0.51
27:14:47:ASP:OD2	27:14:51:LEU:N	2.43	0.51
27:16:94:ILE:N	27:16:99:THR:O	2.40	0.51
2:B:453:TYR:HE1	4:D:288:GLY:HA2	1.74	0.51
1:a:269:ARG:HH21	4:d:243:THR:HB	1.75	0.51
27:2:126:ILE:O	27:2:130:GLU:N	2.43	0.51
37:F:102:LMG:O4	37:F:102:LMG:O5	2.21	0.51
7:G:70:LEU:HD21	7:G:167:PHE:HB2	1.93	0.51
27:3:93:ASN:HA	27:3:100:THR:HA	1.93	0.51
27:3:111:LEU:HD12	27:3:114:ILE:HD12	1.93	0.51
28:9:110:ALA:HB1	28:9:115:ASP:HB3	1.92	0.51
26:10:41:ASP:OD1	26:10:44:GLY:N	2.35	0.51
1:A:22:THR:HB	1:A:136:ARG:HE	1.76	0.51
12:L:33:SER:HB2	12:L:37:PHE:HE2	1.76	0.51
21:V:112:LEU:HD23	21:V:115:ILE:HD12	1.92	0.51
2:b:341:LEU:HB3	2:b:406:LEU:HD12	1.92	0.51
4:d:250:ASN:HD21	19:t:27:PRO:HG3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:224:LYS:HG2	15:o:227:PHE:HB2	1.92	0.51
27:4:37:LEU:HB2	27:4:64:ARG:HH11	1.75	0.51
37:4:316:LMG:H111	37:4:316:LMG:H292	1.93	0.51
27:16:37:LEU:HD13	27:16:167:ARG:HG3	1.92	0.51
27:17:81:TYR:OH	27:17:193:LEU:O	2.28	0.51
27:18:93:ASN:HA	27:18:100:THR:HA	1.92	0.51
27:7:117:ALA:HA	27:7:120:PHE:HD2	1.75	0.51
27:12:52:VAL:HG11	27:12:60:PHE:HD1	1.75	0.51
27:12:151:ILE:O	27:12:151:ILE:HG22	2.10	0.51
31:Z:101:CLA:H2	31:Z:101:CLA:HMA1	1.92	0.51
1:a:22:THR:HB	1:a:136:ARG:HE	1.76	0.51
3:c:453:ALA:O	9:i:33:ASN:ND2	2.44	0.51
21:v:112:LEU:HD23	21:v:115:ILE:HD12	1.92	0.51
27:1:150:PHE:CE2	27:2:151:ILE:CD1	2.94	0.51
43:5:305:A86:O3	45:5:308:KC2:O1A	2.28	0.51
26:10:71:GLY:N	26:10:175:GLN:HE21	2.09	0.51
27:13:62:ARG:NH2	31:13:312:CLA:O1A	2.44	0.51
27:13:111:LEU:HG	31:13:316:CLA:HBC2	1.93	0.51
27:18:40:GLN:O	27:18:44:GLY:N	2.36	0.51
1:A:77:ILE:HD13	12:L:30:VAL:HG13	1.93	0.51
24:Y:44:GLN:HG3	25:Z:29:THR:HG23	1.93	0.51
2:b:326:ARG:NH2	4:d:297:ASP:OD1	2.44	0.51
3:c:302:TYR:HB2	3:c:423:ARG:HH21	1.75	0.51
27:17:64:ARG:HH12	31:17:308:CLA:CGD	2.24	0.51
27:17:117:ALA:HA	27:17:120:PHE:HD2	1.76	0.51
2:B:382:PRO:HG2	2:B:385:ARG:HG2	1.92	0.50
3:C:416:SER:OG	21:V:34:ASN:OD1	2.29	0.50
11:K:35:VAL:HA	11:K:38:MET:HE2	1.92	0.50
2:b:24:LEU:HA	2:b:27:THR:HG22	1.93	0.50
4:d:152:VAL:HG21	4:d:279:LEU:HD22	1.94	0.50
15:o:158:SER:OG	15:o:198:GLN:O	2.29	0.50
27:11:111:LEU:HD12	27:11:114:ILE:HD12	1.93	0.50
27:11:165:LYS:HZ2	27:12:146:PHE:HD1	1.58	0.50
15:O:224:LYS:HG2	15:O:227:PHE:HB2	1.92	0.50
26:0:178:ILE:HG23	26:0:179:LEU:HD12	1.93	0.50
27:3:42:PRO:HG3	31:3:307:CLA:HAB	1.93	0.50
31:8:310:CLA:H2A	31:8:310:CLA:HED2	1.92	0.50
27:12:193:LEU:O	27:12:197:ALA:N	2.44	0.50
27:16:126:ILE:O	27:16:130:GLU:N	2.44	0.50
2:B:24:LEU:HA	2:B:27:THR:HG22	1.93	0.50
2:B:464:PHE:HD2	31:B:611:CLA:HAC2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:158:SER:OG	15:O:198:GLN:O	2.29	0.50
4:d:282:SER:OG	31:d:405:CLA:O1D	2.30	0.50
27:6:106:ASP:HB3	27:6:193:LEU:HD22	1.93	0.50
37:11:317:LMG:HO4	37:11:317:LMG:HO5	1.58	0.50
27:17:89:ARG:NH1	27:17:101:PHE:O	2.39	0.50
37:M:101:LMG:HC61	13:m:30:GLU:HB3	1.93	0.50
16:P:38:GLY:HA3	27:8:48:PRO:HB2	1.94	0.50
2:b:192:PRO:HG3	8:h:61:TYR:CD1	2.46	0.50
3:c:186:TYR:OH	3:c:300:GLU:OE2	2.23	0.50
31:c:505:CLA:C4D	38:c:519:DGD:HB51	2.37	0.50
31:d:402:CLA:H91	35:d:407:PL9:H402	1.93	0.50
35:d:407:PL9:H412	12:l:30:VAL:HG11	1.91	0.50
27:2:65:TYR:HA	27:2:68:LEU:HD12	1.92	0.50
26:10:66:VAL:O	26:10:70:HIS:ND1	2.27	0.50
27:11:136:ASP:O	27:11:138:THR:N	2.45	0.50
27:18:34:GLU:HG3	27:18:35:ASN:H	1.77	0.50
1:A:114:LEU:O	1:A:118:HIS:ND1	2.38	0.50
2:B:311:PHE:O	2:B:317:ASN:ND2	2.43	0.50
3:C:215:ARG:HG2	3:C:221:ASP:HB3	1.94	0.50
3:C:457:LYS:NZ	4:D:227:ASP:O	2.37	0.50
4:D:282:SER:OG	31:D:405:CLA:O1D	2.30	0.50
12:l:33:SER:HB2	12:l:37:PHE:HE2	1.76	0.50
26:0:145:UNK:HA	31:0:314:CLA:HAA2	1.94	0.50
27:11:162:THR:HA	27:11:166:LYS:HB2	1.93	0.50
27:15:192:PRO:HB2	27:15:196:ASP:HB3	1.92	0.50
1:A:27:ARG:NH2	19:T:21:VAL:O	2.44	0.50
2:B:341:LEU:HB3	2:B:406:LEU:HD12	1.92	0.50
3:C:302:TYR:HB2	3:C:423:ARG:HH21	1.75	0.50
31:C:505:CLA:H93	38:C:520:DGD:HB92	1.94	0.50
5:E:56:PHE:HB2	21:V:1:ILE:HG21	1.93	0.50
5:E:65:LEU:HB2	7:G:66:ARG:HH12	1.76	0.50
18:R:52:UNK:HA	27:1:138:THR:HG21	1.93	0.50
3:c:215:ARG:HG2	3:c:221:ASP:HB3	1.94	0.50
27:1:121:GLN:NE2	37:1:301:LMG:O7	2.44	0.50
27:1:150:PHE:CZ	31:1:313:CLA:H121	2.47	0.50
27:2:72:ARG:HB3	31:2:312:CLA:HAC2	1.94	0.50
27:5:131:VAL:HG12	27:5:137:ILE:HD11	1.93	0.50
27:6:39:ALA:HB2	27:6:175:ARG:HH12	1.76	0.50
27:8:106:ASP:HB3	27:8:193:LEU:HD22	1.93	0.50
2:B:357:ARG:HH22	7:G:62:ALA:HB2	1.77	0.50
10:J:23:THR:HG22	37:J:101:LMG:H232	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:162:PHE:CD2	31:b:607:CLA:HHD	2.47	0.50
27:16:120:PHE:O	27:16:124:ALA:N	2.39	0.50
6:F:44:GLN:HE22	17:Q:81:ALA:HB2	1.76	0.50
1:a:58:VAL:HB	1:a:83:VAL:HG21	1.94	0.50
1:a:114:LEU:O	1:a:118:HIS:ND1	2.39	0.50
2:b:156:PHE:HB3	2:b:162:PHE:HB3	1.94	0.50
3:c:83:GLU:OE2	21:v:103:ARG:NH1	2.44	0.50
3:c:320:ARG:NH1	21:v:49:ASN:OD1	2.45	0.50
7:g:70:LEU:HD21	7:g:167:PHE:HB2	1.93	0.50
15:o:145:VAL:HG21	15:o:154:LYS:HD3	1.93	0.50
35:D:407:PL9:H202	36:D:408:LHG:H142	1.94	0.50
2:b:122:LEU:O	8:h:27:ASN:ND2	2.38	0.50
27:3:76:LEU:HA	27:3:79:VAL:HG12	1.94	0.50
27:5:126:ILE:O	27:5:130:GLU:N	2.44	0.50
1:A:258:LEU:O	4:D:128:ARG:NH1	2.42	0.49
31:D:402:CLA:H91	35:D:407:PL9:H402	1.94	0.49
5:e:13:ILE:HD13	41:e:101:HEM:HAD1	1.94	0.49
5:e:23:HIS:NE2	41:e:101:HEM:ND	2.60	0.49
15:o:162:THR:HG21	15:o:195:THR:HA	1.94	0.49
23:x:96:VAL:O	23:x:100:VAL:N	2.41	0.49
27:3:57:GLN:HA	27:3:60:PHE:HB3	1.93	0.49
27:4:40:GLN:HE21	27:4:172:ASN:HD21	1.59	0.49
27:5:193:LEU:HD12	27:5:194:GLY:H	1.77	0.49
1:A:183:MET:HE1	31:D:405:CLA:HBB1	1.94	0.49
36:C:521:LHG:H322	36:C:521:LHG:H161	1.94	0.49
31:W:202:CLA:H51	31:W:202:CLA:H203	1.94	0.49
31:c:505:CLA:H93	38:c:520:DGD:HB92	1.94	0.49
4:d:344:GLU:HB3	7:g:179:ARG:NH2	2.27	0.49
27:11:64:ARG:HH21	27:11:171:LEU:HD11	1.77	0.49
27:14:201:ILE:O	27:14:203:GLY:N	2.45	0.49
2:B:192:PRO:HG3	8:H:61:TYR:CD1	2.46	0.49
3:c:286:ALA:HA	3:c:289:TYR:HD2	1.77	0.49
27:2:76:LEU:HA	27:2:79:VAL:HG12	1.93	0.49
27:3:169:ILE:O	27:3:173:GLN:N	2.36	0.49
27:11:90:LEU:HD13	37:11:317:LMG:H292	1.93	0.49
27:13:57:GLN:O	27:13:61:ASP:N	2.41	0.49
5:E:36:LEU:HA	5:E:39:SER:HB3	1.95	0.49
15:O:145:VAL:HG21	15:O:154:LYS:HD3	1.93	0.49
31:w:203:CLA:H203	31:w:203:CLA:H51	1.94	0.49
25:z:29:THR:HG22	25:z:32:GLU:H	1.77	0.49
27:6:42:PRO:HG2	27:6:43:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:18:48:PRO:CG	43:18:303:A86:O4	2.60	0.49
27:18:81:TYR:CE1	27:18:85:LYS:HE3	2.47	0.49
31:B:608:CLA:HBA1	37:D:409:LMG:H111	1.93	0.49
8:H:63:SER:HB2	8:H:72:VAL:HG21	1.94	0.49
1:a:136:ARG:NH2	9:i:27:ASP:OD1	2.43	0.49
35:d:407:PL9:H202	36:d:408:LHG:H142	1.94	0.49
36:w:202:LHG:H322	36:w:202:LHG:H161	1.94	0.49
27:1:146:PHE:HB3	27:4:165:LYS:NZ	2.27	0.49
27:3:117:ALA:HA	27:3:120:PHE:HD2	1.76	0.49
27:7:64:ARG:HH12	31:7:308:CLA:CGD	2.25	0.49
27:8:159:ASP:OD1	27:8:160:GLU:N	2.46	0.49
31:14:306:CLA:O2D	31:14:306:CLA:H2A	2.11	0.49
4:D:152:VAL:HG21	4:D:279:LEU:HD22	1.94	0.49
16:P:1:PRO:HG3	27:8:55:GLY:HA2	1.93	0.49
27:1:189:LYS:NZ	43:1:306:A86:O	2.36	0.49
27:2:64:ARG:HH12	31:2:307:CLA:CGD	2.25	0.49
27:4:193:LEU:O	27:4:197:ALA:N	2.45	0.49
27:7:39:ALA:HB2	27:7:175:ARG:HH12	1.78	0.49
27:11:68:LEU:HD11	27:11:167:ARG:HH12	1.77	0.49
27:11:150:PHE:CE2	27:12:151:ILE:HD12	2.05	0.49
15:O:232:ASP:HB3	15:O:286:GLN:HE21	1.78	0.49
27:1:175:ARG:NH2	31:1:308:CLA:O1D	2.40	0.49
27:12:111:LEU:HD12	27:12:114:ILE:HD12	1.95	0.49
43:18:305:A86:C19	43:18:305:A86:C23	2.85	0.49
28:19:38:LYS:NZ	28:19:99:GLU:OE1	2.46	0.49
2:B:323:GLY:HA2	4:D:294:ARG:H	1.78	0.49
3:C:83:GLU:OE2	21:V:103:ARG:NH1	2.45	0.49
21:V:126:ALA:HB1	21:V:129:LYS:HB2	1.95	0.49
21:v:126:ALA:HB1	21:v:129:LYS:HB2	1.95	0.49
27:8:93:ASN:HA	27:8:100:THR:HA	1.94	0.49
1:A:15:GLU:OE1	22:W:123:ARG:NE	2.46	0.49
31:C:509:CLA:HED2	31:C:509:CLA:H2A	1.95	0.49
37:K:101:LMG:H132	24:Y:25:LEU:HD11	1.95	0.49
1:a:183:MET:HB3	31:a:403:CLA:HBC2	1.95	0.49
2:b:443:PHE:HE2	15:o:262:PRO:HG2	1.77	0.49
7:g:78:LEU:HD23	7:g:90:ILE:HD13	1.95	0.49
8:h:63:SER:HB2	8:h:72:VAL:HG21	1.94	0.49
17:q:146:GLU:HG2	17:q:149:ARG:HH22	1.78	0.49
27:7:165:LYS:HD2	27:8:146:PHE:HB3	1.95	0.49
27:18:166:LYS:HA	27:18:169:ILE:HG12	1.94	0.49
28:19:110:ALA:HB1	28:19:115:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:SER:HA	7:G:179:ARG:HH22	1.78	0.49
31:B:612:CLA:H61	31:B:612:CLA:H102	1.59	0.49
3:c:99:ILE:HD11	3:c:103:GLY:HA2	1.94	0.49
27:8:109:ALA:HB2	34:8:301:SQD:H3	1.94	0.49
26:10:178:ILE:HG23	26:10:179:LEU:HD12	1.94	0.49
31:C:503:CLA:H62	31:C:503:CLA:H41	1.54	0.48
27:4:126:ILE:O	27:4:130:GLU:N	2.44	0.48
27:5:107:GLY:O	43:5:303:A86:O2	2.31	0.48
27:17:75:MET:HE1	31:17:313:CLA:HBB1	1.94	0.48
31:18:309:CLA:HED2	31:18:309:CLA:H2A	1.94	0.48
2:B:318:ASN:HB2	2:B:321:LYS:HB2	1.95	0.48
3:C:286:ALA:HA	3:C:289:TYR:HD2	1.77	0.48
17:Q:146:GLU:HG2	17:Q:149:ARG:HH22	1.78	0.48
5:e:74:GLN:HB2	7:g:99:LEU:HD21	1.95	0.48
27:4:85:LYS:HZ3	27:4:106:ASP:HB3	1.78	0.48
37:10:319:LMG:HC91	31:18:311:CLA:HAA1	1.94	0.48
27:13:64:ARG:HH21	27:13:171:LEU:HD11	1.78	0.48
27:14:169:ILE:HG22	31:14:306:CLA:CGD	2.43	0.48
27:17:152:ASP:OD1	27:17:153:PHE:N	2.46	0.48
1:A:58:VAL:HB	1:A:83:VAL:HG21	1.94	0.48
1:A:305:SER:HA	10:J:39:SER:HB3	1.93	0.48
3:C:217:PRO:HD2	37:W:201:LMG:HC91	1.94	0.48
15:O:176:THR:OG1	15:O:183:THR:OG1	2.31	0.48
1:a:127:MET:HE2	1:a:127:MET:HB3	1.66	0.48
27:2:161:GLU:HG3	27:2:165:LYS:HE2	1.95	0.48
3:C:99:ILE:HD11	3:C:103:GLY:HA2	1.94	0.48
37:C:522:LMG:O5	37:C:522:LMG:O4	2.29	0.48
21:V:55:ASP:O	21:V:59:LEU:N	2.46	0.48
21:V:99:ASP:O	21:V:105:ARG:NH2	2.45	0.48
2:b:273:TYR:OH	4:d:164:GLN:O	2.23	0.48
31:1:308:CLA:H62	31:1:308:CLA:H122	1.95	0.48
31:2:309:CLA:H3A	31:2:309:CLA:HBA1	1.55	0.48
27:4:69:LYS:HE3	27:4:73:ILE:HD11	1.94	0.48
37:14:316:LMG:H201	37:14:316:LMG:H382	1.96	0.48
27:18:107:GLY:O	43:18:303:A86:O2	2.31	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.48
7:G:78:LEU:HD23	7:G:90:ILE:HD13	1.95	0.48
7:G:123:PHE:HA	7:G:126:ILE:HG12	1.95	0.48
15:O:104:LYS:HG2	22:W:93:ARG:NH1	2.23	0.48
1:a:183:MET:HE1	31:d:405:CLA:HBB1	1.95	0.48
2:b:382:PRO:HG2	2:b:385:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:9:GLN:O	37:m:101:LMG:O3	2.29	0.48
27:3:119:LEU:HD23	27:3:122:LEU:HD12	1.95	0.48
27:5:93:ASN:HA	27:5:100:THR:HA	1.96	0.48
27:6:65:TYR:HA	27:6:68:LEU:HD12	1.95	0.48
4:D:262:SER:N	36:D:408:LHG:O5	2.41	0.48
38:H:102:DGD:O5D	38:H:102:DGD:O4D	2.27	0.48
1:a:198:HIS:HA	1:a:286:THR:HG22	1.96	0.48
31:c:509:CLA:HED2	31:c:509:CLA:H2A	1.95	0.48
5:e:10:PHE:HB2	6:f:19:ARG:HH22	1.78	0.48
15:o:232:ASP:HB3	15:o:286:GLN:HE21	1.78	0.48
1:A:102:VAL:HG21	34:A:411:SQD:H462	1.96	0.48
2:B:162:PHE:CD2	31:B:606:CLA:HHD	2.47	0.48
5:E:13:ILE:HD13	41:E:101:HEM:HAD1	1.96	0.48
1:a:273:PHE:CZ	36:a:410:LHG:HC92	2.49	0.48
2:b:23:HIS:ND1	31:b:616:CLA:OBD	2.39	0.48
2:b:323:GLY:HA2	4:d:294:ARG:H	1.78	0.48
27:18:43:LEU:HD23	27:18:46:PHE:CG	2.47	0.48
3:C:195:ASP:HB2	17:Q:155:ARG:HD3	1.95	0.48
15:O:162:THR:HG21	15:O:195:THR:HA	1.94	0.48
17:Q:127:ARG:HB2	17:Q:151:MET:HE3	1.95	0.48
41:V:201:HEM:HHA	41:V:201:HEM:HBA2	1.96	0.48
31:b:615:CLA:H2	31:b:615:CLA:H8	1.96	0.48
3:c:396:MET:HE1	21:v:48:THR:HA	1.96	0.48
31:1:321:CLA:CGD	27:4:169:ILE:HG22	2.44	0.48
31:11:316:CLA:HHC	31:11:316:CLA:HBB1	1.96	0.48
27:12:158:PHE:HB3	27:12:161:GLU:HB3	1.95	0.48
27:14:182:LEU:HB3	31:14:314:CLA:HBC2	1.96	0.48
27:15:125:PHE:O	27:15:129:LEU:N	2.45	0.48
3:C:396:MET:HE1	21:V:48:THR:HA	1.95	0.48
16:P:6:TRP:NE1	27:8:48:PRO:O	2.44	0.48
16:P:126:MET:HG2	31:P:606:CLA:HMC2	1.95	0.48
4:d:193:LEU:HD11	4:d:315:TYR:HE1	1.79	0.48
27:2:117:ALA:HA	27:2:120:PHE:HD2	1.78	0.48
27:11:161:GLU:OE2	27:12:148:ASN:ND2	2.47	0.48
27:15:108:PHE:CE2	27:15:185:MET:HA	2.48	0.48
43:15:304:A86:C26	31:15:312:CLA:HAB	2.44	0.48
27:17:76:LEU:HA	27:17:79:VAL:HG12	1.95	0.48
34:L:102:SQD:H322	19:T:16:VAL:HG22	1.96	0.48
16:P:20:ALA:HB1	16:P:24:LEU:HD12	1.96	0.48
1:a:89:ILE:O	1:a:92:HIS:ND1	2.29	0.48
2:b:112:ILE:HG12	33:b:618:BCR:H271	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:339:LYS:HD3	20:u:98:ASN:HD22	1.79	0.48
3:c:406:SER:HA	3:c:420:VAL:HG23	1.96	0.48
3:c:457:LYS:NZ	4:d:227:ASP:O	2.37	0.48
15:o:102:GLN:HE22	17:q:188:LYS:NZ	2.11	0.48
20:u:79:TYR:HD1	20:u:82:ARG:HD3	1.79	0.48
37:0:317:LMG:O10	31:8:312:CLA:H3A	2.13	0.48
27:4:182:LEU:HB3	31:4:314:CLA:HBC2	1.96	0.48
27:15:57:GLN:O	27:15:61:ASP:N	2.37	0.48
31:A:403:CLA:H201	36:D:408:LHG:H321	1.96	0.47
35:D:407:PL9:H401	36:D:408:LHG:H212	1.96	0.47
12:L:13:LEU:H	13:M:29:THR:HG21	1.79	0.47
16:P:9:SER:HB2	16:P:19:ARG:HB3	1.96	0.47
7:g:123:PHE:HA	7:g:126:ILE:HG12	1.95	0.47
27:5:88:ILE:HG23	37:5:315:LMG:H151	1.95	0.47
27:14:172:ASN:HA	27:14:175:ARG:HB2	1.96	0.47
27:17:119:LEU:HD23	27:17:122:LEU:HD12	1.95	0.47
27:18:42:PRO:HG3	31:18:306:CLA:CAB	2.44	0.47
28:19:21:VAL:HG11	28:19:29:PHE:HD1	1.78	0.47
5:E:23:HIS:NE2	41:E:101:HEM:ND	2.62	0.47
1:a:84:PRO:HB2	1:a:169:SER:HA	1.96	0.47
31:a:403:CLA:H201	36:d:408:LHG:H321	1.96	0.47
34:b:601:SQD:H383	38:b:622:DGD:HBN2	1.96	0.47
34:l:101:SQD:H322	19:t:16:VAL:HG22	1.96	0.47
31:z:101:CLA:H2	31:z:101:CLA:HMA1	1.94	0.47
27:1:42:PRO:HD3	31:1:307:CLA:HMB1	1.95	0.47
27:1:68:LEU:HD11	27:1:167:ARG:HH12	1.79	0.47
27:1:150:PHE:CD2	31:1:313:CLA:H41	2.48	0.47
31:3:313:CLA:H12	31:3:313:CLA:H3A	1.95	0.47
27:7:166:LYS:HA	27:7:169:ILE:HG12	1.96	0.47
31:14:311:CLA:HBA1	31:14:311:CLA:H3A	1.62	0.47
1:A:183:MET:HB3	31:A:403:CLA:HBC2	1.94	0.47
5:e:36:LEU:HA	5:e:39:SER:HB3	1.95	0.47
15:o:176:THR:OG1	15:o:183:THR:OG1	2.31	0.47
27:1:153:PHE:CD2	31:1:313:CLA:H43	2.48	0.47
43:19:305:A86:O3	45:19:309:KC2:O1A	2.32	0.47
20:U:79:TYR:HD1	20:U:82:ARG:HD3	1.79	0.47
1:a:92:HIS:CD2	22:w:93:ARG:HD3	2.49	0.47
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.26	0.47
16:p:42:VAL:HG11	27:18:46:PHE:HD1	1.79	0.47
17:q:127:ARG:HB2	17:q:151:MET:HE3	1.95	0.47
21:v:99:ASP:O	21:v:105:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:111:LEU:HD12	27:4:114:ILE:HD12	1.97	0.47
27:5:138:THR:OG1	27:5:139:GLY:N	2.48	0.47
31:5:307:CLA:H62	31:5:307:CLA:H41	1.63	0.47
31:11:312:CLA:HBB1	31:11:312:CLA:HHC	1.95	0.47
1:A:198:HIS:HA	1:A:286:THR:HG22	1.96	0.47
1:A:212:SER:HB2	4:D:211:CYS:HB2	1.97	0.47
4:D:193:LEU:HD11	4:D:315:TYR:HE1	1.79	0.47
1:a:91:MET:HE1	1:a:163:ILE:HA	1.95	0.47
37:d:404:LMG:H292	37:d:409:LMG:HC92	1.96	0.47
6:f:44:GLN:HE22	17:q:81:ALA:HB2	1.80	0.47
12:l:24:LEU:HD12	36:l:102:LHG:H132	1.96	0.47
16:p:9:SER:HB2	16:p:19:ARG:HB3	1.96	0.47
16:p:20:ALA:HB1	16:p:24:LEU:HD12	1.95	0.47
27:1:93:ASN:O	43:1:303:A86:O3	2.31	0.47
27:5:65:TYR:CZ	27:5:142:PHE:HA	2.49	0.47
27:14:89:ARG:NH2	27:14:106:ASP:OD1	2.36	0.47
28:19:6:LEU:O	28:19:33:ARG:NH2	2.47	0.47
1:A:328:ILE:HD11	4:D:325:ILE:HD11	1.96	0.47
1:a:258:LEU:O	4:d:128:ARG:NH1	2.44	0.47
2:b:318:ASN:HB2	2:b:321:LYS:HB2	1.95	0.47
37:c:521:LMG:O5	37:c:521:LMG:O4	2.30	0.47
5:e:65:LEU:HB2	7:g:66:ARG:NH1	2.29	0.47
10:j:36:LEU:H	10:j:36:LEU:HG	1.52	0.47
37:4:316:LMG:H352	37:4:316:LMG:H322	1.61	0.47
28:9:6:LEU:O	28:9:33:ARG:NH2	2.48	0.47
27:11:135:LYS:HB3	27:11:137:ILE:HG12	1.96	0.47
27:17:126:ILE:O	27:17:130:GLU:N	2.48	0.47
2:B:174:ILE:HD11	2:B:309:LEU:HD12	1.97	0.47
2:B:392:ILE:HD12	2:B:418:LYS:HG2	1.97	0.47
10:J:36:LEU:H	10:J:36:LEU:HG	1.52	0.47
11:K:55:ALA:HB1	24:Y:40:ILE:HD11	1.95	0.47
12:L:24:LEU:HD12	36:L:101:LHG:H132	1.96	0.47
2:b:243:SER:HB3	2:b:466:HIS:CE1	2.50	0.47
2:b:399:VAL:HB	2:b:411:PHE:HB2	1.96	0.47
34:b:601:SQD:H351	38:b:622:DGD:HBH1	1.96	0.47
3:c:317:PHE:HA	3:c:320:ARG:HG2	1.97	0.47
16:p:126:MET:HG2	31:p:606:CLA:HMC2	1.95	0.47
20:u:28:ILE:HD11	20:u:62:LEU:HD13	1.97	0.47
21:v:55:ASP:O	21:v:59:LEU:N	2.46	0.47
26:0:190:SER:HB3	26:0:193:PRO:HD2	1.97	0.47
27:2:39:ALA:HB2	27:2:175:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:183:ALA:C	27:5:187:HIS:HD1	2.21	0.47
27:6:62:ARG:HH12	45:6:310:KC2:CGA	2.28	0.47
27:7:111:LEU:HD12	27:7:114:ILE:HD12	1.96	0.47
27:8:126:ILE:O	27:8:130:GLU:N	2.48	0.47
28:9:21:VAL:HG11	28:9:29:PHE:HD1	1.80	0.47
37:11:317:LMG:H322	37:11:317:LMG:H291	1.69	0.47
27:14:117:ALA:HA	27:14:120:PHE:HD2	1.79	0.47
31:15:307:CLA:H62	31:15:307:CLA:H41	1.61	0.47
27:17:194:GLY:HA2	27:17:197:ALA:HB3	1.97	0.47
3:C:453:ALA:O	9:I:33:ASN:ND2	2.48	0.47
7:G:150:LEU:HD13	7:G:173:ALA:H	1.79	0.47
25:Z:32:GLU:O	25:Z:36:SER:OG	2.29	0.47
2:b:392:ILE:HD12	2:b:418:LYS:HG2	1.97	0.47
41:v:201:HEM:HHA	41:v:201:HEM:HBA2	1.96	0.47
27:2:111:LEU:HD12	27:2:114:ILE:HD12	1.97	0.47
1:A:18:CYS:HB2	22:W:123:ARG:HH22	1.78	0.47
1:A:91:MET:HE1	1:A:163:ILE:HA	1.95	0.47
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.97	0.47
4:D:113:PHE:O	4:D:117:HIS:ND1	2.40	0.47
27:1:64:ARG:HH21	27:1:171:LEU:HD11	1.79	0.47
31:4:312:CLA:HED3	31:4:312:CLA:H2A	1.96	0.47
27:13:93:ASN:HA	27:13:100:THR:HA	1.96	0.47
27:18:82:LEU:HD13	43:18:305:A86:C9	2.44	0.47
1:A:84:PRO:HB2	1:A:169:SER:HA	1.96	0.47
1:A:195:HIS:HD2	1:A:196:PRO:HD2	1.80	0.47
2:B:11:VAL:HG11	31:B:614:CLA:HED2	1.97	0.47
31:P:601:CLA:H3A	3:c:253:PHE:CE1	2.50	0.47
3:c:387:TRP:NE1	17:q:149:ARG:O	2.35	0.47
27:6:158:PHE:HE2	27:6:162:THR:N	2.13	0.47
27:8:53:GLU:OE1	27:8:53:GLU:N	2.41	0.47
27:8:190:LEU:HB2	27:8:191:ILE:HD12	1.97	0.47
28:19:41:ARG:NE	28:19:140:GLU:OE2	2.47	0.47
1:A:257:ARG:O	4:D:128:ARG:NH2	2.48	0.46
2:B:251:VAL:HG22	31:B:602:CLA:H92	1.97	0.46
33:B:617:BCR:H313	37:B:620:LMG:H322	1.96	0.46
3:C:317:PHE:HA	3:C:320:ARG:HG2	1.97	0.46
4:D:338:ASN:HD21	7:G:66:ARG:HD2	1.81	0.46
5:E:64:PRO:HB2	5:E:79:LEU:HD13	1.97	0.46
16:P:74:ILE:HD13	31:P:606:CLA:HBC3	1.97	0.46
35:d:407:PL9:H401	36:d:408:LHG:H212	1.96	0.46
16:p:188:VAL:HG11	44:p:612:DD6:C24	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:CZ	36:A:410:LHG:HC92	2.49	0.46
2:B:87:ASN:HD22	34:i:101:SQD:H61	1.80	0.46
2:B:112:ILE:HG12	33:B:617:BCR:H271	1.96	0.46
2:B:248:ALA:HB2	31:B:603:CLA:H61	1.97	0.46
2:B:399:VAL:HB	2:B:411:PHE:HB2	1.96	0.46
38:B:621:DGD:HBF1	34:B:623:SQD:H351	1.98	0.46
3:C:324:LEU:HD13	20:U:33:ILE:HD13	1.98	0.46
1:a:212:SER:HB2	4:d:211:CYS:HB2	1.97	0.46
33:y:101:BCR:H20C	33:y:101:BCR:H361	1.82	0.46
26:10:81:TYR:CD2	26:10:181:LEU:HD21	2.50	0.46
27:12:126:ILE:O	27:12:130:GLU:N	2.48	0.46
1:A:202:VAL:HG23	31:A:403:CLA:HMB2	1.97	0.46
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.51	0.46
31:B:607:CLA:H161	31:B:607:CLA:H141	1.74	0.46
1:a:84:PRO:HA	1:a:112:TYR:CG	2.51	0.46
1:a:202:VAL:HG23	31:a:403:CLA:HMB2	1.97	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.95	0.46
38:1:318:DGD:HB92	38:1:318:DGD:HB61	1.64	0.46
37:15:315:LMG:H142	37:15:315:LMG:H112	1.81	0.46
1:A:195:HIS:ND1	1:A:293:MET:SD	2.89	0.46
3:C:339:LYS:HD3	20:U:98:ASN:HD22	1.79	0.46
2:b:98:LEU:HD21	38:b:622:DGD:HBW1	1.97	0.46
4:d:103:ARG:HH21	5:e:77:GLU:HG2	1.81	0.46
27:7:76:LEU:HA	27:7:79:VAL:HG12	1.97	0.46
28:9:38:LYS:NZ	28:9:99:GLU:OE1	2.46	0.46
31:10:308:CLA:H2A	31:10:308:CLA:HED3	1.97	0.46
27:11:93:ASN:HA	27:11:100:THR:HA	1.98	0.46
1:A:127:MET:HE2	1:A:127:MET:HB3	1.66	0.46
31:A:406:CLA:H122	37:W:201:LMG:H162	1.98	0.46
3:C:197:ARG:HE	17:Q:179:GLU:CD	2.24	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.96	0.46
16:P:153:GLN:NE2	16:P:165:TYR:O	2.44	0.46
31:b:616:CLA:H152	31:b:616:CLA:H112	1.79	0.46
12:l:13:LEU:H	13:m:29:THR:HG21	1.80	0.46
27:4:147:ARG:HA	27:4:148:ASN:HA	1.67	0.46
27:5:68:LEU:HD11	27:5:167:ARG:NH1	2.31	0.46
27:7:62:ARG:HH12	45:7:309:KC2:CGA	2.28	0.46
43:9:305:A86:O3	45:9:309:KC2:O1A	2.33	0.46
31:11:307:CLA:HBA1	27:12:134:MET:HA	1.98	0.46
31:13:313:CLA:HBA1	31:13:313:CLA:H12	1.80	0.46
27:16:62:ARG:HH12	45:16:309:KC2:CGA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:16:310:CLA:HED2	31:16:310:CLA:H2A	1.98	0.46
2:B:243:SER:HB3	2:B:466:HIS:CE1	2.50	0.46
2:B:258:TYR:OH	4:D:162:LEU:O	2.27	0.46
2:B:332:LYS:HA	2:B:437:LEU:HD11	1.97	0.46
1:a:195:HIS:HD2	1:a:196:PRO:HD2	1.80	0.46
1:a:257:ARG:O	4:d:128:ARG:NH2	2.48	0.46
31:b:612:CLA:H71	36:l:102:LHG:H292	1.97	0.46
3:c:324:LEU:HD13	20:u:33:ILE:HD13	1.97	0.46
3:c:416:SER:OG	21:v:34:ASN:OD1	2.33	0.46
31:c:503:CLA:H62	31:c:503:CLA:H41	1.54	0.46
7:g:150:LEU:HD13	7:g:173:ALA:H	1.79	0.46
15:o:241:GLY:HA3	15:o:252:THR:HG23	1.98	0.46
27:12:151:ILE:O	27:12:151:ILE:CG2	2.63	0.46
27:14:111:LEU:HD12	27:14:114:ILE:HD12	1.98	0.46
1:A:40:THR:HG21	1:A:121:LEU:HB2	1.98	0.46
2:B:192:PRO:HG3	8:H:61:TYR:HD1	1.80	0.46
1:a:40:THR:HG21	1:a:121:LEU:HB2	1.98	0.46
1:a:246:TYR:OH	40:d:401:BCT:O2	2.34	0.46
2:b:357:ARG:HH22	7:g:62:ALA:HB2	1.81	0.46
16:p:74:ILE:HD13	31:p:606:CLA:HBC3	1.97	0.46
27:2:62:ARG:HH12	45:2:308:KC2:CGA	2.28	0.46
31:2:306:CLA:O2D	31:2:306:CLA:H2A	2.15	0.46
27:3:134:MET:O	27:3:147:ARG:NH2	2.49	0.46
27:5:57:GLN:O	27:5:61:ASP:N	2.35	0.46
27:7:119:LEU:HD23	27:7:122:LEU:HD12	1.97	0.46
27:7:169:ILE:O	27:7:173:GLN:N	2.34	0.46
1:A:103:ASP:OD1	38:b:622:DGD:O2D	2.23	0.46
2:B:18:ARG:NH2	12:L:5:ASN:HD21	2.14	0.46
13:M:30:GLU:HB3	37:m:101:LMG:HC61	1.97	0.46
15:O:241:GLY:HA3	15:O:252:THR:HG23	1.98	0.46
2:b:155:ALA:O	2:b:159:THR:OG1	2.33	0.46
2:b:226:TYR:CD1	2:b:231:MET:HB2	2.50	0.46
4:d:52:THR:HG23	4:d:78:VAL:HG23	1.98	0.46
27:13:193:LEU:HD12	27:13:196:ASP:H	1.81	0.46
27:15:179:MET:HE2	31:15:307:CLA:HMC2	1.98	0.46
31:19:313:CLA:H91	31:19:313:CLA:H111	1.78	0.46
34:B:623:SQD:H252	19:t:18:PHE:HE1	1.80	0.46
4:D:193:LEU:O	12:L:35:TYR:OH	2.32	0.46
4:D:336:HIS:CD2	4:D:337:GLU:HG3	2.51	0.46
21:V:60:SER:HA	21:V:65:ARG:HG3	1.97	0.46
1:a:195:HIS:ND1	1:a:293:MET:SD	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:304:GLN:HG2	1:a:313:VAL:HG11	1.97	0.46
5:e:64:PRO:HB2	5:e:79:LEU:HD13	1.97	0.46
11:k:34:ILE:HA	24:y:24:VAL:HG11	1.97	0.46
13:m:28:GLN:HE21	13:m:32:ARG:HH21	1.64	0.46
27:2:169:ILE:HG22	31:2:306:CLA:CGD	2.46	0.46
27:2:172:ASN:ND2	31:2:306:CLA:O1D	2.44	0.46
31:2:315:CLA:HAC1	31:2:315:CLA:HHD	1.51	0.46
27:5:37:LEU:HD21	27:5:167:ARG:HG3	1.96	0.46
27:7:152:ASP:CG	27:8:151:ILE:HB	2.41	0.46
31:7:307:CLA:O2D	31:7:307:CLA:H2A	2.16	0.46
27:8:52:VAL:O	27:8:54:ASP:N	2.48	0.46
26:10:26:ALA:C	26:10:164:ARG:NH1	2.74	0.46
27:17:192:PRO:HB2	27:17:196:ASP:HB3	1.96	0.46
43:17:302:A86:O	31:17:307:CLA:HAC2	2.16	0.46
1:A:27:ARG:HB3	34:b:601:SQD:H442	1.98	0.46
2:B:384:ARG:HA	15:O:253:THR:HG22	1.98	0.46
2:b:251:VAL:HG22	31:b:603:CLA:H92	1.97	0.46
2:b:332:LYS:HA	2:b:437:LEU:HD11	1.98	0.46
27:4:148:ASN:N	31:4:312:CLA:HBA2	2.30	0.46
27:7:193:LEU:HD12	27:7:196:ASP:H	1.81	0.46
26:10:62:ARG:NH2	45:10:310:KC2:O2D	2.46	0.46
27:17:57:GLN:O	27:17:61:ASP:N	2.49	0.46
27:17:169:ILE:O	27:17:173:GLN:N	2.35	0.46
32:D:403:PHO:H3A	31:D:405:CLA:H142	1.96	0.45
9:I:7:LEU:O	9:I:10:THR:OG1	2.28	0.45
20:U:28:ILE:HD11	20:U:62:LEU:HD13	1.97	0.45
4:d:254:SER:HB2	19:t:24:ARG:HH12	1.81	0.45
27:2:75:MET:HE1	31:2:312:CLA:HBB1	1.97	0.45
27:3:64:ARG:HH12	31:3:308:CLA:CGD	2.28	0.45
27:18:169:ILE:HG22	31:18:306:CLA:CGD	2.47	0.45
31:18:306:CLA:H2A	31:18:306:CLA:O2D	2.15	0.45
1:A:32:TRP:CD2	9:I:22:GLY:HA3	2.51	0.45
33:B:618:BCR:HC41	37:B:620:LMG:H342	1.97	0.45
38:B:621:DGD:HG31	33:a:407:BCR:H401	1.97	0.45
15:O:182:ILE:HB	15:O:227:PHE:HZ	1.81	0.45
2:b:174:ILE:HD11	2:b:309:LEU:HD12	1.97	0.45
2:b:248:ALA:HB2	31:b:604:CLA:H61	1.97	0.45
3:c:68:VAL:HG21	31:c:504:CLA:HED2	1.98	0.45
3:c:335:THR:HA	15:o:239:ARG:HH11	1.81	0.45
4:d:113:PHE:O	4:d:117:HIS:ND1	2.40	0.45
4:d:303:LEU:O	4:d:306:ALA:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:336:HIS:CD2	4:d:337:GLU:HG3	2.51	0.45
32:d:403:PHO:H3A	31:d:405:CLA:H142	1.97	0.45
37:4:316:LMG:H401	37:4:316:LMG:H212	1.98	0.45
31:9:308:CLA:H62	31:9:308:CLA:H41	1.62	0.45
27:11:149:GLY:H	31:11:313:CLA:CGA	2.29	0.45
27:15:111:LEU:HD12	27:15:114:ILE:HD12	1.99	0.45
13:M:28:GLN:HE21	13:M:32:ARG:HH21	1.64	0.45
15:O:198:GLN:HE21	15:O:202:GLY:HA2	1.82	0.45
2:b:22:VAL:HG13	31:b:615:CLA:HMB2	1.99	0.45
3:c:217:PRO:HD2	37:w:201:LMG:HC91	1.97	0.45
3:c:273:SER:O	3:c:441:HIS:ND1	2.40	0.45
15:o:122:LYS:HG2	15:o:222:THR:HG22	1.99	0.45
21:v:60:SER:HA	21:v:65:ARG:HG3	1.97	0.45
26:0:65:TYR:OH	26:0:135:ARG:NH2	2.49	0.45
27:5:194:GLY:HA2	27:5:197:ALA:HB3	1.98	0.45
27:6:133:VAL:HG12	27:6:134:MET:HG3	1.98	0.45
27:7:158:PHE:CE1	27:8:155:TRP:HD1	2.34	0.45
1:a:106:LEU:HD11	33:a:407:BCR:H402	1.98	0.45
1:a:245:THR:O	4:d:265:ARG:NH2	2.50	0.45
1:a:328:ILE:HD11	4:d:325:ILE:HD11	1.97	0.45
31:a:406:CLA:H122	37:w:201:LMG:H162	1.98	0.45
33:c:517:BCR:H24C	33:c:517:BCR:H371	1.75	0.45
20:u:34:ARG:NH2	21:v:51:ASN:OD1	2.48	0.45
31:2:315:CLA:HBB1	31:2:315:CLA:HHC	1.99	0.45
27:3:77:ALA:HA	31:3:310:CLA:HAB	1.99	0.45
31:12:310:CLA:HED2	31:12:310:CLA:H2A	1.99	0.45
27:17:72:ARG:NH2	27:17:145:ASP:OD2	2.40	0.45
34:B:623:SQD:H442	1:a:27:ARG:HB3	1.98	0.45
31:C:503:CLA:H2	31:C:504:CLA:H193	1.98	0.45
38:C:519:DGD:HA22	10:J:29:ILE:HG21	1.97	0.45
15:O:326:LEU:HD21	15:O:328:LYS:HE3	1.99	0.45
3:c:311:GLN:HE21	3:c:358:PHE:HB2	1.81	0.45
31:c:503:CLA:H2	31:c:504:CLA:H193	1.98	0.45
8:h:72:VAL:O	38:h:102:DGD:O3E	2.28	0.45
31:6:311:CLA:HED2	31:6:311:CLA:H2A	1.99	0.45
27:18:111:LEU:HD12	27:18:114:ILE:HD12	1.97	0.45
4:D:52:THR:HG23	4:D:78:VAL:HG23	1.98	0.45
9:I:9:TYR:HB3	22:W:109:ARG:NH1	2.28	0.45
31:b:616:CLA:H161	8:h:19:LEU:HD11	1.97	0.45
37:b:621:LMG:H351	13:m:10:ALA:HB1	1.99	0.45
33:c:517:BCR:H15C	33:c:517:BCR:H351	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:406:CLA:H41	31:d:406:CLA:H61	1.64	0.45
16:p:123:PHE:HA	16:p:126:MET:HE2	1.99	0.45
27:5:175:ARG:HA	27:5:178:MET:HE3	1.99	0.45
27:6:75:MET:HE1	31:6:314:CLA:HAB	1.97	0.45
28:9:75:ASN:OD1	28:9:76:GLY:N	2.50	0.45
27:11:150:PHE:C	27:11:152:ASP:H	2.23	0.45
27:17:42:PRO:HG2	27:17:43:LEU:HD12	1.99	0.45
27:17:57:GLN:HA	27:17:60:PHE:HB3	1.99	0.45
27:17:111:LEU:HD12	27:17:114:ILE:HD12	1.97	0.45
31:19:312:CLA:H62	31:19:312:CLA:H41	1.77	0.45
2:B:155:ALA:O	2:B:159:THR:OG1	2.33	0.45
31:B:615:CLA:H112	31:B:615:CLA:H152	1.82	0.45
3:C:311:GLN:HE21	3:C:358:PHE:HB2	1.81	0.45
15:O:122:LYS:HG2	15:O:222:THR:HG22	1.99	0.45
34:i:101:SQD:H81	34:i:101:SQD:H45	1.81	0.45
15:o:129:LEU:HB2	15:o:184:PHE:HE1	1.81	0.45
31:0:311:CLA:H92	31:0:311:CLA:H61	1.81	0.45
27:1:91:PRO:HG2	37:1:317:LMG:HC71	1.98	0.45
27:3:150:PHE:CZ	31:3:313:CLA:H121	2.51	0.45
31:4:311:CLA:HBA1	31:4:311:CLA:H3A	1.63	0.45
31:7:313:CLA:HAA1	31:7:313:CLA:HED3	1.98	0.45
27:8:111:LEU:HD12	27:8:114:ILE:HD12	1.97	0.45
37:14:316:LMG:H401	37:14:316:LMG:H212	1.99	0.45
1:A:84:PRO:HA	1:A:112:TYR:CG	2.51	0.45
31:B:602:CLA:H101	8:H:58:LEU:HD12	1.99	0.45
3:C:68:VAL:HG21	31:C:504:CLA:HED2	1.98	0.45
8:H:72:VAL:O	38:H:102:DGD:O3E	2.28	0.45
16:P:48:PHE:HB3	27:5:132:PHE:HE1	1.81	0.45
1:a:223:LEU:HD23	1:a:246:TYR:HB3	1.99	0.45
2:b:388:SER:HA	7:g:179:ARG:HH22	1.82	0.45
31:b:611:CLA:HHC	31:b:611:CLA:HBB1	1.98	0.45
27:2:153:PHE:HE2	27:3:151:ILE:HB	1.82	0.45
27:3:39:ALA:HB2	27:3:175:ARG:HH12	1.80	0.45
27:5:179:MET:HE2	31:5:307:CLA:HMC2	1.99	0.45
27:8:130:GLU:HG2	31:8:312:CLA:NB	2.32	0.45
27:14:184:LEU:HA	27:14:184:LEU:HD12	1.74	0.45
1:A:106:LEU:HD11	33:A:407:BCR:H402	1.98	0.45
1:A:315:ASN:O	4:D:64:ALA:N	2.46	0.45
4:D:200:GLY:HA3	4:D:282:SER:HB2	1.99	0.45
37:J:101:LMG:H111	37:J:101:LMG:H141	1.54	0.45
16:p:6:TRP:NE1	27:18:48:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:p:602:CLA:H41	31:p:602:CLA:H61	1.79	0.45
27:3:149:GLY:H	31:3:313:CLA:CGA	2.29	0.45
27:5:144:GLY:C	27:5:146:PHE:H	2.23	0.45
31:12:310:CLA:H3A	31:12:310:CLA:HBA1	1.52	0.45
27:13:150:PHE:C	27:13:152:ASP:H	2.24	0.45
27:14:145:ASP:HB2	31:14:312:CLA:OBD	2.16	0.45
27:15:117:ALA:HB1	37:15:315:LMG:H111	1.99	0.45
31:A:403:CLA:H152	32:A:405:PHO:H61	1.99	0.45
2:B:64:PRO:HB3	2:B:267:LEU:HG	1.99	0.45
33:B:618:BCR:H20C	33:B:618:BCR:H361	1.85	0.45
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.52	0.45
31:a:404:CLA:HMD3	4:d:182:LEU:HD11	1.98	0.45
2:b:167:TRP:HD1	2:b:264:PRO:HG3	1.82	0.45
27:6:166:LYS:HA	27:6:169:ILE:HG12	1.98	0.45
27:14:89:ARG:NH1	27:14:101:PHE:O	2.49	0.45
27:16:191:ILE:HD12	27:16:191:ILE:HG23	1.84	0.45
1:A:223:LEU:HD23	1:A:246:TYR:HB3	1.99	0.44
1:A:223:LEU:HB3	4:D:265:ARG:HH12	1.82	0.44
24:Y:17:LEU:O	24:Y:21:ALA:N	2.48	0.44
1:a:77:ILE:HD13	12:l:30:VAL:HG13	1.99	0.44
2:b:192:PRO:HG3	8:h:61:TYR:HD1	1.81	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.44
4:d:330:ALA:HA	4:d:333:ASP:HB3	1.99	0.44
27:2:93:ASN:HA	27:2:100:THR:HA	1.98	0.44
27:6:169:ILE:O	27:6:173:GLN:N	2.35	0.44
27:8:175:ARG:HA	27:8:178:MET:HE3	1.99	0.44
33:A:407:BCR:H20C	33:A:407:BCR:H361	1.81	0.44
2:B:341:LEU:HD21	2:B:431:GLU:HB2	1.99	0.44
4:D:330:ALA:HA	4:D:333:ASP:HB3	1.99	0.44
17:Q:93:PRO:HA	17:Q:101:GLY:HA2	1.99	0.44
23:X:96:VAL:O	23:X:100:VAL:N	2.41	0.44
21:v:5:GLU:O	21:v:9:THR:OG1	2.35	0.44
27:1:153:PHE:CZ	27:2:151:ILE:HG23	2.14	0.44
31:6:314:CLA:HED3	31:6:314:CLA:HBD	1.86	0.44
28:19:58:ARG:HG3	28:19:71:ALA:HA	2.00	0.44
31:19:308:CLA:H41	31:19:308:CLA:H62	1.64	0.44
3:C:335:THR:HA	15:O:239:ARG:HH11	1.83	0.44
2:b:341:LEU:HD21	2:b:431:GLU:HB2	2.00	0.44
4:d:68:LEU:HB2	6:f:40:MET:HE2	1.99	0.44
4:d:262:SER:N	36:d:408:LHG:O5	2.41	0.44
6:f:40:MET:HB3	37:f:102:LMG:HC62	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:101:SQD:H142	34:l:101:SQD:H341	2.00	0.44
37:1:317:LMG:H321	37:1:317:LMG:H352	1.68	0.44
31:5:314:CLA:HHC	31:5:314:CLA:HBB1	1.99	0.44
27:8:46:PHE:CZ	27:8:48:PRO:HG3	2.52	0.44
27:15:72:ARG:HB3	31:15:312:CLA:HAC1	1.98	0.44
27:15:93:ASN:HA	27:15:100:THR:HA	1.99	0.44
27:18:179:MET:HE2	31:18:307:CLA:HMC2	1.99	0.44
28:19:8:ALA:HB2	31:19:308:CLA:HED2	1.99	0.44
28:19:75:ASN:OD1	28:19:76:GLY:N	2.50	0.44
3:C:387:TRP:NE1	17:Q:149:ARG:O	2.40	0.44
37:J:101:LMG:HC62	17:Q:84:THR:HG22	1.98	0.44
21:V:5:GLU:O	21:V:9:THR:OG1	2.35	0.44
31:b:613:CLA:H61	31:b:613:CLA:H102	1.59	0.44
3:c:164:HIS:ND1	31:c:508:CLA:OBD	2.41	0.44
5:e:41:GLY:HA3	17:q:66:VAL:HG21	2.00	0.44
15:o:198:GLN:HE21	15:o:202:GLY:HA2	1.82	0.44
27:1:149:GLY:H	31:1:313:CLA:CGA	2.29	0.44
43:5:304:A86:C26	31:5:312:CLA:HAB	2.47	0.44
37:5:315:LMG:H191	37:5:315:LMG:H302	1.99	0.44
31:8:308:CLA:H62	31:8:308:CLA:H41	1.72	0.44
26:10:27:PHE:HE2	26:10:140:UNK:HA	1.83	0.44
27:11:186:VAL:HG21	31:11:315:CLA:HAC1	1.99	0.44
33:C:516:BCR:H323	31:W:202:CLA:HBB2	1.99	0.44
1:a:223:LEU:HB3	4:d:265:ARG:HH12	1.82	0.44
2:b:299:SER:OG	2:b:407:ASN:OD1	2.35	0.44
2:b:451:TYR:OH	31:b:605:CLA:O2D	2.29	0.44
3:c:342:MET:HE2	3:c:342:MET:HB3	1.69	0.44
15:o:326:LEU:HD21	15:o:328:LYS:HE3	1.99	0.44
27:3:153:PHE:HD1	27:3:162:THR:HB	1.83	0.44
27:5:111:LEU:HD12	27:5:114:ILE:HD12	1.99	0.44
27:12:104:ILE:HG12	27:12:113:LYS:HE2	1.98	0.44
31:15:312:CLA:HED3	31:15:312:CLA:HBD	1.78	0.44
27:16:150:PHE:C	27:16:152:ASP:H	2.25	0.44
43:18:303:A86:C39	43:18:303:A86:C33	2.95	0.44
2:B:167:TRP:HD1	2:B:264:PRO:HG3	1.82	0.44
34:B:623:SQD:H331	34:B:623:SQD:H362	1.88	0.44
5:E:41:GLY:HA3	17:Q:66:VAL:HG21	1.99	0.44
7:G:178:VAL:O	20:U:103:ARG:NH1	2.32	0.44
34:b:601:SQD:H371	38:b:622:DGD:HBH1	2.00	0.44
31:c:504:CLA:H72	31:c:504:CLA:H111	1.79	0.44
31:3:313:CLA:HED3	31:3:313:CLA:HAA1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:150:PHE:C	27:6:152:ASP:H	2.26	0.44
27:7:65:TYR:HA	27:7:68:LEU:HD12	1.99	0.44
28:9:98:LEU:HA	28:9:102:VAL:HB	2.00	0.44
27:12:57:GLN:O	27:12:61:ASP:N	2.38	0.44
27:15:137:ILE:HB	31:15:311:CLA:HMA1	1.99	0.44
27:18:175:ARG:HA	27:18:178:MET:HE3	2.00	0.44
28:19:98:LEU:HA	28:19:102:VAL:HB	1.99	0.44
1:A:245:THR:O	4:D:265:ARG:NH2	2.50	0.44
31:B:604:CLA:H111	31:B:615:CLA:H42	1.99	0.44
38:b:622:DGD:HG32	38:b:622:DGD:HD2	1.54	0.44
31:c:502:CLA:HBC3	31:c:504:CLA:H92	2.00	0.44
7:g:154:ASN:HB2	7:g:157:ILE:HG22	1.99	0.44
11:k:28:TYR:HE1	25:z:9:THR:HG21	1.82	0.44
26:0:36:PRO:HG3	31:0:308:CLA:HBB1	1.99	0.44
27:4:204:HIS:HD2	36:4:317:LHG:H192	1.82	0.44
37:4:316:LMG:H201	37:4:316:LMG:H382	1.99	0.44
26:10:160:GLN:HE21	26:10:164:ARG:HD3	1.82	0.44
1:A:131:TRP:CZ3	31:C:506:CLA:HAA2	2.52	0.44
34:A:411:SQD:H81	34:A:411:SQD:H45	1.81	0.44
31:C:502:CLA:HBC3	31:C:504:CLA:H92	2.00	0.44
31:D:402:CLA:H141	31:D:402:CLA:H161	1.77	0.44
16:P:123:PHE:HA	16:P:126:MET:HE2	1.98	0.44
34:l:101:SQD:H132	34:l:101:SQD:H162	1.67	0.44
27:11:65:TYR:HB2	27:11:141:GLU:HG3	1.99	0.44
27:11:193:LEU:HD12	27:11:196:ASP:H	1.81	0.44
31:15:307:CLA:H172	31:15:307:CLA:H13	1.71	0.44
27:17:62:ARG:HH12	45:17:309:KC2:CGA	2.31	0.44
2:B:367:PRO:O	2:B:425:GLN:NE2	2.50	0.44
15:O:196:THR:HA	15:O:206:PRO:HA	2.00	0.44
31:P:602:CLA:H41	31:P:602:CLA:H61	1.79	0.44
21:V:49:ASN:ND2	41:V:201:HEM:O1D	2.51	0.44
21:V:76:ILE:HD13	21:V:112:LEU:HD22	1.99	0.44
1:a:188:ALA:HB2	1:a:328:ILE:HB	2.00	0.44
31:b:605:CLA:H111	31:b:616:CLA:H42	1.99	0.44
3:c:63:TRP:CH2	31:c:503:CLA:HHB	2.53	0.44
15:o:182:ILE:HB	15:o:227:PHE:HZ	1.81	0.44
43:5:301:A86:O	31:5:306:CLA:HAC2	2.18	0.44
27:11:38:GLY:HA3	27:11:171:LEU:HD22	1.99	0.44
27:11:91:PRO:HD2	37:11:317:LMG:H301	1.99	0.44
43:11:302:A86:O	31:11:307:CLA:HAC2	2.18	0.44
27:12:72:ARG:HB3	31:12:313:CLA:HAC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:VAL:HG13	31:B:614:CLA:HMB2	1.99	0.43
4:D:80:THR:HG22	4:D:111:TRP:CE2	2.53	0.43
5:E:74:GLN:HB2	7:G:99:LEU:HD21	2.00	0.43
31:a:403:CLA:H152	32:a:405:PHO:H61	1.99	0.43
31:b:605:CLA:HAC1	31:b:605:CLA:HHD	1.79	0.43
3:c:423:ARG:HA	3:c:423:ARG:HD3	1.82	0.43
31:c:502:CLA:H202	31:c:502:CLA:H161	1.82	0.43
21:v:49:ASN:ND2	41:v:201:HEM:O1D	2.51	0.43
26:0:26:ALA:O	26:0:164:ARG:NH1	2.48	0.43
27:6:94:ILE:N	27:6:99:THR:O	2.40	0.43
28:9:138:ALA:O	28:9:142:ASN:ND2	2.51	0.43
31:9:310:CLA:H91	31:9:310:CLA:H111	1.78	0.43
27:14:158:PHE:HB3	27:14:161:GLU:HB3	1.99	0.43
31:16:308:CLA:H41	31:16:308:CLA:H62	1.74	0.43
27:18:76:LEU:HA	27:18:79:VAL:HG12	2.00	0.43
2:B:378:ARG:NH1	7:G:157:ILE:O	2.51	0.43
2:B:442:VAL:HG23	15:O:262:PRO:HD2	2.00	0.43
3:C:189:TRP:HH2	3:C:367:GLU:HG3	1.83	0.43
7:G:75:ILE:O	7:G:138:TYR:OH	2.36	0.43
2:b:98:LEU:HD11	38:b:622:DGD:HBT2	1.98	0.43
31:b:604:CLA:HAB	31:b:606:CLA:H152	2.00	0.43
31:b:608:CLA:H11	37:b:621:LMG:H121	2.00	0.43
31:c:506:CLA:H93	31:c:506:CLA:H111	1.83	0.43
31:c:509:CLA:H72	11:k:46:PHE:HZ	1.83	0.43
4:d:200:GLY:HA3	4:d:282:SER:HB2	1.99	0.43
16:p:196:GLN:HB3	36:18:316:LHG:H141	2.01	0.43
27:1:51:LEU:HD13	31:1:308:CLA:H72	1.99	0.43
37:1:301:LMG:H152	37:1:301:LMG:H121	1.82	0.43
27:5:72:ARG:HB3	31:5:312:CLA:HAC1	2.00	0.43
27:6:169:ILE:HG22	31:6:308:CLA:CGD	2.48	0.43
27:7:151:ILE:H	27:7:151:ILE:HG13	1.57	0.43
27:15:148:ASN:HB3	31:15:312:CLA:HBA2	2.00	0.43
31:B:603:CLA:HAB	31:B:605:CLA:H152	2.01	0.43
31:C:502:CLA:H92	31:C:502:CLA:H62	1.81	0.43
7:G:154:ASN:HB2	7:G:157:ILE:HG22	1.99	0.43
16:P:48:PHE:HB3	27:5:132:PHE:CE1	2.53	0.43
24:Y:32:LEU:HA	24:Y:35:ILE:HD12	2.00	0.43
4:d:157:PHE:CE1	4:d:171:PRO:HG2	2.52	0.43
5:e:74:GLN:NE2	7:g:95:ASN:OD1	2.51	0.43
15:o:266:LEU:HD23	15:o:266:LEU:HA	1.85	0.43
31:3:307:CLA:H2A	31:3:307:CLA:O2D	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:37:LEU:HD11	27:6:167:ARG:HG3	2.00	0.43
27:6:119:LEU:HD23	27:6:122:LEU:HD12	2.00	0.43
31:14:306:CLA:HMB3	31:14:306:CLA:HHB	1.58	0.43
31:A:404:CLA:HMD3	4:D:182:LEU:HD11	1.99	0.43
31:B:615:CLA:H161	8:H:19:LEU:HD11	2.00	0.43
3:C:63:TRP:CH2	31:C:503:CLA:HHB	2.53	0.43
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.83	0.43
31:C:505:CLA:C4D	38:C:519:DGD:HB51	2.37	0.43
31:C:507:CLA:H171	31:C:507:CLA:H13	1.79	0.43
1:a:131:TRP:CZ3	31:c:506:CLA:HAA2	2.53	0.43
31:b:603:CLA:H91	31:b:603:CLA:H111	1.79	0.43
37:j:101:LMG:H141	37:j:101:LMG:H111	1.54	0.43
27:13:141:GLU:HG2	27:13:142:PHE:CG	2.52	0.43
43:15:301:A86:O	31:15:306:CLA:HAC2	2.18	0.43
27:16:119:LEU:HD23	27:16:122:LEU:HD12	2.00	0.43
27:18:65:TYR:HB2	27:18:141:GLU:O	2.17	0.43
2:B:443:PHE:CE2	15:O:262:PRO:HG2	2.53	0.43
4:D:12:ARG:NH1	4:D:16:ASP:HB3	2.33	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.99	0.43
34:L:102:SQD:H142	34:L:102:SQD:H341	2.01	0.43
13:M:28:GLN:NE2	37:M:101:LMG:O1	2.51	0.43
37:P:614:LMG:H112	37:P:614:LMG:H141	1.87	0.43
33:h:101:BCR:H24C	33:h:101:BCR:H371	1.84	0.43
25:z:32:GLU:O	25:z:36:SER:OG	2.26	0.43
26:0:65:TYR:O	26:0:68:ILE:N	2.48	0.43
31:3:316:CLA:HHD	31:3:316:CLA:HAC1	1.72	0.43
31:6:309:CLA:H41	31:6:309:CLA:H62	1.79	0.43
43:10:301:A86:O	31:10:308:CLA:HAC2	2.19	0.43
31:12:307:CLA:C2B	27:13:133:VAL:HG21	2.49	0.43
31:17:307:CLA:O2D	31:17:307:CLA:H2A	2.18	0.43
27:18:131:VAL:HG13	27:18:132:PHE:HD1	1.83	0.43
1:A:188:ALA:HB2	1:A:328:ILE:HB	2.00	0.43
3:C:116:VAL:HG11	33:C:515:BCR:HC42	2.00	0.43
15:O:129:LEU:HB2	15:O:184:PHE:HE1	1.82	0.43
1:a:29:TYR:HB2	4:d:255:GLN:HG3	2.01	0.43
1:a:95:PRO:HD2	1:a:98:GLU:HB2	1.99	0.43
2:b:64:PRO:HB3	2:b:267:LEU:HG	2.00	0.43
2:b:96:VAL:O	2:b:100:HIS:ND1	2.48	0.43
3:c:449:ARG:NH2	9:i:28:PRO:HG3	2.33	0.43
38:c:520:DGD:O2D	10:j:32:SER:O	2.35	0.43
31:d:405:CLA:H62	31:d:405:CLA:H101	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:101:BCR:H372	37:f:102:LMG:H292	2.00	0.43
27:1:130:GLU:HG2	31:1:312:CLA:NB	2.34	0.43
27:2:185:MET:HE2	31:2:315:CLA:HMA3	2.00	0.43
27:6:126:ILE:O	27:6:130:GLU:N	2.51	0.43
27:13:34:GLU:N	27:13:36:GLU:OE1	2.51	0.43
1:A:207:GLY:HA3	1:A:278:TRP:HE1	1.83	0.43
34:b:601:SQD:H331	34:b:601:SQD:H362	1.88	0.43
3:c:189:TRP:HH2	3:c:367:GLU:HG3	1.83	0.43
4:d:299:VAL:H	12:l:38:ASN:HB3	1.84	0.43
17:q:93:PRO:HA	17:q:101:GLY:HA2	1.99	0.43
27:2:175:ARG:HB3	31:2:307:CLA:HAC2	2.00	0.43
31:4:309:CLA:H62	31:4:309:CLA:H2	1.85	0.43
31:8:307:CLA:O2D	31:8:307:CLA:H2A	2.18	0.43
26:10:184:HIS:O	26:10:188:GLY:N	2.51	0.43
27:12:76:LEU:HA	27:12:79:VAL:HG12	2.00	0.43
27:15:137:ILE:HD12	31:15:311:CLA:HMA1	2.00	0.43
27:15:191:ILE:H	27:15:191:ILE:HG13	1.40	0.43
2:B:375:GLY:HA3	7:G:65:ASN:HD21	1.83	0.43
3:C:191:PRO:HG2	17:Q:179:GLU:HA	1.99	0.43
38:C:519:DGD:HA41	37:J:101:LMG:H352	2.01	0.43
33:F:101:BCR:H372	37:F:102:LMG:H292	2.00	0.43
31:b:617:CLA:H62	31:b:617:CLA:H101	1.82	0.43
12:l:13:LEU:HD13	13:m:25:LEU:HB2	2.00	0.43
21:v:76:ILE:HD13	21:v:112:LEU:HD22	1.99	0.43
27:2:169:ILE:HD13	27:2:169:ILE:HG21	1.75	0.43
27:4:85:LYS:NZ	27:4:193:LEU:HB2	2.34	0.43
27:8:166:LYS:HE3	27:8:166:LYS:HB3	1.65	0.43
27:11:64:ARG:NH2	27:11:67:GLU:OE1	2.51	0.43
27:15:121:GLN:NE2	37:15:315:LMG:O7	2.51	0.43
33:Y:101:BCR:H24C	33:Y:101:BCR:H371	1.68	0.43
33:h:101:BCR:H20C	33:h:101:BCR:H361	1.85	0.43
27:1:45:PHE:HA	31:1:308:CLA:HED2	2.00	0.43
27:3:169:ILE:HG22	31:3:307:CLA:CGD	2.47	0.43
27:11:133:VAL:C	27:11:135:LYS:H	2.27	0.43
27:15:149:GLY:HA2	43:18:305:A86:C34	2.48	0.43
1:A:246:TYR:OH	40:D:401:BCT:O2	2.34	0.43
1:A:249:VAL:HG12	2:B:490:VAL:HG23	2.01	0.43
2:B:450:TRP:CE2	31:B:607:CLA:HBA1	2.53	0.43
31:B:611:CLA:H111	31:B:611:CLA:H142	1.78	0.43
3:C:119:LEU:O	3:C:122:SER:OG	2.33	0.43
4:D:185:LEU:HD12	31:D:405:CLA:HMD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:250:ASN:HD21	19:T:27:PRO:HG3	1.83	0.43
2:b:450:TRP:CE2	31:b:608:CLA:HBA1	2.54	0.43
38:c:519:DGD:HA41	37:j:101:LMG:H352	2.01	0.43
7:g:153:ILE:HB	7:g:158:GLY:HA2	2.01	0.43
21:v:13:ASP:OD1	21:v:14:ASN:N	2.51	0.43
31:1:321:CLA:H2A	31:1:321:CLA:O2D	2.19	0.43
27:7:42:PRO:HG2	27:7:43:LEU:HD12	2.00	0.43
27:8:169:ILE:HG22	31:8:307:CLA:CGD	2.49	0.43
27:14:81:TYR:CE1	27:14:184:LEU:HD11	2.53	0.43
27:17:94:ILE:HG22	27:17:99:THR:HB	2.01	0.43
31:B:610:CLA:H102	31:B:615:CLA:HAA1	2.01	0.42
16:P:9:SER:O	16:P:19:ARG:NH2	2.32	0.42
4:d:12:ARG:NH1	4:d:16:ASP:HB3	2.33	0.42
15:o:196:THR:HA	15:o:206:PRO:HA	2.00	0.42
21:v:81:THR:OG1	21:v:83:ASP:OD1	2.26	0.42
27:6:111:LEU:HD12	27:6:114:ILE:HD12	2.01	0.42
27:7:192:PRO:HB2	27:7:196:ASP:HB3	2.01	0.42
28:9:58:ARG:HG3	28:9:71:ALA:HA	1.99	0.42
28:9:103:MET:HE1	31:9:310:CLA:H18	2.01	0.42
31:12:308:CLA:H62	31:12:308:CLA:H41	1.71	0.42
31:18:312:CLA:H92	31:18:312:CLA:H61	1.90	0.42
31:B:607:CLA:H11	37:B:620:LMG:H121	2.00	0.42
11:K:48:LEU:HD13	24:Y:32:LEU:HG	2.01	0.42
2:b:341:LEU:HD12	2:b:429:VAL:HG12	2.01	0.42
3:c:95:LEU:HD13	31:c:503:CLA:H143	2.02	0.42
4:d:178:ILE:HD11	32:d:403:PHO:H201	2.01	0.42
10:j:23:THR:HG22	37:j:101:LMG:H232	2.01	0.42
16:p:153:GLN:NE2	16:p:165:TYR:O	2.44	0.42
38:1:318:DGD:O5E	38:1:318:DGD:O4E	2.35	0.42
27:4:81:TYR:CE1	27:4:184:LEU:HD11	2.55	0.42
27:4:117:ALA:HA	27:4:120:PHE:HD2	1.84	0.42
31:11:313:CLA:H61	31:11:313:CLA:H92	1.68	0.42
31:13:316:CLA:H202	31:13:316:CLA:H161	1.84	0.42
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.99	0.42
2:b:367:PRO:O	2:b:425:GLN:NE2	2.52	0.42
31:b:607:CLA:H72	33:b:620:BCR:H311	2.01	0.42
31:b:611:CLA:H102	31:b:616:CLA:HAA1	2.01	0.42
4:d:216:ALA:O	4:d:220:ASN:ND2	2.52	0.42
16:p:37:LEU:HD13	43:18:303:A86:O5	2.19	0.42
20:u:27:ASP:OD1	20:u:28:ILE:N	2.53	0.42
22:w:99:PRO:HG2	37:w:201:LMG:HC71	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:0:301:A86:O	31:0:308:CLA:HAC2	2.19	0.42
27:1:133:VAL:O	27:1:135:LYS:N	2.49	0.42
27:3:175:ARG:HA	27:3:178:MET:HE3	2.02	0.42
27:5:66:VAL:O	27:5:70:HIS:ND1	2.27	0.42
26:10:168:LEU:HD12	26:10:168:LEU:HA	1.81	0.42
31:14:306:CLA:H93	31:14:306:CLA:H111	1.96	0.42
27:15:68:LEU:HD21	27:15:167:ARG:NH2	2.34	0.42
31:15:306:CLA:CHB	27:16:133:VAL:HG13	2.50	0.42
31:A:403:CLA:H151	31:D:402:CLA:H151	2.01	0.42
34:A:408:SQD:H341	31:C:509:CLA:H18	2.02	0.42
2:B:91:TRP:CD1	37:N:101:LMG:HC2	2.54	0.42
2:B:340:TRP:HD1	2:B:430:PHE:CE1	2.37	0.42
3:C:321:ASP:OD2	3:C:340:TYR:OH	2.26	0.42
13:M:31:ALA:HB2	13:m:28:GLN:HG3	2.01	0.42
1:a:189:GLU:OE2	1:a:332:HIS:NE2	2.53	0.42
2:b:74:SER:HB2	2:b:93:PHE:HD2	1.84	0.42
2:b:359:MET:HB3	2:b:359:MET:HE2	1.82	0.42
31:b:603:CLA:H101	8:h:58:LEU:HD12	2.01	0.42
3:c:109:VAL:HG11	31:z:101:CLA:H52	2.02	0.42
3:c:190:ALA:HA	3:c:191:PRO:HD3	1.83	0.42
3:c:344:SER:N	3:c:348:GLU:O	2.42	0.42
31:c:503:CLA:H202	31:c:503:CLA:H162	1.84	0.42
27:1:52:VAL:HG21	31:1:308:CLA:O1A	2.19	0.42
27:1:179:MET:HE2	31:1:308:CLA:HMC2	2.02	0.42
27:3:194:GLY:HA2	27:3:197:ALA:HB3	2.00	0.42
27:6:131:VAL:HG13	27:6:132:PHE:H	1.84	0.42
27:7:75:MET:HB3	27:7:75:MET:HE2	1.79	0.42
43:7:301:A86:O	31:7:307:CLA:HAC2	2.19	0.42
27:8:43:LEU:HD23	27:8:46:PHE:CG	2.54	0.42
27:8:137:ILE:HD11	31:8:312:CLA:HMA3	2.01	0.42
26:10:163:LYS:HA	26:10:166:ILE:HD12	2.01	0.42
27:13:37:LEU:HD21	27:13:167:ARG:HG3	2.01	0.42
37:14:316:LMG:H291	37:14:316:LMG:H321	1.90	0.42
2:B:451:TYR:OH	31:B:604:CLA:O2D	2.29	0.42
31:B:607:CLA:HMC3	33:B:618:BCR:HC7	2.01	0.42
4:D:216:ALA:O	4:D:220:ASN:ND2	2.52	0.42
15:O:178:ASP:OD1	15:O:179:GLY:N	2.53	0.42
1:a:249:VAL:HG12	2:b:490:VAL:HG23	2.01	0.42
34:a:408:SQD:H341	31:c:509:CLA:H18	2.01	0.42
27:3:153:PHE:HZ	27:4:150:PHE:HA	1.84	0.42
27:5:117:ALA:HB1	37:5:316:LMG:H111	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:11:75:MET:HE1	31:11:313:CLA:HHC	2.01	0.42
27:18:48:PRO:HG3	43:18:303:A86:O4	2.20	0.42
27:18:106:ASP:HB3	27:18:193:LEU:HD22	2.02	0.42
28:19:138:ALA:O	28:19:142:ASN:ND2	2.52	0.42
43:19:305:A86:C6	31:19:312:CLA:H161	2.49	0.42
2:B:299:SER:OG	2:B:407:ASN:OD1	2.35	0.42
2:B:341:LEU:HD12	2:B:429:VAL:HG12	2.02	0.42
31:B:606:CLA:H193	31:B:606:CLA:H162	1.88	0.42
31:D:406:CLA:H61	31:D:406:CLA:H41	1.64	0.42
33:H:101:BCR:H15C	33:H:101:BCR:H351	1.91	0.42
31:P:601:CLA:H101	36:P:615:LHG:H122	2.02	0.42
1:a:207:GLY:HA3	1:a:278:TRP:HE1	1.83	0.42
1:a:267:ASN:HD22	34:a:408:SQD:H3	1.84	0.42
2:b:340:TRP:HD1	2:b:430:PHE:CE1	2.37	0.42
2:b:383:PHE:N	4:d:344:GLU:O	2.48	0.42
31:b:608:CLA:H161	31:b:608:CLA:H141	1.74	0.42
4:d:80:THR:HG22	4:d:111:TRP:CE2	2.53	0.42
4:d:338:ASN:HD21	7:g:66:ARG:HD2	1.85	0.42
37:p:614:LMG:H302	27:18:49:LEU:HD22	2.01	0.42
24:y:32:LEU:HA	24:y:35:ILE:HD12	2.00	0.42
26:0:31:LEU:HB2	26:0:64:ARG:NH2	2.32	0.42
27:1:65:TYR:HB2	27:1:141:GLU:HA	2.02	0.42
27:6:158:PHE:HE2	27:6:162:THR:H	1.68	0.42
27:6:193:LEU:HD12	27:6:196:ASP:H	1.84	0.42
27:7:134:MET:O	27:7:147:ARG:NH2	2.52	0.42
28:9:33:ARG:NH2	31:9:308:CLA:HED3	2.34	0.42
26:10:129:LEU:HD23	26:10:133:VAL:HB	2.02	0.42
27:11:41:PRO:HA	27:11:43:LEU:H	1.84	0.42
27:14:126:ILE:O	27:14:130:GLU:N	2.49	0.42
1:A:89:ILE:O	1:A:92:HIS:ND1	2.29	0.42
31:B:609:CLA:HBA1	31:B:610:CLA:HBB1	2.02	0.42
4:D:85:VAL:HG11	4:D:90:LEU:HD11	2.01	0.42
2:b:358:ARG:HH12	2:b:427:GLY:C	2.28	0.42
3:c:116:VAL:HG11	33:c:515:BCR:HC42	2.01	0.42
3:c:331:ALA:O	15:o:192:TYR:OH	2.32	0.42
31:p:606:CLA:HHC	31:p:606:CLA:HMC1	1.87	0.42
27:3:169:ILE:HD13	27:3:169:ILE:HG21	1.80	0.42
27:14:85:LYS:HA	27:14:85:LYS:HD3	1.89	0.42
37:14:316:LMG:H322	37:14:316:LMG:H352	1.59	0.42
27:16:111:LEU:HD12	27:16:114:ILE:HD12	2.01	0.42
27:16:133:VAL:HG12	27:16:134:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HD22	34:A:408:SQD:H3	1.84	0.42
33:B:619:BCR:H402	34:B:623:SQD:H441	2.02	0.42
3:C:151:TRP:CE3	3:C:268:GLY:HA2	2.55	0.42
7:G:153:ILE:HB	7:G:158:GLY:HA2	2.01	0.42
1:a:341:LEU:H	3:c:313:GLN:HE22	1.67	0.42
1:a:341:LEU:H	3:c:313:GLN:NE2	2.18	0.42
2:b:442:VAL:HG23	15:o:262:PRO:HD2	2.01	0.42
3:c:191:PRO:HG2	17:q:179:GLU:HA	2.01	0.42
4:d:185:LEU:HD12	31:d:405:CLA:HMD2	2.01	0.42
7:g:153:ILE:HG12	7:g:173:ALA:HA	2.01	0.42
31:p:601:CLA:H101	36:p:615:LHG:H122	2.02	0.42
27:5:93:ASN:O	43:5:302:A86:O3	2.37	0.42
27:11:158:PHE:HE1	27:12:155:TRP:CD1	2.37	0.42
27:12:64:ARG:NH2	27:12:67:GLU:OE1	2.53	0.42
27:12:77:ALA:HA	31:12:310:CLA:HAB	2.02	0.42
28:19:103:MET:HE1	31:19:310:CLA:H18	2.01	0.42
1:A:189:GLU:OE2	1:A:332:HIS:NE2	2.53	0.42
1:A:201:GLY:HA3	1:A:286:THR:HG23	2.01	0.42
2:B:162:PHE:HD2	31:B:606:CLA:HHD	1.85	0.42
3:C:95:LEU:HD13	31:C:503:CLA:H143	2.02	0.42
3:C:191:PRO:HB2	17:Q:178:LEU:HD23	2.01	0.42
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.85	0.42
4:D:329:MET:O	4:D:333:ASP:N	2.53	0.42
13:M:32:ARG:HB2	13:m:31:ALA:HB1	2.02	0.42
20:U:27:ASP:OD1	20:U:28:ILE:N	2.52	0.42
20:U:43:TYR:OH	21:V:51:ASN:ND2	2.53	0.42
31:b:603:CLA:H171	38:h:102:DGD:HAF2	2.02	0.42
33:y:101:BCR:H24C	33:y:101:BCR:H371	1.68	0.42
27:6:137:ILE:HD11	31:6:313:CLA:HMA2	2.01	0.42
31:6:308:CLA:H2A	31:6:308:CLA:O2D	2.20	0.42
27:8:169:ILE:HD13	27:8:169:ILE:HG21	1.83	0.42
27:13:76:LEU:HA	27:13:79:VAL:HG12	2.01	0.42
27:14:60:PHE:O	27:14:64:ARG:N	2.48	0.42
27:15:175:ARG:HA	27:15:178:MET:HE3	2.01	0.42
32:A:405:PHO:C2B	31:D:402:CLA:H2	2.50	0.42
31:B:606:CLA:H72	33:B:619:BCR:H311	2.01	0.42
32:a:405:PHO:C2B	31:d:402:CLA:H2	2.50	0.42
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.55	0.42
38:b:622:DGD:HO4D	38:b:622:DGD:HO2E	1.61	0.42
33:c:516:BCR:H323	31:w:203:CLA:HBB2	2.02	0.42
27:2:42:PRO:HG2	27:2:43:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:312:CLA:HMB3	31:2:312:CLA:HHB	1.73	0.42
27:8:179:MET:HE2	31:8:308:CLA:HMC2	2.01	0.42
27:11:76:LEU:HA	27:11:79:VAL:HG12	2.00	0.42
27:11:151:ILE:H	27:11:151:ILE:HG13	1.50	0.42
31:14:309:CLA:H62	31:14:309:CLA:H2	1.81	0.42
27:18:52:VAL:HG11	27:18:60:PHE:HD1	1.85	0.42
27:18:64:ARG:HH21	27:18:171:LEU:HD11	1.85	0.42
1:A:56:PRO:HA	1:A:73:TYR:CE2	2.52	0.41
2:B:74:SER:HA	2:B:92:SER:HB2	2.02	0.41
2:B:98:LEU:HD11	38:B:621:DGD:HBT1	2.01	0.41
3:C:164:HIS:ND1	31:C:508:CLA:OBD	2.41	0.41
31:b:617:CLA:HHC	31:b:617:CLA:HBB1	2.02	0.41
10:j:15:LEU:HD11	24:y:33:PHE:CE1	2.55	0.41
23:x:80:MET:HG3	23:x:84:LEU:HD22	2.02	0.41
31:0:308:CLA:HED3	31:0:308:CLA:H2A	2.02	0.41
27:4:89:ARG:NH1	27:4:101:PHE:O	2.53	0.41
27:6:169:ILE:HG21	27:6:169:ILE:HD13	1.78	0.41
27:7:150:PHE:C	27:7:152:ASP:H	2.26	0.41
28:9:8:ALA:HB2	31:9:308:CLA:HED2	2.01	0.41
26:10:162:LYS:HE2	26:10:166:ILE:HD11	2.01	0.41
28:19:142:ASN:ND2	31:19:307:CLA:O1D	2.46	0.41
1:A:29:TYR:HB2	4:D:255:GLN:HG3	2.02	0.41
2:B:383:PHE:N	4:D:344:GLU:O	2.47	0.41
33:C:516:BCR:H15C	33:C:516:BCR:H351	1.86	0.41
11:K:24:LEU:HD11	11:K:35:VAL:HG21	2.02	0.41
37:K:101:LMG:H141	37:K:101:LMG:H112	1.51	0.41
20:U:14:TYR:O	20:U:17:ILE:HG13	2.20	0.41
31:a:403:CLA:H151	31:d:402:CLA:H151	2.01	0.41
2:b:277:SER:HA	7:g:60:SER:HA	2.03	0.41
5:e:10:PHE:HB2	6:f:19:ARG:NH2	2.34	0.41
11:k:24:LEU:HD11	11:k:35:VAL:HG21	2.02	0.41
26:0:81:TYR:CD2	26:0:181:LEU:HD21	2.55	0.41
27:2:64:ARG:NH1	31:2:307:CLA:H2A	2.35	0.41
27:5:121:GLN:NE2	37:5:316:LMG:O7	2.52	0.41
27:11:144:GLY:O	27:11:146:PHE:N	2.53	0.41
27:16:37:LEU:HG	27:16:171:LEU:HD13	2.02	0.41
31:18:309:CLA:H2	31:18:309:CLA:H61	1.92	0.41
1:A:91:MET:HB2	1:A:91:MET:HE2	1.80	0.41
2:B:98:LEU:HD22	31:B:606:CLA:H172	2.02	0.41
3:C:193:GLY:HA2	17:Q:152:TYR:CD1	2.54	0.41
3:C:342:MET:HE2	3:C:342:MET:HB3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:218:LYS:HD3	15:o:102:GLN:HA	2.02	0.41
1:a:315:ASN:O	4:d:64:ALA:N	2.50	0.41
3:c:41:ARG:NH1	31:c:512:CLA:OBD	2.54	0.41
3:c:151:TRP:CE3	3:c:268:GLY:HA2	2.55	0.41
31:c:505:CLA:H92	31:c:505:CLA:H62	1.86	0.41
15:o:229:MET:HB2	15:o:291:MET:HB2	2.02	0.41
37:p:614:LMG:H112	37:p:614:LMG:H141	1.87	0.41
27:3:158:PHE:HE2	27:4:151:ILE:HA	1.85	0.41
27:7:133:VAL:H	27:7:133:VAL:HG22	1.54	0.41
31:12:307:CLA:HHB	31:12:307:CLA:HMB1	1.86	0.41
31:14:312:CLA:H12	31:14:312:CLA:CHB	2.50	0.41
27:17:52:VAL:O	27:17:54:ASP:N	2.54	0.41
2:B:214:ILE:HG21	31:R:101:CLA:H3A	2.02	0.41
31:B:616:CLA:HBB1	31:B:616:CLA:HHC	2.01	0.41
3:C:64:ALA:HB1	31:C:504:CLA:HED3	2.02	0.41
3:C:329:SER:HB3	3:C:341:LEU:HD12	2.01	0.41
37:M:101:LMG:H172	37:M:101:LMG:H372	2.01	0.41
31:a:403:CLA:H122	32:a:405:PHO:H3A	2.02	0.41
35:a:409:PL9:H251	35:a:409:PL9:H272	1.87	0.41
2:b:392:ILE:HG23	2:b:397:VAL:HB	2.02	0.41
24:y:17:LEU:O	24:y:21:ALA:N	2.48	0.41
27:5:137:ILE:HD12	31:5:311:CLA:HMA1	2.02	0.41
27:18:183:ALA:O	27:18:187:HIS:N	2.43	0.41
2:B:16:PRO:HB2	2:B:123:PHE:CD1	2.56	0.41
2:B:358:ARG:HH12	2:B:427:GLY:C	2.28	0.41
31:B:616:CLA:H91	31:B:616:CLA:H111	1.80	0.41
3:C:31:THR:HG23	3:C:33:PHE:H	1.86	0.41
31:C:503:CLA:H202	31:C:503:CLA:H162	1.84	0.41
4:D:303:LEU:O	4:D:306:ALA:N	2.47	0.41
5:E:65:LEU:HB2	7:G:66:ARG:NH1	2.36	0.41
37:J:101:LMG:H362	37:K:101:LMG:H191	2.03	0.41
1:a:93:PHE:CD2	37:w:201:LMG:HC1	2.56	0.41
33:b:619:BCR:H20C	33:b:619:BCR:H361	1.85	0.41
3:c:31:THR:HG23	3:c:33:PHE:H	1.86	0.41
31:c:510:CLA:H141	31:c:510:CLA:H161	1.87	0.41
4:d:24:LYS:HD2	4:d:26:ARG:NH1	2.36	0.41
26:0:108:PHE:HE2	26:0:185:GLU:HB2	1.84	0.41
26:0:178:ILE:O	26:0:182:MET:HG2	2.21	0.41
26:0:184:HIS:O	26:0:188:GLY:N	2.54	0.41
31:2:306:CLA:C3B	27:3:133:VAL:HG21	2.50	0.41
27:4:131:VAL:HG12	27:4:132:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:190:LEU:HB3	27:4:191:ILE:HD12	2.02	0.41
27:6:89:ARG:NH1	27:6:101:PHE:O	2.48	0.41
43:9:305:A86:C6	31:9:312:CLA:H161	2.51	0.41
27:14:131:VAL:HG12	27:14:132:PHE:CD1	2.56	0.41
27:16:169:ILE:O	27:16:173:GLN:N	2.36	0.41
28:19:62:THR:HG22	28:19:69:THR:HG22	2.02	0.41
2:B:392:ILE:HG23	2:B:397:VAL:HB	2.02	0.41
4:D:144:ILE:O	4:D:147:SER:OG	2.33	0.41
4:D:156:VAL:HG22	4:D:286:ILE:HG12	2.01	0.41
7:G:153:ILE:HG12	7:G:173:ALA:HA	2.01	0.41
2:b:383:PHE:CD2	4:d:347:PRO:HA	2.56	0.41
31:b:606:CLA:H193	31:b:610:CLA:HBB2	2.02	0.41
31:b:609:CLA:H3A	31:b:609:CLA:HBA2	1.81	0.41
4:d:156:VAL:HG22	4:d:286:ILE:HG12	2.02	0.41
7:g:68:ARG:HA	7:g:100:PHE:HE1	1.85	0.41
15:o:129:LEU:HD21	15:o:335:VAL:HG22	2.03	0.41
26:0:65:TYR:OH	26:0:135:ARG:NE	2.53	0.41
27:5:81:TYR:CE1	27:5:184:LEU:HD11	2.55	0.41
27:8:64:ARG:HH21	27:8:171:LEU:HD11	1.86	0.41
27:8:68:LEU:HD11	27:8:167:ARG:HH12	1.86	0.41
27:11:89:ARG:NH1	27:11:101:PHE:O	2.54	0.41
27:11:182:LEU:O	27:11:186:VAL:HG23	2.20	0.41
38:11:318:DGD:HB92	38:11:318:DGD:HB61	1.67	0.41
31:14:312:CLA:HHB	31:14:312:CLA:HMB1	1.72	0.41
27:16:57:GLN:O	27:16:61:ASP:N	2.44	0.41
27:16:172:ASN:ND2	31:16:307:CLA:O1D	2.47	0.41
34:B:623:SQD:H121	34:B:623:SQD:H241	2.03	0.41
3:C:56:HIS:ND1	31:C:510:CLA:HHB	2.36	0.41
31:D:406:CLA:H91	8:H:52:ILE:HD11	2.03	0.41
31:P:601:CLA:H192	31:P:601:CLA:H162	1.86	0.41
1:a:186:PHE:O	1:a:190:HIS:HB2	2.21	0.41
1:a:340:PRO:HD2	3:c:313:GLN:HE21	1.85	0.41
2:b:98:LEU:HD22	31:b:607:CLA:H172	2.02	0.41
2:b:384:ARG:HA	15:o:253:THR:HG22	2.01	0.41
2:b:475:PHE:HD2	4:d:140:PRO:HD3	1.86	0.41
4:d:157:PHE:HE1	4:d:171:PRO:HG2	1.85	0.41
37:j:101:LMG:H362	37:k:101:LMG:H191	2.03	0.41
20:u:14:TYR:O	20:u:17:ILE:HG13	2.20	0.41
26:0:65:TYR:CE2	26:0:69:LYS:HB2	2.56	0.41
27:1:128:PHE:CE2	27:1:133:VAL:HG21	2.56	0.41
27:5:65:TYR:OH	27:5:142:PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:6:182:LEU:HB3	31:6:316:CLA:HBC2	2.02	0.41
27:7:69:LYS:NZ	27:7:130:GLU:OE2	2.48	0.41
27:8:64:ARG:HH12	31:8:308:CLA:CGD	2.29	0.41
27:11:73:ILE:HD13	31:11:312:CLA:HBC3	2.03	0.41
27:11:186:VAL:HG11	31:11:315:CLA:CHD	2.50	0.41
27:16:161:GLU:HG3	27:16:165:LYS:HE2	2.02	0.41
27:17:175:ARG:HB3	31:17:308:CLA:HAC2	2.02	0.41
27:18:159:ASP:OD1	27:18:160:GLU:N	2.54	0.41
28:19:6:LEU:HB3	28:19:33:ARG:HH12	1.85	0.41
28:19:33:ARG:NH2	31:19:308:CLA:HED3	2.35	0.41
1:A:57:PRO:HD3	1:A:73:TYR:CE2	2.56	0.41
31:B:602:CLA:H93	31:B:602:CLA:H61	1.84	0.41
2:b:352:ARG:NH1	2:b:378:ARG:HH21	2.18	0.41
31:b:608:CLA:HMC3	33:b:619:BCR:HC7	2.01	0.41
33:b:620:BCR:H15C	33:b:620:BCR:H351	1.93	0.41
4:d:235:PHE:CD1	4:d:243:THR:HG21	2.56	0.41
11:k:48:LEU:HA	11:k:51:VAL:HB	2.03	0.41
26:0:73:ILE:HD12	31:0:313:CLA:HMD3	2.02	0.41
27:3:63:LEU:HB3	31:3:308:CLA:HHB	2.03	0.41
27:8:131:VAL:HG13	27:8:132:PHE:HD1	1.86	0.41
31:8:308:CLA:H3A	31:8:308:CLA:HBA2	1.82	0.41
27:13:65:TYR:HA	27:13:68:LEU:HD12	2.03	0.41
27:14:34:GLU:HG3	27:14:36:GLU:H	1.85	0.41
27:14:106:ASP:HB2	27:14:193:LEU:HD13	2.03	0.41
27:15:181:ILE:HA	27:15:184:LEU:HB3	2.03	0.41
2:B:74:SER:HB2	2:B:93:PHE:HD2	1.85	0.41
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.55	0.41
2:B:475:PHE:HE1	4:D:134:ARG:HD3	1.86	0.41
31:B:602:CLA:H61	31:B:602:CLA:H41	1.84	0.41
38:B:621:DGD:HBE1	34:B:623:SQD:H371	2.02	0.41
3:C:41:ARG:NH1	31:C:512:CLA:OBD	2.54	0.41
3:C:449:ARG:NH2	9:I:28:PRO:HG3	2.35	0.41
4:D:89:LEU:HG	8:H:62:ASN:ND2	2.36	0.41
5:E:51:ARG:NH1	17:Q:66:VAL:HG22	2.31	0.41
11:K:28:TYR:CE1	25:Z:9:THR:HG21	2.54	0.41
12:L:29:ALA:O	12:L:33:SER:HB3	2.20	0.41
15:O:102:GLN:HE22	17:Q:188:LYS:NZ	2.19	0.41
15:O:229:MET:HB2	15:O:291:MET:HB2	2.02	0.41
21:V:92:HIS:NE2	41:V:201:HEM:NC	2.69	0.41
23:X:80:MET:HG3	23:X:84:LEU:HD22	2.01	0.41
1:a:196:PRO:HA	1:a:199:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:201:GLY:HA3	1:a:286:THR:HG23	2.01	0.41
2:b:18:ARG:NH2	12:l:5:ASN:HD21	2.19	0.41
2:b:91:TRP:CD1	37:n:701:LMG:HC2	2.56	0.41
2:b:162:PHE:HD2	31:b:607:CLA:HHD	1.84	0.41
3:c:56:HIS:ND1	31:c:510:CLA:HHB	2.36	0.41
3:c:329:SER:HB3	3:c:341:LEU:HD12	2.01	0.41
4:d:85:VAL:HG11	4:d:90:LEU:HD11	2.01	0.41
4:d:329:MET:O	4:d:333:ASP:N	2.53	0.41
20:u:33:ILE:HG12	20:u:43:TYR:CE1	2.56	0.41
26:0:127:GLY:HA2	26:0:130:GLU:HB3	2.02	0.41
27:1:62:ARG:O	27:1:66:VAL:HG23	2.21	0.41
27:2:153:PHE:CE2	27:3:151:ILE:HB	2.56	0.41
27:3:151:ILE:H	27:3:151:ILE:HG13	1.43	0.41
27:6:172:ASN:ND2	31:6:308:CLA:O1D	2.43	0.41
27:7:152:ASP:N	27:7:152:ASP:OD1	2.48	0.41
27:7:153:PHE:HD1	27:7:162:THR:HB	1.86	0.41
27:8:76:LEU:HA	27:8:79:VAL:HG12	2.03	0.41
27:8:137:ILE:O	27:8:139:GLY:N	2.45	0.41
27:8:193:LEU:O	27:8:197:ALA:N	2.54	0.41
28:9:6:LEU:HB3	28:9:33:ARG:HH12	1.86	0.41
26:10:95:ASP:OD2	26:10:97:SER:OG	2.36	0.41
38:11:318:DGD:HB92	38:11:318:DGD:HBW1	1.61	0.41
27:12:62:ARG:O	27:12:66:VAL:HG23	2.21	0.41
27:12:68:LEU:HD11	27:12:167:ARG:HH12	1.85	0.41
27:12:158:PHE:HZ	27:13:154:GLY:H	1.69	0.41
27:13:112:SER:HA	31:13:316:CLA:HBC3	2.02	0.41
27:15:81:TYR:CE1	27:15:184:LEU:HD11	2.56	0.41
31:19:308:CLA:H141	31:19:308:CLA:H161	1.76	0.41
2:B:96:VAL:O	2:B:100:HIS:ND1	2.48	0.41
31:B:604:CLA:H71	31:B:604:CLA:H112	1.68	0.41
31:C:510:CLA:H142	31:C:510:CLA:H112	1.91	0.41
38:C:519:DGD:HA41	38:C:519:DGD:HA72	1.87	0.41
4:D:48:TRP:HA	4:D:78:VAL:HG21	2.03	0.41
4:D:157:PHE:HE1	4:D:171:PRO:HG2	1.85	0.41
7:G:68:ARG:HA	7:G:100:PHE:HE1	1.85	0.41
33:H:101:BCR:H24C	33:H:101:BCR:H371	1.84	0.41
21:V:13:ASP:OD1	21:V:14:ASN:N	2.51	0.41
34:b:601:SQD:H441	33:b:620:BCR:H402	2.03	0.41
31:b:608:CLA:H93	31:b:608:CLA:H61	1.82	0.41
3:c:69:LEU:HA	3:c:69:LEU:HD23	1.91	0.41
3:c:186:TYR:HA	3:c:196:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:30:THR:HG22	33:f:101:BCR:H17C	2.02	0.41
26:0:40:PHE:HB3	31:0:309:CLA:CAD	2.51	0.41
37:0:317:LMG:HC91	31:8:312:CLA:HAA1	2.03	0.41
31:4:312:CLA:H12	31:4:312:CLA:CHB	2.51	0.41
27:5:148:ASN:HD21	31:5:312:CLA:HBD	1.86	0.41
27:6:51:LEU:HD13	31:6:309:CLA:H52	2.03	0.41
27:6:75:MET:HB3	27:6:75:MET:HE2	1.87	0.41
27:7:169:ILE:HG22	31:7:307:CLA:CGD	2.51	0.41
26:10:73:ILE:HD12	31:10:313:CLA:HMD3	2.03	0.41
27:15:107:GLY:O	43:15:303:A86:O2	2.38	0.41
27:16:69:LYS:NZ	27:16:130:GLU:OE2	2.41	0.41
27:16:169:ILE:HG22	31:16:307:CLA:CGD	2.51	0.41
27:16:182:LEU:HB3	31:16:315:CLA:HBC2	2.02	0.41
31:16:313:CLA:HED3	31:16:313:CLA:HBD	1.99	0.41
31:A:403:CLA:H122	32:A:405:PHO:H3A	2.02	0.40
2:B:359:MET:HE2	2:B:359:MET:HB3	1.81	0.40
31:B:609:CLA:H92	31:B:609:CLA:H62	1.84	0.40
4:D:24:LYS:HD2	4:D:26:ARG:NH1	2.35	0.40
34:b:601:SQD:H242	34:b:601:SQD:H271	1.89	0.40
31:b:602:CLA:H93	33:h:101:BCR:H402	2.03	0.40
31:b:605:CLA:H71	31:b:605:CLA:H112	1.68	0.40
3:c:27:ASP:OD1	11:k:59:ARG:HD3	2.21	0.40
31:c:507:CLA:H171	31:c:507:CLA:H13	1.79	0.40
12:l:29:ALA:O	12:l:33:SER:HB3	2.20	0.40
21:v:92:HIS:NE2	41:v:201:HEM:NC	2.69	0.40
31:1:313:CLA:H61	31:1:313:CLA:H92	1.86	0.40
27:7:66:VAL:HA	31:7:312:CLA:HED1	2.03	0.40
27:7:175:ARG:HB3	31:7:308:CLA:HAC2	2.03	0.40
27:12:175:ARG:HA	27:12:178:MET:HE3	2.03	0.40
27:14:51:LEU:O	27:14:56:ASN:ND2	2.54	0.40
27:15:169:ILE:HG22	31:15:306:CLA:CGD	2.52	0.40
27:17:169:ILE:HG22	31:17:307:CLA:CGD	2.51	0.40
27:18:140:GLY:HA3	27:18:143:VAL:HG22	2.02	0.40
31:B:610:CLA:HBB1	31:B:610:CLA:HHC	2.02	0.40
3:C:186:TYR:HA	3:C:196:VAL:HA	2.02	0.40
31:C:505:CLA:H91	31:C:505:CLA:H112	1.79	0.40
31:D:406:CLA:H61	31:D:406:CLA:H92	1.95	0.40
33:Y:101:BCR:H11C	33:Y:101:BCR:H341	1.98	0.40
1:a:260:PHE:HB2	1:a:263:ALA:HB3	2.03	0.40
3:c:195:ASP:HB2	17:q:155:ARG:HD3	2.02	0.40
31:c:505:CLA:H112	31:c:505:CLA:H91	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:57:SER:OG	4:d:65:SER:OG	2.30	0.40
31:d:402:CLA:H141	31:d:402:CLA:H161	1.77	0.40
15:o:171:ILE:HA	15:o:189:GLY:HA3	2.04	0.40
31:1:315:CLA:HBB1	31:1:315:CLA:HHC	2.03	0.40
27:7:137:ILE:HD11	31:7:312:CLA:HMA2	2.03	0.40
27:14:56:ASN:O	27:14:60:PHE:N	2.45	0.40
27:14:175:ARG:HB3	43:14:301:A86:C23	2.51	0.40
27:15:51:LEU:HD12	31:15:307:CLA:H52	2.03	0.40
27:17:75:MET:HE2	27:17:75:MET:HB3	1.84	0.40
31:18:309:CLA:HBA2	31:18:309:CLA:H3A	1.74	0.40
1:A:93:PHE:CD2	37:W:201:LMG:HC1	2.56	0.40
1:A:186:PHE:O	1:A:190:HIS:HB2	2.21	0.40
1:A:196:PRO:HA	1:A:199:MET:HB2	2.02	0.40
1:A:260:PHE:HB2	1:A:263:ALA:HB3	2.03	0.40
2:B:247:PHE:HE1	31:B:602:CLA:H122	1.86	0.40
33:B:617:BCR:H383	34:l:101:SQD:H112	2.03	0.40
3:C:273:SER:O	3:C:441:HIS:ND1	2.40	0.40
3:C:393:ALA:HB1	41:V:201:HEM:HBC1	2.03	0.40
4:D:235:PHE:CD1	4:D:243:THR:HG21	2.56	0.40
2:b:340:TRP:HD1	2:b:430:PHE:HE1	1.68	0.40
34:b:601:SQD:H241	34:b:601:SQD:H121	2.03	0.40
31:b:604:CLA:H41	31:b:604:CLA:H62	1.85	0.40
31:b:612:CLA:H111	31:b:612:CLA:H142	1.79	0.40
3:c:92:LEU:HD21	3:c:114:VAL:HG11	2.03	0.40
3:c:95:LEU:O	3:c:178:LYS:NZ	2.49	0.40
31:c:510:CLA:H3A	31:c:510:CLA:HBA1	1.88	0.40
31:d:402:CLA:H91	31:d:402:CLA:H112	1.90	0.40
31:d:405:CLA:H91	31:d:405:CLA:H111	1.81	0.40
33:f:101:BCR:H19C	37:f:102:LMG:H351	2.02	0.40
31:p:602:CLA:H142	31:p:602:CLA:H111	1.89	0.40
26:0:29:ASP:OD1	26:0:30:GLU:N	2.54	0.40
27:2:144:GLY:O	27:2:146:PHE:N	2.54	0.40
27:4:165:LYS:HD2	27:4:165:LYS:HA	1.81	0.40
27:5:200:PRO:HB2	27:5:201:ILE:H	1.66	0.40
31:5:309:CLA:HBA2	31:5:309:CLA:H3A	1.67	0.40
27:8:76:LEU:HA	27:8:76:LEU:HD23	1.90	0.40
31:11:308:CLA:O1A	31:11:308:CLA:H3A	2.22	0.40
27:14:204:HIS:HD2	36:14:317:LHG:H192	1.86	0.40
27:17:150:PHE:C	27:17:152:ASP:H	2.28	0.40
31:18:307:CLA:H62	31:18:307:CLA:H41	1.84	0.40
1:A:140:ARG:HB3	1:A:142:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:603:CLA:H62	31:B:603:CLA:H41	1.85	0.40
33:B:617:BCR:H20C	33:B:617:BCR:H361	1.87	0.40
38:C:518:DGD:HA21	38:C:518:DGD:HB31	2.04	0.40
37:M:101:LMG:H111	13:m:27:ILE:HG13	2.03	0.40
15:O:102:GLN:HB2	16:p:218:LYS:HA	2.04	0.40
1:a:140:ARG:HB3	1:a:142:TRP:CZ3	2.56	0.40
2:b:122:LEU:HD11	8:h:23:LEU:HB2	2.03	0.40
31:b:617:CLA:H111	31:b:617:CLA:H91	1.81	0.40
38:c:518:DGD:HA21	38:c:518:DGD:HB31	2.04	0.40
15:o:103:VAL:HG13	15:o:108:LEU:HB3	2.04	0.40
17:q:140:TRP:HZ3	17:q:193:VAL:HG21	1.87	0.40
31:1:308:CLA:O1A	31:1:308:CLA:H3A	2.22	0.40
27:7:151:ILE:HD13	27:7:151:ILE:HG21	1.83	0.40
28:9:62:THR:HG22	28:9:69:THR:HG22	2.04	0.40
31:10:313:CLA:HMB2	37:10:319:LMG:H312	2.03	0.40
27:12:93:ASN:HA	27:12:100:THR:HA	2.02	0.40
43:13:301:A86:O	31:13:307:CLA:HAC2	2.21	0.40
27:16:42:PRO:HG2	27:16:43:LEU:HD12	2.02	0.40
27:18:69:LYS:HD2	27:18:137:ILE:HD12	2.03	0.40
36:B:622:LHG:O4	4:D:141:TYR:OH	2.23	0.40
3:C:69:LEU:HD23	3:C:69:LEU:HA	1.91	0.40
37:C:522:LMG:H231	37:C:522:LMG:H201	1.96	0.40
31:D:405:CLA:H62	31:D:405:CLA:H101	1.84	0.40
33:F:101:BCR:H19C	37:F:102:LMG:H351	2.02	0.40
15:O:129:LEU:HD21	15:O:335:VAL:HG22	2.03	0.40
17:Q:140:TRP:HZ3	17:Q:193:VAL:HG21	1.87	0.40
20:U:33:ILE:HG12	20:U:43:TYR:CE1	2.56	0.40
1:a:57:PRO:HD3	1:a:73:TYR:CE2	2.56	0.40
38:b:622:DGD:HB42	38:b:622:DGD:HA72	2.04	0.40
31:c:505:CLA:H61	31:c:505:CLA:H41	1.86	0.40
33:c:517:BCR:HC42	11:k:28:TYR:CE1	2.56	0.40
4:d:48:TRP:HA	4:d:78:VAL:HG21	2.03	0.40
37:k:101:LMG:H132	24:y:25:LEU:HD11	2.03	0.40
31:2:309:CLA:HED2	31:2:309:CLA:H2A	2.04	0.40
27:3:130:GLU:OE2	27:3:137:ILE:HD13	2.22	0.40
27:3:185:MET:O	27:3:189:LYS:N	2.55	0.40
27:4:64:ARG:NH1	27:4:171:LEU:HD22	2.37	0.40
31:4:312:CLA:HHB	31:4:312:CLA:HMB1	1.69	0.40
27:5:138:THR:OG1	27:5:141:GLU:HB3	2.21	0.40
27:8:77:ALA:HB3	27:8:181:ILE:HD11	2.04	0.40
28:9:41:ARG:NE	28:9:140:GLU:OE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:18:126:ILE:O	27:18:130:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
13	m	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
15	O	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	30	63
15	o	247/249 (99%)	217 (88%)	29 (12%)	1 (0%)	30	63
16	P	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	63
16	p	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	63
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%)	3	17
24	y	31/33 (94%)	27 (87%)	3 (10%)	1 (3%)	3	17
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%)	9	34
26	10	145/178 (82%)	130 (90%)	15 (10%)	0	100	100
27	1	170/172 (99%)	141 (83%)	27 (16%)	2 (1%)	10	38
27	11	170/172 (99%)	146 (86%)	22 (13%)	2 (1%)	10	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	12	170/172 (99%)	146 (86%)	23 (14%)	1 (1%)	21 54
27	13	170/172 (99%)	150 (88%)	18 (11%)	2 (1%)	10 38
27	14	170/172 (99%)	148 (87%)	19 (11%)	3 (2%)	6 29
27	15	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	21 54
27	16	170/172 (99%)	146 (86%)	21 (12%)	3 (2%)	6 29
27	17	170/172 (99%)	146 (86%)	18 (11%)	6 (4%)	3 15
27	18	170/172 (99%)	142 (84%)	25 (15%)	3 (2%)	6 29
27	2	170/172 (99%)	147 (86%)	19 (11%)	4 (2%)	4 23
27	3	170/172 (99%)	145 (85%)	23 (14%)	2 (1%)	10 38
27	4	170/172 (99%)	149 (88%)	21 (12%)	0	100 100
27	5	170/172 (99%)	140 (82%)	29 (17%)	1 (1%)	21 54
27	6	170/172 (99%)	143 (84%)	24 (14%)	3 (2%)	6 29
27	7	170/172 (99%)	142 (84%)	24 (14%)	4 (2%)	4 23
27	8	170/172 (99%)	136 (80%)	32 (19%)	2 (1%)	10 38
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%)	26 59

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

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Mol	Chain	Res	Type
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
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
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%)	29	62
10	j	26/26 (100%)	25 (96%)	1 (4%)	29	62
11	K	32/32 (100%)	31 (97%)	1 (3%)	35	67
11	k	32/32 (100%)	31 (97%)	1 (3%)	35	67
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%)	81	88
15	o	201/201 (100%)	200 (100%)	1 (0%)	81	88
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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%)	118 (100%)	0	100	100
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%)	131 (99%)	1 (1%)	73	85
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%)	76	85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	7709 (100%)	8 (0%)	87 92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	36	LEU
11	K	41	ILE
15	O	156	VAL
10	j	36	LEU
11	k	41	ILE
15	o	156	VAL
27	2	192	PRO
27	14	169	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	230	ASN
1	A	234	ASN
1	A	241	GLN
1	A	322	ASN
1	A	338	ASN
2	B	26	HIS
2	B	58	GLN
2	B	87	ASN
2	B	179	GLN
2	B	274	GLN
2	B	287	GLN
2	B	318	ASN
2	B	394	GLN
2	B	425	GLN
2	B	496	GLN
3	C	311	GLN
3	C	313	GLN
3	C	322	GLN
3	C	332	GLN

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Mol	Chain	Res	Type
3	C	385	GLN
3	C	415	ASN
4	D	87	HIS
4	D	106	GLN
4	D	142	ASN
4	D	189	HIS
4	D	190	ASN
4	D	292	ASN
4	D	338	ASN
5	E	74	GLN
6	F	41	GLN
6	F	44	GLN
7	G	65	ASN
11	K	32	ASN
11	K	53	GLN
12	L	5	ASN
13	M	28	GLN
13	M	40	GLN
15	O	96	ASN
15	O	102	GLN
15	O	110	ASN
15	O	198	GLN
15	O	286	GLN
15	O	311	GLN
17	Q	86	GLN
20	U	16	ASN
20	U	30	ASN
20	U	53	HIS
20	U	98	ASN
21	V	70	ASN
25	Z	45	GLN
1	a	181	ASN
1	a	230	ASN
1	a	234	ASN
1	a	241	GLN
1	a	322	ASN
1	a	338	ASN
2	b	58	GLN
2	b	87	ASN
2	b	179	GLN
2	b	274	GLN
2	b	287	GLN

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Mol	Chain	Res	Type
2	b	318	ASN
2	b	394	GLN
2	b	425	GLN
3	c	311	GLN
3	c	313	GLN
3	c	322	GLN
3	c	385	GLN
4	d	87	HIS
4	d	106	GLN
4	d	142	ASN
4	d	189	HIS
4	d	190	ASN
4	d	250	ASN
4	d	292	ASN
4	d	338	ASN
5	e	74	GLN
6	f	44	GLN
7	g	65	ASN
11	k	32	ASN
12	l	5	ASN
12	l	38	ASN
13	m	28	GLN
13	m	40	GLN
15	o	96	ASN
15	o	102	GLN
15	o	110	ASN
15	o	164	GLN
15	o	198	GLN
15	o	286	GLN
15	o	311	GLN
17	q	86	GLN
20	u	30	ASN
20	u	53	HIS
20	u	98	ASN
25	z	45	GLN
26	0	170	GLN
27	1	187	HIS
27	2	35	ASN
27	2	70	HIS
27	2	173	GLN
27	3	40	GLN
27	3	70	HIS

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Mol	Chain	Res	Type
27	3	173	GLN
27	4	56	ASN
27	4	172	ASN
27	4	173	GLN
27	5	173	GLN
27	6	35	ASN
27	6	121	GLN
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	26	GLN
28	9	157	HIS
26	10	160	GLN
26	10	170	GLN
27	11	187	HIS
27	14	173	GLN
27	14	204	HIS
27	15	173	GLN
27	15	187	HIS
27	16	70	HIS
27	16	121	GLN
27	16	173	GLN
27	17	35	ASN
27	17	70	HIS
27	17	173	GLN
27	17	187	HIS
27	18	70	HIS
27	18	173	GLN
27	18	187	HIS
28	19	9	GLN
28	19	26	GLN
28	19	142	ASN
28	19	157	HIS

5.3.3 RNA

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 oligosaccharides 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	$\#\|Z\| > 2$
31	CLA	12	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.57	6 (11%)
43	A86	18	302	-	44,50,50	1.34	4 (9%)	51,76,76	2.48	18 (35%)
31	CLA	p	602	-	69,73,73	1.29	10 (14%)	83,113,113	1.38	8 (9%)
38	DGD	1	318	-	55,55,67	1.04	3 (5%)	69,69,81	1.36	8 (11%)
43	A86	17	316	-	44,50,50	1.62	7 (15%)	51,76,76	4.91	33 (64%)
42	KC1	14	313	27	49,53,53	2.68	19 (38%)	63,89,89	5.20	40 (63%)
45	KC2	0	310	26	49,53,53	2.73	19 (38%)	62,89,89	4.31	35 (56%)
37	LMG	W	201	-	48,48,55	0.97	6 (12%)	56,56,63	1.40	9 (16%)
31	CLA	14	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.32	9 (10%)
43	A86	0	306	-	44,50,50	1.65	8 (18%)	51,76,76	3.10	18 (35%)
43	A86	6	306	31	44,50,50	1.45	4 (9%)	51,76,76	3.79	22 (43%)
37	LMG	Z	102	-	31,31,55	1.16	3 (9%)	39,39,63	1.20	3 (7%)
31	CLA	A	403	1	69,73,73	1.31	10 (14%)	83,113,113	1.43	11 (13%)
42	KC1	0	315	-	49,53,53	2.66	20 (40%)	63,89,89	5.42	38 (60%)
31	CLA	B	610	-	69,73,73	1.27	10 (14%)	83,113,113	1.41	10 (12%)
31	CLA	17	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.57	7 (12%)
43	A86	12	305	-	44,50,50	1.33	4 (9%)	51,76,76	3.04	21 (41%)
45	KC2	8	311	-	49,53,53	2.83	20 (40%)	62,89,89	5.04	37 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	7	305	-	44,50,50	1.44	5 (11%)	51,76,76	3.74	23 (45%)
43	A86	3	306	-	44,50,50	1.30	3 (6%)	51,76,76	4.65	24 (47%)
45	KC2	1	311	-	49,53,53	2.78	18 (36%)	62,89,89	4.35	37 (59%)
31	CLA	8	308	-	65,69,73	1.33	12 (18%)	78,108,113	1.59	11 (14%)
31	CLA	p	608	16	55,59,73	1.42	10 (18%)	66,96,113	1.52	7 (10%)
36	LHG	a	410	1	36,36,48	0.76	1 (2%)	39,42,54	1.24	4 (10%)
31	CLA	6	308	-	46,50,73	1.48	7 (15%)	55,85,113	1.99	11 (20%)
31	CLA	D	406	-	69,73,73	1.23	9 (13%)	83,113,113	1.38	6 (7%)
31	CLA	11	310	-	54,58,73	1.36	9 (16%)	65,95,113	1.56	7 (10%)
31	CLA	1	316	43	46,50,73	1.53	9 (19%)	55,85,113	1.59	7 (12%)
33	BCR	h	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.36	8 (14%)
43	A86	19	303	-	44,50,50	1.30	5 (11%)	51,76,76	3.32	22 (43%)
37	LMG	10	319	-	31,31,55	1.41	4 (12%)	39,39,63	1.32	4 (10%)
31	CLA	c	504	31	69,73,73	1.29	11 (15%)	83,113,113	1.49	15 (18%)
33	BCR	C	516	-	41,41,41	1.24	5 (12%)	56,56,56	1.35	9 (16%)
31	CLA	C	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.47	9 (10%)
37	LMG	b	621	-	51,51,55	0.89	4 (7%)	59,59,63	1.50	11 (18%)
43	A86	10	304	-	44,50,50	1.28	4 (9%)	51,76,76	4.45	25 (49%)
37	LMG	f	102	-	46,46,55	0.96	4 (8%)	54,54,63	1.49	9 (16%)
43	A86	16	306	31	44,50,50	1.45	5 (11%)	51,76,76	3.81	24 (47%)
43	A86	13	306	43	44,50,50	1.37	3 (6%)	51,76,76	4.62	23 (45%)
31	CLA	D	405	4	69,73,73	1.39	12 (17%)	83,113,113	1.61	11 (13%)
43	A86	8	306	-	44,50,50	1.43	6 (13%)	51,76,76	3.66	22 (43%)
31	CLA	4	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	9 (10%)
37	LMG	D	404	4	40,40,55	1.10	4 (10%)	48,48,63	1.52	7 (14%)
43	A86	12	301	-	44,50,50	1.36	4 (9%)	51,76,76	4.70	26 (50%)
42	KC1	16	314	27	49,53,53	2.95	19 (38%)	63,89,89	6.04	38 (60%)
42	KC1	P	609	-	49,53,53	2.67	18 (36%)	63,89,89	4.23	38 (60%)
36	LHG	b	623	-	42,42,48	0.73	1 (2%)	45,48,54	1.21	4 (8%)
43	A86	4	305	-	44,50,50	1.52	9 (20%)	51,76,76	4.09	23 (45%)
31	CLA	9	312	43	69,73,73	1.27	9 (13%)	83,113,113	1.41	10 (12%)
45	KC2	15	308	-	49,53,53	2.94	22 (44%)	62,89,89	4.82	39 (62%)
31	CLA	14	311	-	50,54,73	1.44	10 (20%)	60,90,113	1.68	11 (18%)
38	DGD	H	102	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	8 (10%)
31	CLA	B	608	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	BCR	y	101	-	41,41,41	1.33	4 (9%)	56,56,56	1.59	12 (21%)
43	A86	6	301	43	44,50,50	1.30	4 (9%)	51,76,76	4.04	28 (54%)
43	A86	15	301	31	44,50,50	1.61	7 (15%)	51,76,76	4.24	23 (45%)
45	KC2	17	309	-	49,53,53	2.97	21 (42%)	62,89,89	4.38	30 (48%)
43	A86	1	306	-	44,50,50	1.42	7 (15%)	51,76,76	4.32	25 (49%)
37	LMG	w	201	-	48,48,55	0.97	6 (12%)	56,56,63	1.41	9 (16%)
31	CLA	10	317	-	52,56,73	1.47	11 (21%)	62,92,113	1.55	9 (14%)
31	CLA	15	306	-	46,50,73	1.53	7 (15%)	55,85,113	1.84	12 (21%)
31	CLA	15	312	-	51,55,73	1.61	12 (23%)	61,91,113	1.77	16 (26%)
42	KC1	1	314	-	49,53,53	2.80	18 (36%)	63,89,89	4.31	36 (57%)
31	CLA	2	311	-	49,53,73	1.52	10 (20%)	59,89,113	1.52	8 (13%)
31	CLA	z	103	-	52,56,73	1.48	11 (21%)	62,92,113	1.57	10 (16%)
31	CLA	9	311	43	50,54,73	1.47	6 (12%)	60,90,113	1.85	8 (13%)
43	A86	11	319	-	44,50,50	1.29	4 (9%)	51,76,76	3.28	18 (35%)
31	CLA	19	310	-	69,73,73	1.25	7 (10%)	83,113,113	1.39	7 (8%)
37	LMG	M	101	-	40,40,55	0.88	1 (2%)	48,48,63	1.31	5 (10%)
33	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.46	11 (19%)
31	CLA	p	605	16	45,49,73	1.52	9 (20%)	54,84,113	1.67	10 (18%)
45	KC2	2	308	-	49,53,53	2.99	21 (42%)	62,89,89	4.41	31 (50%)
45	KC2	6	310	-	49,53,53	2.94	22 (44%)	62,89,89	4.35	32 (51%)
36	LHG	D	408	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	7 (13%)
36	LHG	18	316	-	30,30,48	0.83	1 (3%)	33,36,54	1.22	2 (6%)
43	A86	18	301	-	44,50,50	1.47	5 (11%)	51,76,76	4.91	26 (50%)
42	KC1	12	314	-	49,53,53	2.77	17 (34%)	63,89,89	4.27	36 (57%)
36	LHG	z	102	-	24,24,48	0.95	0	27,30,54	1.30	3 (11%)
41	HEM	e	101	5,6	50,50,50	1.48	5 (10%)	66,82,82	1.13	5 (7%)
43	A86	5	301	31	44,50,50	1.50	5 (11%)	51,76,76	4.25	27 (52%)
36	LHG	15	316	-	24,24,48	0.79	0	27,30,54	1.25	2 (7%)
43	A86	2	303	-	44,50,50	1.35	5 (11%)	51,76,76	3.33	25 (49%)
43	A86	13	304	-	44,50,50	1.66	8 (18%)	51,76,76	5.39	27 (52%)
31	CLA	b	603	2	69,73,73	1.30	13 (18%)	83,113,113	1.46	12 (14%)
31	CLA	3	307	-	46,50,73	1.50	7 (15%)	55,85,113	1.93	15 (27%)
31	CLA	B	603	2	69,73,73	1.29	9 (13%)	83,113,113	1.57	15 (18%)
43	A86	9	306	-	44,50,50	1.61	8 (18%)	51,76,76	3.12	19 (37%)
31	CLA	0	314	-	51,55,73	1.49	11 (21%)	61,91,113	1.54	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	12	308	-	69,73,73	1.27	11 (15%)	83,113,113	1.52	12 (14%)
31	CLA	6	314	-	46,50,73	1.73	10 (21%)	55,85,113	2.03	13 (23%)
43	A86	14	304	-	44,50,50	1.31	5 (11%)	51,76,76	3.18	23 (45%)
31	CLA	9	310	-	69,73,73	1.24	7 (10%)	83,113,113	1.38	7 (8%)
41	HEM	E	101	5,6	50,50,50	1.48	4 (8%)	66,82,82	1.12	4 (6%)
31	CLA	R	101	-	51,55,73	1.43	9 (17%)	61,91,113	1.50	6 (9%)
33	BCR	C	515	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	8 (14%)
31	CLA	5	307	-	69,73,73	1.27	11 (15%)	83,113,113	1.28	10 (12%)
31	CLA	11	315	-	45,49,73	1.57	9 (20%)	54,84,113	1.87	13 (24%)
37	LMG	c	522	-	31,31,55	1.16	3 (9%)	39,39,63	1.20	3 (7%)
37	LMG	14	316	-	49,49,55	0.79	0	57,57,63	1.41	11 (19%)
42	KC1	2	313	27	49,53,53	2.82	19 (38%)	63,89,89	4.68	34 (53%)
43	A86	2	301	-	44,50,50	1.35	5 (11%)	51,76,76	3.44	24 (47%)
31	CLA	10	308	-	54,58,73	1.41	10 (18%)	65,95,113	1.59	8 (12%)
34	SQD	10	320	31	40,41,54	1.12	6 (15%)	49,52,65	1.73	10 (20%)
43	A86	0	301	-	44,50,50	1.37	5 (11%)	51,76,76	4.30	27 (52%)
34	SQD	i	101	-	39,40,54	1.10	5 (12%)	48,51,65	2.00	12 (25%)
42	KC1	7	314	27	49,53,53	2.87	19 (38%)	63,89,89	4.42	35 (55%)
45	KC2	12	311	-	49,53,53	2.89	21 (42%)	62,89,89	4.68	35 (56%)
45	KC2	7	311	27	49,53,53	2.89	22 (44%)	62,89,89	4.69	38 (61%)
33	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.47	9 (16%)
31	CLA	13	307	-	46,50,73	1.51	7 (15%)	55,85,113	1.79	12 (21%)
43	A86	16	303	43	44,50,50	1.44	5 (11%)	51,76,76	5.37	24 (47%)
31	CLA	B	616	-	69,73,73	1.29	10 (14%)	83,113,113	1.52	13 (15%)
31	CLA	B	604	-	69,73,73	1.49	13 (18%)	83,113,113	2.30	19 (22%)
43	A86	11	305	-	44,50,50	1.44	5 (11%)	51,76,76	3.87	34 (66%)
31	CLA	c	503	3,31	69,73,73	1.49	12 (17%)	83,113,113	2.40	21 (25%)
31	CLA	b	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
33	BCR	c	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	7 (12%)
32	PHO	d	403	-	58,69,69	1.92	9 (15%)	56,99,99	1.78	11 (19%)
31	CLA	1	312	-	50,54,73	1.53	12 (24%)	60,90,113	1.56	10 (16%)
31	CLA	2	315	43	50,54,73	1.62	10 (20%)	60,90,113	2.54	20 (33%)
31	CLA	10	314	-	51,55,73	1.49	11 (21%)	61,91,113	1.65	12 (19%)
31	CLA	C	509	3	69,73,73	1.39	11 (15%)	83,113,113	1.77	14 (16%)
31	CLA	C	514	-	53,57,73	1.39	11 (20%)	62,93,113	1.56	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	1	303	-	44,50,50	1.54	7 (15%)	51,76,76	4.68	27 (52%)
31	CLA	C	513	-	69,73,73	1.25	11 (15%)	83,113,113	1.40	9 (10%)
31	CLA	a	406	1	64,68,73	1.26	11 (17%)	77,107,113	1.41	8 (10%)
43	A86	1	302	-	44,50,50	1.29	3 (6%)	51,76,76	4.93	31 (60%)
37	LMG	d	409	4	37,37,55	0.90	2 (5%)	45,45,63	1.36	6 (13%)
43	A86	12	306	-	44,50,50	1.49	9 (20%)	51,76,76	3.91	27 (52%)
31	CLA	19	311	43	50,54,73	1.47	8 (16%)	60,90,113	1.80	7 (11%)
43	A86	7	306	-	44,50,50	1.31	5 (11%)	51,76,76	3.95	23 (45%)
31	CLA	b	617	-	69,73,73	1.29	10 (14%)	83,113,113	1.53	14 (16%)
43	A86	2	305	31	44,50,50	1.46	4 (9%)	51,76,76	3.76	24 (47%)
31	CLA	14	309	-	69,73,73	1.22	8 (11%)	83,113,113	1.44	7 (8%)
31	CLA	16	312	-	51,55,73	1.49	9 (17%)	61,91,113	1.44	8 (13%)
31	CLA	13	312	-	49,53,73	1.48	7 (14%)	59,89,113	1.58	7 (11%)
33	BCR	b	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.38	10 (17%)
43	A86	0	305	-	44,50,50	1.31	4 (9%)	51,76,76	3.36	25 (49%)
36	LHG	14	317	-	34,34,48	0.71	1 (2%)	37,40,54	1.27	4 (10%)
33	BCR	A	407	-	41,41,41	1.25	3 (7%)	56,56,56	1.21	6 (10%)
31	CLA	13	315	-	48,52,73	1.53	8 (16%)	56,87,113	1.41	7 (12%)
31	CLA	B	602	2	69,73,73	1.31	13 (18%)	83,113,113	1.47	12 (14%)
31	CLA	p	604	-	52,56,73	1.45	11 (21%)	62,92,113	1.60	11 (17%)
31	CLA	16	308	-	69,73,73	1.24	11 (15%)	83,113,113	1.50	10 (12%)
31	CLA	p	610	-	45,49,73	1.50	11 (24%)	54,84,113	1.67	10 (18%)
31	CLA	7	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.59	7 (12%)
31	CLA	3	315	-	48,52,73	1.50	8 (16%)	56,87,113	1.50	7 (12%)
37	LMG	k	101	-	46,46,55	1.06	4 (8%)	54,54,63	1.45	8 (14%)
31	CLA	6	309	-	69,73,73	1.24	11 (15%)	83,113,113	1.47	9 (10%)
31	CLA	8	315	-	47,51,73	1.48	11 (23%)	56,86,113	1.58	6 (10%)
31	CLA	14	315	-	47,51,73	1.48	9 (19%)	56,86,113	1.98	9 (16%)
31	CLA	P	605	16	45,49,73	1.53	9 (20%)	54,84,113	1.66	11 (20%)
31	CLA	5	311	-	49,53,73	1.51	10 (20%)	59,89,113	1.89	13 (22%)
43	A86	5	304	-	44,50,50	1.33	5 (11%)	51,76,76	3.90	29 (56%)
31	CLA	15	311	27	49,53,73	1.64	11 (22%)	59,89,113	2.11	17 (28%)
45	KC2	4	310	-	49,53,53	2.89	20 (40%)	62,89,89	4.25	35 (56%)
31	CLA	C	502	-	69,73,73	1.26	11 (15%)	83,113,113	1.46	11 (13%)
43	A86	14	303	-	44,50,50	1.29	4 (9%)	51,76,76	3.02	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	1	310	-	54,58,73	1.35	9 (16%)	65,95,113	1.61	8 (12%)
40	BCT	d	401	30	2,3,3	1.38	0	2,3,3	3.94	1 (50%)
42	KC1	18	313	27,31	49,53,53	2.76	20 (40%)	63,89,89	5.84	37 (58%)
31	CLA	P	610	-	45,49,73	1.49	11 (24%)	54,84,113	1.68	10 (18%)
45	KC2	2	310	-	49,53,53	2.91	22 (44%)	62,89,89	4.80	38 (61%)
31	CLA	7	307	-	45,49,73	1.54	7 (15%)	54,84,113	2.07	18 (33%)
31	CLA	19	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.59	8 (14%)
31	CLA	17	308	-	45,49,73	1.55	11 (24%)	54,84,113	1.63	9 (16%)
36	LHG	L	101	-	48,48,48	0.78	3 (6%)	51,54,54	1.29	7 (13%)
43	A86	3	305	-	44,50,50	1.72	9 (20%)	51,76,76	5.48	28 (54%)
31	CLA	2	312	-	52,56,73	1.76	11 (21%)	62,92,113	2.05	14 (22%)
31	CLA	w	203	-	69,73,73	1.27	10 (14%)	83,113,113	1.52	12 (14%)
31	CLA	12	310	-	47,51,73	1.47	8 (17%)	56,86,113	1.56	7 (12%)
43	A86	18	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.66	19 (37%)
36	LHG	18	315	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
41	HEM	v	201	21	50,50,50	1.40	4 (8%)	66,82,82	1.64	15 (22%)
31	CLA	0	312	26,34	50,54,73	1.50	9 (18%)	60,90,113	1.80	11 (18%)
31	CLA	16	310	-	45,49,73	1.49	7 (15%)	54,84,113	1.70	8 (14%)
43	A86	15	305	27	44,50,50	1.45	5 (11%)	51,76,76	4.12	23 (45%)
43	A86	9	305	-	44,50,50	1.58	6 (13%)	51,76,76	5.12	24 (47%)
31	CLA	10	307	-	52,56,73	1.51	9 (17%)	62,92,113	1.77	15 (24%)
43	A86	19	306	-	44,50,50	1.36	4 (9%)	51,76,76	2.97	14 (27%)
31	CLA	c	507	-	69,73,73	1.30	10 (14%)	83,113,113	1.45	8 (9%)
43	A86	1	305	-	44,50,50	1.55	6 (13%)	51,76,76	3.97	34 (66%)
45	KC2	6	312	27	49,53,53	2.93	21 (42%)	62,89,89	4.68	38 (61%)
43	A86	0	302	26	44,50,50	1.55	6 (13%)	51,76,76	3.58	23 (45%)
31	CLA	C	511	3	69,73,73	1.27	10 (14%)	83,113,113	1.41	10 (12%)
43	A86	17	305	-	44,50,50	1.73	9 (20%)	51,76,76	5.58	24 (47%)
34	SQD	B	623	-	53,54,54	0.91	5 (9%)	62,65,65	1.74	12 (19%)
31	CLA	c	509	3	69,73,73	1.39	11 (15%)	83,113,113	1.76	14 (16%)
43	A86	5	302	-	44,50,50	1.50	5 (11%)	51,76,76	3.24	26 (50%)
43	A86	14	301	-	44,50,50	1.37	4 (9%)	51,76,76	2.76	22 (43%)
45	KC2	7	309	-	49,53,53	2.97	22 (44%)	62,89,89	4.40	31 (50%)
43	A86	14	302	43	44,50,50	1.44	5 (11%)	51,76,76	2.43	17 (33%)
33	BCR	C	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	12	312	-	49,53,73	1.46	9 (18%)	59,89,113	1.67	9 (15%)
43	A86	8	305	-	44,50,50	1.56	6 (13%)	51,76,76	4.36	25 (49%)
31	CLA	11	313	-	69,73,73	1.36	10 (14%)	83,113,113	1.52	12 (14%)
38	DGD	W	203	-	57,57,67	1.15	8 (14%)	71,71,81	1.48	10 (14%)
43	A86	16	305	43	44,50,50	1.70	7 (15%)	51,76,76	5.47	29 (56%)
43	A86	13	305	-	44,50,50	1.34	4 (9%)	51,76,76	3.10	19 (37%)
43	A86	12	303	-	44,50,50	1.36	4 (9%)	51,76,76	3.21	21 (41%)
33	BCR	B	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.38	10 (17%)
31	CLA	B	611	2	69,73,73	1.45	11 (15%)	83,113,113	1.77	12 (14%)
43	A86	13	302	-	44,50,50	1.51	4 (9%)	51,76,76	4.78	27 (52%)
45	KC2	11	311	-	49,53,53	2.80	19 (38%)	62,89,89	4.37	36 (58%)
31	CLA	2	314	-	45,49,73	1.53	8 (17%)	54,84,113	1.62	9 (16%)
31	CLA	11	307	27	47,51,73	1.51	8 (17%)	56,86,113	2.21	20 (35%)
31	CLA	13	316	-	69,73,73	1.22	7 (10%)	83,113,113	1.44	10 (12%)
31	CLA	15	313	-	45,49,73	1.57	9 (20%)	54,84,113	1.64	11 (20%)
31	CLA	b	607	-	69,73,73	1.29	11 (15%)	83,113,113	1.95	22 (26%)
37	LMG	c	521	-	51,51,55	0.90	2 (3%)	59,59,63	1.24	4 (6%)
31	CLA	10	313	26	46,50,73	1.53	9 (19%)	55,85,113	1.89	8 (14%)
31	CLA	10	316	-	50,54,73	1.45	9 (18%)	60,90,113	1.50	7 (11%)
31	CLA	B	607	-	69,73,73	1.28	10 (14%)	83,113,113	1.40	7 (8%)
43	A86	p	613	31	44,50,50	1.42	4 (9%)	51,76,76	3.70	29 (56%)
43	A86	1	320	-	44,50,50	1.39	5 (11%)	51,76,76	3.60	26 (50%)
43	A86	6	303	-	44,50,50	1.42	5 (11%)	51,76,76	4.20	26 (50%)
31	CLA	B	609	-	69,73,73	1.22	9 (13%)	83,113,113	1.36	10 (12%)
37	LMG	5	315	-	37,37,55	1.00	4 (10%)	45,45,63	1.17	3 (6%)
35	PL9	D	407	-	55,55,55	2.03	15 (27%)	68,69,69	1.42	12 (17%)
42	KC1	6	315	27	49,53,53	2.91	20 (40%)	63,89,89	6.52	39 (61%)
43	A86	6	302	-	44,50,50	1.43	5 (11%)	51,76,76	3.58	23 (45%)
38	DGD	c	519	-	63,63,67	1.12	10 (15%)	77,77,81	1.52	15 (19%)
31	CLA	p	603	-	54,58,73	1.41	11 (20%)	65,95,113	1.57	12 (18%)
31	CLA	z	101	-	55,59,73	1.40	11 (20%)	66,96,113	1.45	6 (9%)
31	CLA	b	612	2	69,73,73	1.45	11 (15%)	83,113,113	1.77	12 (14%)
37	LMG	K	101	-	46,46,55	1.06	4 (8%)	54,54,63	1.45	8 (14%)
43	A86	17	301	-	44,50,50	1.48	8 (18%)	51,76,76	4.54	24 (47%)
31	CLA	17	313	27	54,58,73	1.65	11 (20%)	65,95,113	1.88	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	a	403	1	69,73,73	1.31	10 (14%)	83,113,113	1.43	11 (13%)
31	CLA	C	505	-	69,73,73	1.23	12 (17%)	83,113,113	1.61	8 (9%)
31	CLA	8	312	-	50,54,73	1.48	10 (20%)	60,90,113	1.65	11 (18%)
45	KC2	12	309	-	49,53,53	2.88	18 (36%)	62,89,89	4.38	38 (61%)
38	DGD	h	102	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	8 (10%)
35	PL9	d	407	-	55,55,55	2.04	15 (27%)	68,69,69	1.42	12 (17%)
31	CLA	c	513	-	69,73,73	1.24	11 (15%)	83,113,113	1.40	8 (9%)
31	CLA	5	312	-	51,55,73	1.51	11 (21%)	61,91,113	1.62	11 (18%)
43	A86	0	303	-	44,50,50	1.51	7 (15%)	51,76,76	3.57	25 (49%)
31	CLA	W	202	-	69,73,73	1.26	10 (14%)	83,113,113	1.52	12 (14%)
45	KC2	5	310	27	49,53,53	2.81	22 (44%)	62,89,89	4.31	36 (58%)
31	CLA	P	603	-	54,58,73	1.42	11 (20%)	65,95,113	1.57	12 (18%)
31	CLA	7	308	-	45,49,73	1.55	10 (22%)	54,84,113	1.65	9 (16%)
37	LMG	C	522	-	51,51,55	0.89	2 (3%)	59,59,63	1.24	4 (6%)
31	CLA	16	315	-	47,51,73	1.50	6 (12%)	56,86,113	1.54	7 (12%)
31	CLA	2	306	-	46,50,73	1.49	5 (10%)	55,85,113	2.11	14 (25%)
37	LMG	4	316	-	49,49,55	0.82	1 (2%)	57,57,63	1.45	13 (22%)
37	LMG	5	316	-	36,36,55	1.22	4 (11%)	44,44,63	1.76	8 (18%)
44	DD6	p	612	-	39,45,45	2.20	6 (15%)	52,67,67	3.59	26 (50%)
37	LMG	D	409	4	37,37,55	0.90	1 (2%)	45,45,63	1.36	6 (13%)
31	CLA	18	306	42	54,58,73	1.41	11 (20%)	65,95,113	1.75	14 (21%)
31	CLA	8	310	-	56,60,73	1.36	10 (17%)	67,97,113	1.62	8 (11%)
31	CLA	9	307	-	65,69,73	1.28	7 (10%)	78,108,113	1.48	8 (10%)
43	A86	7	304	-	44,50,50	1.53	6 (13%)	51,76,76	5.71	31 (60%)
45	KC2	19	309	28	49,53,53	2.90	20 (40%)	62,89,89	4.69	38 (61%)
42	KC1	11	314	-	49,53,53	2.76	20 (40%)	63,89,89	4.49	37 (58%)
31	CLA	9	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.58	8 (14%)
43	A86	19	304	-	44,50,50	1.29	4 (9%)	51,76,76	4.23	20 (39%)
31	CLA	18	314	27	47,51,73	1.47	10 (21%)	56,86,113	1.67	7 (12%)
45	KC2	17	311	27	49,53,53	2.91	21 (42%)	62,89,89	4.55	37 (59%)
31	CLA	1	315	27	45,49,73	1.58	7 (15%)	54,84,113	1.53	3 (5%)
31	CLA	b	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.44	8 (9%)
31	CLA	13	313	-	69,73,73	1.41	12 (17%)	83,113,113	1.56	13 (15%)
32	PHO	D	403	-	58,69,69	1.93	9 (15%)	56,99,99	1.78	12 (21%)
31	CLA	c	510	3	69,73,73	1.26	11 (15%)	83,113,113	1.55	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	b	606	-	69,73,73	1.32	11 (15%)	83,113,113	1.55	9 (10%)
31	CLA	7	313	-	54,58,73	1.65	12 (22%)	65,95,113	1.86	15 (23%)
31	CLA	3	313	-	69,73,73	1.45	11 (15%)	83,113,113	1.57	11 (13%)
31	CLA	B	615	-	69,73,73	1.28	10 (14%)	83,113,113	1.53	9 (10%)
37	LMG	P	614	-	31,31,55	0.93	1 (3%)	39,39,63	1.70	9 (23%)
33	BCR	Y	101	-	41,41,41	1.34	4 (9%)	56,56,56	1.59	14 (25%)
43	A86	13	303	-	44,50,50	1.32	3 (6%)	51,76,76	2.92	18 (35%)
45	KC2	13	311	-	49,53,53	3.02	21 (42%)	62,89,89	4.37	33 (53%)
31	CLA	P	606	-	47,51,73	2.06	10 (21%)	56,86,113	3.99	29 (51%)
34	SQD	a	408	38	53,54,54	0.96	6 (11%)	62,65,65	1.56	12 (19%)
42	KC1	5	313	-	49,53,53	2.81	20 (40%)	63,89,89	5.41	40 (63%)
43	A86	10	306	-	44,50,50	1.44	4 (9%)	51,76,76	3.10	19 (37%)
42	KC1	3	314	27	49,53,53	2.84	19 (38%)	63,89,89	5.62	36 (57%)
31	CLA	A	404	-	53,57,73	1.43	10 (18%)	62,93,113	1.60	11 (17%)
37	LMG	N	101	14	28,28,55	1.12	4 (14%)	36,36,63	1.31	6 (16%)
43	A86	6	305	43	44,50,50	1.73	10 (22%)	51,76,76	5.46	30 (58%)
31	CLA	P	604	-	52,56,73	1.45	12 (23%)	62,92,113	1.59	11 (17%)
36	LHG	w	202	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	4 (9%)
42	KC1	15	317	27	49,53,53	2.82	19 (38%)	63,89,89	4.78	40 (63%)
45	KC2	14	308	27	49,53,53	2.88	21 (42%)	62,89,89	4.74	34 (54%)
31	CLA	c	502	-	69,73,73	1.26	11 (15%)	83,113,113	1.46	11 (13%)
31	CLA	A	406	1	64,68,73	1.26	10 (15%)	77,107,113	1.41	8 (10%)
31	CLA	0	309	-	63,67,73	1.30	10 (15%)	75,105,113	1.48	10 (13%)
43	A86	15	303	-	44,50,50	1.42	5 (11%)	51,76,76	4.15	23 (45%)
31	CLA	0	316	-	50,54,73	1.46	9 (18%)	60,90,113	1.50	8 (13%)
31	CLA	9	313	-	69,73,73	1.20	9 (13%)	83,113,113	1.98	13 (15%)
43	A86	10	303	-	44,50,50	1.47	7 (15%)	51,76,76	3.57	25 (49%)
33	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.42	8 (14%)
43	A86	12	304	-	44,50,50	1.39	5 (11%)	51,76,76	3.94	18 (35%)
43	A86	17	306	-	44,50,50	1.44	4 (9%)	51,76,76	3.70	22 (43%)
31	CLA	D	402	-	69,73,73	1.25	11 (15%)	83,113,113	1.52	11 (13%)
31	CLA	3	308	-	47,51,73	1.52	10 (21%)	56,86,113	1.68	8 (14%)
31	CLA	6	316	-	47,51,73	1.51	7 (14%)	56,86,113	1.54	8 (14%)
31	CLA	1	313	-	69,73,73	1.36	10 (14%)	83,113,113	1.45	13 (15%)
31	CLA	4	309	-	69,73,73	1.23	8 (11%)	83,113,113	1.45	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	7	302	-	44,50,50	1.60	8 (18%)	51,76,76	4.10	25 (49%)
31	CLA	5	314	-	45,49,73	1.55	7 (15%)	54,84,113	1.53	7 (12%)
37	LMG	d	404	-	40,40,55	1.07	4 (10%)	48,48,63	1.55	7 (14%)
42	KC1	19	314	-	49,53,53	2.87	22 (44%)	63,89,89	4.45	38 (60%)
37	LMG	B	620	-	51,51,55	0.90	4 (7%)	59,59,63	1.50	11 (18%)
33	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	8 (14%)
43	A86	6	304	-	44,50,50	1.36	6 (13%)	51,76,76	3.40	22 (43%)
36	LHG	B	622	-	42,42,48	0.74	1 (2%)	45,48,54	1.21	4 (8%)
45	KC2	13	309	-	49,53,53	2.91	20 (40%)	62,89,89	4.12	31 (50%)
31	CLA	b	610	-	69,73,73	1.22	9 (13%)	83,113,113	1.37	10 (12%)
43	A86	17	303	-	44,50,50	1.41	6 (13%)	51,76,76	3.72	22 (43%)
38	DGD	C	518	-	56,56,67	1.23	10 (17%)	70,70,81	1.68	17 (24%)
37	LMG	0	317	-	31,31,55	1.35	3 (9%)	39,39,63	1.39	6 (15%)
38	DGD	C	520	34	63,63,67	1.18	10 (15%)	77,77,81	1.58	13 (16%)
43	A86	17	304	-	44,50,50	1.33	4 (9%)	51,76,76	3.13	13 (25%)
31	CLA	14	306	-	65,69,73	1.49	12 (18%)	78,108,113	2.24	21 (26%)
38	DGD	w	204	-	57,57,67	1.15	7 (12%)	71,71,81	1.48	10 (14%)
45	KC2	9	309	28	49,53,53	2.89	20 (40%)	62,89,89	4.63	38 (61%)
43	A86	11	306	-	44,50,50	1.77	8 (18%)	51,76,76	5.16	25 (49%)
33	BCR	c	516	-	41,41,41	1.24	5 (12%)	56,56,56	1.35	8 (14%)
31	CLA	16	313	-	46,50,73	1.85	13 (28%)	55,85,113	2.44	20 (36%)
43	A86	10	301	-	44,50,50	1.39	5 (11%)	51,76,76	4.35	28 (54%)
45	KC2	15	310	27	49,53,53	2.80	23 (46%)	62,89,89	4.44	36 (58%)
31	CLA	B	614	2	69,73,73	1.25	11 (15%)	83,113,113	1.49	11 (13%)
43	A86	P	611	-	44,50,50	1.87	10 (22%)	51,76,76	6.02	30 (58%)
45	KC2	18	308	-	49,53,53	2.84	22 (44%)	62,89,89	4.43	34 (54%)
37	LMG	m	101	-	40,40,55	0.95	1 (2%)	48,48,63	1.34	3 (6%)
45	KC2	5	308	-	49,53,53	2.92	23 (46%)	62,89,89	4.67	39 (62%)
31	CLA	C	512	3	69,73,73	1.31	10 (14%)	83,113,113	1.56	11 (13%)
31	CLA	11	312	27	50,54,73	1.53	10 (20%)	60,90,113	1.60	9 (15%)
37	LMG	p	614	-	31,31,55	0.94	1 (3%)	39,39,63	1.69	9 (23%)
42	KC1	13	314	-	49,53,53	2.83	18 (36%)	63,89,89	4.78	40 (63%)
31	CLA	5	306	-	46,50,73	1.53	8 (17%)	55,85,113	1.77	16 (29%)
31	CLA	C	504	31	69,73,73	1.28	11 (15%)	83,113,113	1.49	15 (18%)
34	SQD	b	601	38	53,54,54	0.90	5 (9%)	62,65,65	1.74	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	10	312	26,34	50,54,73	1.48	9 (18%)	60,90,113	1.78	11 (18%)
42	KC1	p	609	-	49,53,53	2.67	19 (38%)	63,89,89	4.23	38 (60%)
43	A86	11	303	-	44,50,50	1.49	4 (9%)	51,76,76	4.52	28 (54%)
43	A86	4	304	-	44,50,50	1.30	4 (9%)	51,76,76	3.07	20 (39%)
45	KC2	1	309	-	49,53,53	2.88	21 (42%)	62,89,89	4.31	34 (54%)
43	A86	5	303	-	44,50,50	1.33	5 (11%)	51,76,76	4.15	24 (47%)
43	A86	11	302	-	44,50,50	1.48	6 (13%)	51,76,76	5.53	30 (58%)
43	A86	12	302	-	44,50,50	1.48	5 (11%)	51,76,76	4.72	30 (58%)
31	CLA	19	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.42	12 (14%)
43	A86	15	302	-	44,50,50	1.47	5 (11%)	51,76,76	4.46	29 (56%)
43	A86	10	302	-	44,50,50	1.45	5 (11%)	51,76,76	3.12	20 (39%)
31	CLA	1	308	-	69,73,73	1.27	9 (13%)	83,113,113	1.41	9 (10%)
36	LHG	A	410	1	36,36,48	0.76	1 (2%)	39,42,54	1.24	4 (10%)
31	CLA	p	607	43	47,51,73	1.50	11 (23%)	56,86,113	1.68	10 (17%)
43	A86	P	613	31	44,50,50	1.42	4 (9%)	51,76,76	3.70	29 (56%)
37	LMG	j	101	-	50,50,55	0.95	3 (6%)	58,58,63	1.32	4 (6%)
31	CLA	0	313	-	46,50,73	1.55	10 (21%)	55,85,113	2.09	11 (20%)
31	CLA	B	612	2	69,73,73	1.26	11 (15%)	83,113,113	1.60	12 (14%)
31	CLA	C	503	3,31	69,73,73	1.49	12 (17%)	83,113,113	2.40	21 (25%)
43	A86	7	303	-	44,50,50	1.30	4 (9%)	51,76,76	3.07	13 (25%)
31	CLA	18	311	27	50,54,73	1.54	10 (20%)	60,90,113	1.67	11 (18%)
40	BCT	D	401	30	2,3,3	1.38	0	2,3,3	3.94	1 (50%)
43	A86	17	302	-	44,50,50	1.79	9 (20%)	51,76,76	3.62	25 (49%)
31	CLA	b	613	2	69,73,73	1.26	11 (15%)	83,113,113	1.59	12 (14%)
33	BCR	a	407	-	41,41,41	1.25	3 (7%)	56,56,56	1.22	6 (10%)
42	KC1	17	314	27	49,53,53	2.79	19 (38%)	63,89,89	5.20	36 (57%)
31	CLA	P	601	16	69,73,73	1.26	11 (15%)	83,113,113	1.31	6 (7%)
45	KC2	16	311	-	49,53,53	2.93	21 (42%)	62,89,89	4.66	37 (59%)
43	A86	4	306	-	44,50,50	1.38	5 (11%)	51,76,76	3.99	25 (49%)
43	A86	14	305	-	44,50,50	1.48	8 (18%)	51,76,76	4.18	29 (56%)
31	CLA	b	615	2	69,73,73	1.25	11 (15%)	83,113,113	1.51	12 (14%)
31	CLA	c	505	-	69,73,73	1.23	12 (17%)	83,113,113	1.61	9 (10%)
31	CLA	p	606	-	47,51,73	2.06	10 (21%)	56,86,113	3.98	30 (53%)
43	A86	16	304	-	44,50,50	1.35	6 (13%)	51,76,76	3.49	24 (47%)
38	DGD	b	622	34	56,56,67	1.30	9 (16%)	70,70,81	1.62	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	KC1	9	314	-	49,53,53	2.87	22 (44%)	63,89,89	4.45	38 (60%)
37	LMG	11	317	-	45,45,55	0.96	2 (4%)	53,53,63	1.25	5 (9%)
43	A86	11	320	-	44,50,50	1.37	3 (6%)	51,76,76	3.74	22 (43%)
31	CLA	13	308	-	47,51,73	1.52	10 (21%)	56,86,113	1.62	10 (17%)
31	CLA	c	511	3	69,73,73	1.27	11 (15%)	83,113,113	1.42	10 (12%)
31	CLA	B	613	2	69,73,73	1.29	11 (15%)	83,113,113	1.26	7 (8%)
34	SQD	A	408	38	53,54,54	0.96	6 (11%)	62,65,65	1.56	13 (20%)
31	CLA	C	510	3	69,73,73	1.26	11 (15%)	83,113,113	1.56	10 (12%)
43	A86	8	302	-	44,50,50	1.74	7 (15%)	51,76,76	4.70	35 (68%)
31	CLA	0	307	-	52,56,73	1.48	11 (21%)	62,92,113	1.60	11 (17%)
35	PL9	a	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.46	6 (14%)
36	LHG	P	615	-	26,26,48	0.87	1 (3%)	29,32,54	1.35	3 (10%)
34	SQD	l	101	-	53,54,54	0.94	5 (9%)	62,65,65	1.51	11 (17%)
31	CLA	d	405	4	69,73,73	1.39	12 (17%)	83,113,113	1.61	11 (13%)
42	KC1	10	315	-	49,53,53	2.69	17 (34%)	63,89,89	5.41	41 (65%)
43	A86	3	302	-	44,50,50	1.38	5 (11%)	51,76,76	3.58	27 (52%)
31	CLA	19	313	-	69,73,73	1.21	8 (11%)	83,113,113	2.01	14 (16%)
31	CLA	4	315	-	47,51,73	1.49	11 (23%)	56,86,113	1.82	8 (14%)
42	KC1	4	313	-	49,53,53	2.66	17 (34%)	63,89,89	4.91	40 (63%)
33	BCR	H	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	8 (14%)
43	A86	1	304	31	44,50,50	1.43	5 (11%)	51,76,76	2.85	18 (35%)
31	CLA	19	307	-	65,69,73	1.28	7 (10%)	78,108,113	1.48	9 (11%)
31	CLA	7	312	-	51,55,73	1.51	10 (19%)	61,91,113	1.42	8 (13%)
31	CLA	5	309	-	59,63,73	1.31	9 (15%)	71,101,113	1.62	13 (18%)
31	CLA	14	312	-	55,59,73	1.61	11 (20%)	66,96,113	1.84	16 (24%)
43	A86	3	301	-	44,50,50	1.62	9 (20%)	51,76,76	4.06	26 (50%)
45	KC2	8	309	-	49,53,53	2.82	21 (42%)	62,89,89	4.39	34 (54%)
31	CLA	17	310	-	49,53,73	1.48	7 (14%)	59,89,113	1.61	7 (11%)
31	CLA	c	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.49	10 (12%)
45	KC2	10	310	26	49,53,53	2.72	20 (40%)	62,89,89	4.36	35 (56%)
31	CLA	12	307	-	46,50,73	1.54	9 (19%)	55,85,113	2.01	20 (36%)
43	A86	7	301	-	44,50,50	1.42	5 (11%)	51,76,76	3.49	24 (47%)
31	CLA	B	606	-	69,73,73	1.29	10 (14%)	83,113,113	1.97	22 (26%)
43	A86	8	303	-	44,50,50	1.50	5 (11%)	51,76,76	3.64	27 (52%)
43	A86	19	301	-	44,50,50	1.32	4 (9%)	51,76,76	4.46	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	b	608	-	69,73,73	1.28	10 (14%)	83,113,113	1.39	8 (9%)
31	CLA	3	312	-	49,53,73	1.51	9 (18%)	59,89,113	1.58	8 (13%)
42	KC1	8	314	31,43	49,53,53	2.64	19 (38%)	63,89,89	6.02	36 (57%)
31	CLA	18	312	27	59,63,73	1.50	12 (20%)	71,101,113	1.74	16 (22%)
43	A86	16	302	-	44,50,50	1.56	6 (13%)	51,76,76	3.53	24 (47%)
33	BCR	b	620	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	9 (16%)
43	A86	3	303	-	44,50,50	1.47	4 (9%)	51,76,76	4.77	28 (54%)
31	CLA	P	607	43	47,51,73	1.49	11 (23%)	56,86,113	1.69	11 (19%)
36	LHG	l	102	-	48,48,48	0.79	3 (6%)	51,54,54	1.29	7 (13%)
31	CLA	c	512	3	69,73,73	1.31	10 (14%)	83,113,113	1.56	11 (13%)
31	CLA	3	310	-	45,49,73	1.49	7 (15%)	54,84,113	1.68	9 (16%)
45	KC2	14	310	-	49,53,53	2.88	19 (38%)	62,89,89	4.22	35 (56%)
37	LMG	1	301	-	36,36,55	1.17	4 (11%)	44,44,63	1.44	6 (13%)
43	A86	p	611	-	44,50,50	1.88	10 (22%)	51,76,76	6.01	30 (58%)
33	BCR	F	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.42	8 (14%)
31	CLA	a	404	-	53,57,73	1.43	10 (18%)	62,93,113	1.61	11 (17%)
35	PL9	A	409	-	33,33,55	1.29	5 (15%)	41,42,69	1.47	6 (14%)
43	A86	9	302	-	44,50,50	1.31	4 (9%)	51,76,76	3.02	19 (37%)
31	CLA	15	307	-	69,73,73	1.27	11 (15%)	83,113,113	1.29	9 (10%)
29	OEX	a	401	3,1	0,14,14	-	-	-		
31	CLA	17	312	-	51,55,73	1.49	11 (21%)	61,91,113	1.41	8 (13%)
36	LHG	Z	103	-	24,24,48	0.95	0	27,30,54	1.30	3 (11%)
43	A86	11	304	31	44,50,50	1.42	6 (13%)	51,76,76	2.96	22 (43%)
36	LHG	p	615	-	26,26,48	0.87	1 (3%)	29,32,54	1.35	3 (10%)
36	LHG	4	317	-	34,34,48	0.76	1 (2%)	37,40,54	1.25	3 (8%)
31	CLA	C	506	-	69,73,73	1.22	12 (17%)	83,113,113	1.49	8 (9%)
37	LMG	F	102	-	46,46,55	0.96	4 (8%)	54,54,63	1.49	9 (16%)
33	BCR	c	515	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	8 (14%)
43	A86	4	301	-	44,50,50	1.31	4 (9%)	51,76,76	3.65	22 (43%)
43	A86	9	301	-	44,50,50	1.30	3 (6%)	51,76,76	4.38	25 (49%)
31	CLA	10	309	-	63,67,73	1.29	10 (15%)	75,105,113	1.46	11 (14%)
31	CLA	14	314	-	47,51,73	1.50	10 (21%)	56,86,113	1.64	6 (10%)
44	DD6	P	612	-	39,45,45	2.10	4 (10%)	52,67,67	2.33	17 (32%)
31	CLA	17	307	-	45,49,73	1.53	6 (13%)	54,84,113	2.04	16 (29%)
38	DGD	c	518	-	56,56,67	1.22	10 (17%)	70,70,81	1.68	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	KC2	3	311	-	49,53,53	2.92	20 (40%)	62,89,89	4.66	36 (58%)
31	CLA	c	514	-	53,57,73	1.39	11 (20%)	62,93,113	1.56	8 (12%)
31	CLA	P	608	16	55,59,73	1.41	10 (18%)	66,96,113	1.51	6 (9%)
31	CLA	b	611	-	69,73,73	1.28	11 (15%)	83,113,113	1.41	9 (10%)
37	LMG	11	301	-	36,36,55	1.16	4 (11%)	44,44,63	1.44	6 (13%)
38	DGD	c	520	34	63,63,67	1.18	10 (15%)	77,77,81	1.58	14 (18%)
31	CLA	b	614	2	69,73,73	1.28	11 (15%)	83,113,113	1.27	7 (8%)
31	CLA	B	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
31	CLA	4	312	27	55,59,73	1.62	11 (20%)	66,96,113	2.09	18 (27%)
43	A86	18	303	-	44,50,50	1.51	5 (11%)	51,76,76	2.80	19 (37%)
37	LMG	n	701	14	28,28,55	1.11	4 (14%)	36,36,63	1.32	6 (16%)
31	CLA	1	321	-	65,69,73	1.37	10 (15%)	78,108,113	2.09	21 (26%)
31	CLA	2	307	-	69,73,73	1.26	11 (15%)	83,113,113	1.56	10 (12%)
32	PHO	a	405	-	58,69,69	1.93	10 (17%)	56,99,99	1.76	10 (17%)
31	CLA	11	316	43	45,49,73	1.58	9 (20%)	54,84,113	1.54	8 (14%)
31	CLA	12	316	-	50,54,73	1.51	7 (14%)	60,90,113	1.53	8 (13%)
31	CLA	b	604	2	69,73,73	1.29	9 (13%)	83,113,113	1.56	15 (18%)
43	A86	2	304	-	44,50,50	1.59	7 (15%)	51,76,76	5.40	26 (50%)
43	A86	4	303	-	44,50,50	1.40	7 (15%)	51,76,76	2.98	18 (35%)
31	CLA	p	601	16	69,73,73	1.25	11 (15%)	83,113,113	1.32	6 (7%)
31	CLA	13	310	-	45,49,73	1.49	8 (17%)	54,84,113	1.63	8 (14%)
43	A86	9	303	-	44,50,50	1.29	4 (9%)	51,76,76	3.20	21 (41%)
43	A86	5	305	-	44,50,50	1.51	7 (15%)	51,76,76	3.49	23 (45%)
45	KC2	11	309	-	49,53,53	2.80	18 (36%)	62,89,89	4.58	35 (56%)
43	A86	4	302	-	44,50,50	1.56	5 (11%)	51,76,76	4.11	28 (54%)
31	CLA	0	311	-	59,63,73	1.34	11 (18%)	71,101,113	1.49	10 (14%)
37	LMG	15	314	-	37,37,55	0.98	3 (8%)	45,45,63	1.13	2 (4%)
31	CLA	2	309	-	47,51,73	1.46	7 (14%)	56,86,113	1.61	7 (12%)
36	LHG	C	521	-	39,39,48	0.67	1 (2%)	42,45,54	1.22	4 (9%)
43	A86	0	304	-	44,50,50	1.27	5 (11%)	51,76,76	4.49	25 (49%)
38	DGD	11	318	-	61,61,67	0.93	3 (4%)	75,75,81	1.32	10 (13%)
36	LHG	5	317	-	24,24,48	0.77	0	27,30,54	1.27	2 (7%)
31	CLA	11	308	-	69,73,73	1.26	10 (14%)	83,113,113	1.55	15 (18%)
43	A86	15	304	-	44,50,50	1.38	5 (11%)	51,76,76	4.51	29 (56%)
43	A86	19	305	-	44,50,50	1.54	6 (13%)	51,76,76	5.10	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	5	318	42	44,50,50	1.29	4 (9%)	51,76,76	3.52	22 (43%)
34	SQD	L	102	-	53,54,54	0.94	5 (9%)	62,65,65	1.52	11 (17%)
31	CLA	18	309	-	56,60,73	1.35	10 (17%)	67,97,113	1.65	8 (11%)
31	CLA	d	402	-	69,73,73	1.25	10 (14%)	83,113,113	1.51	10 (12%)
45	KC2	4	308	27	49,53,53	2.88	20 (40%)	62,89,89	4.72	34 (54%)
31	CLA	15	309	-	59,63,73	1.32	9 (15%)	71,101,113	1.62	11 (15%)
45	KC2	16	309	-	49,53,53	2.94	22 (44%)	62,89,89	4.38	32 (51%)
31	CLA	d	406	-	69,73,73	1.23	9 (13%)	83,113,113	1.39	7 (8%)
31	CLA	12	313	-	52,56,73	1.61	10 (19%)	62,92,113	1.63	13 (20%)
43	A86	6	307	-	44,50,50	1.65	9 (20%)	51,76,76	4.37	25 (49%)
45	KC2	3	309	-	49,53,53	2.96	22 (44%)	62,89,89	4.63	34 (54%)
31	CLA	C	507	-	69,73,73	1.30	10 (14%)	83,113,113	1.45	8 (9%)
31	CLA	8	307	42	54,58,73	1.44	10 (18%)	65,95,113	1.80	13 (20%)
43	A86	10	305	-	44,50,50	1.30	4 (9%)	51,76,76	3.34	25 (49%)
31	CLA	6	313	-	51,55,73	1.48	9 (17%)	61,91,113	1.45	8 (13%)
31	CLA	16	307	-	46,50,73	1.52	7 (15%)	55,85,113	1.98	11 (20%)
41	HEM	V	201	21	50,50,50	1.40	4 (8%)	66,82,82	1.64	15 (22%)
43	A86	8	304	-	44,50,50	1.57	8 (18%)	51,76,76	3.32	24 (47%)
31	CLA	3	316	-	69,73,73	1.30	9 (13%)	83,113,113	2.10	20 (24%)
31	CLA	6	311	-	45,49,73	1.48	7 (15%)	54,84,113	1.70	8 (14%)
31	CLA	4	314	-	47,51,73	1.50	10 (21%)	56,86,113	1.61	7 (12%)
31	CLA	0	308	-	54,58,73	1.41	10 (18%)	65,95,113	1.58	9 (13%)
31	CLA	b	605	-	69,73,73	1.48	14 (20%)	83,113,113	2.30	19 (22%)
43	A86	2	302	-	44,50,50	1.44	5 (11%)	51,76,76	4.73	27 (52%)
31	CLA	P	602	-	69,73,73	1.29	11 (15%)	83,113,113	1.38	8 (9%)
37	LMG	1	317	-	45,45,55	0.99	3 (6%)	53,53,63	1.21	5 (9%)
43	A86	10	318	-	44,50,50	1.47	8 (18%)	51,76,76	3.64	24 (47%)
34	SQD	A	411	-	39,40,54	1.10	5 (12%)	48,51,65	2.01	12 (25%)
36	LHG	8	316	-	38,38,48	0.69	1 (2%)	41,44,54	1.28	4 (9%)
31	CLA	19	312	43	69,73,73	1.26	9 (13%)	83,113,113	1.39	11 (13%)
43	A86	3	304	-	44,50,50	1.58	7 (15%)	51,76,76	2.99	21 (41%)
31	CLA	r	101	-	51,55,73	1.43	9 (17%)	61,91,113	1.51	6 (9%)
31	CLA	10	311	-	59,63,73	1.34	11 (18%)	71,101,113	1.50	9 (12%)
43	A86	1	319	-	44,50,50	1.40	4 (9%)	51,76,76	4.70	27 (52%)
31	CLA	1	307	-	47,51,73	1.47	9 (19%)	56,86,113	1.87	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	A86	19	302	-	44,50,50	1.43	4 (9%)	51,76,76	5.35	23 (45%)
38	DGD	B	621	-	55,55,67	1.34	7 (12%)	69,69,81	1.74	15 (21%)
29	OEX	A	401	3,1	0,14,14	-	-	-		
45	KC2	18	310	27	49,53,53	2.83	20 (40%)	62,89,89	5.08	37 (59%)
32	PHO	A	405	-	58,69,69	1.93	10 (17%)	56,99,99	1.77	10 (17%)
31	CLA	c	506	-	69,73,73	1.23	12 (17%)	83,113,113	1.50	8 (9%)
43	A86	16	301	43	44,50,50	1.36	4 (9%)	51,76,76	4.05	26 (50%)
43	A86	13	301	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	26 (50%)
31	CLA	Z	101	-	55,59,73	1.40	11 (20%)	66,96,113	1.44	6 (9%)
31	CLA	8	313	-	59,63,73	1.54	12 (20%)	71,101,113	1.82	18 (25%)
38	DGD	C	519	-	63,63,67	1.12	9 (14%)	77,77,81	1.52	15 (19%)
31	CLA	9	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.39	11 (13%)
36	LHG	d	408	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
31	CLA	7	310	-	49,53,73	1.46	7 (14%)	59,89,113	1.60	7 (11%)
34	SQD	8	301	31	40,41,54	1.11	5 (12%)	49,52,65	1.79	12 (24%)
31	CLA	18	307	-	65,69,73	1.36	11 (16%)	78,108,113	1.61	15 (19%)
37	LMG	J	101	-	50,50,55	0.95	3 (6%)	58,58,63	1.32	4 (6%)
36	LHG	8	317	-	30,30,48	0.78	1 (3%)	33,36,54	1.26	2 (6%)
31	CLA	b	616	-	69,73,73	1.30	11 (15%)	83,113,113	1.55	9 (10%)
37	LMG	15	315	-	36,36,55	1.20	4 (11%)	44,44,63	1.74	9 (20%)
43	A86	18	304	-	44,50,50	1.44	6 (13%)	51,76,76	4.00	22 (43%)
31	CLA	B	605	-	69,73,73	1.32	11 (15%)	83,113,113	1.55	9 (10%)
31	CLA	4	311	-	50,54,73	1.42	9 (18%)	60,90,113	1.60	9 (15%)
43	A86	9	304	-	44,50,50	1.27	4 (9%)	51,76,76	4.19	18 (35%)

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
31	CLA	12	315	-	-	2/10/86/115	-
43	A86	18	302	-	-	8/34/90/90	0/3/3/3
31	CLA	p	602	-	-	16/39/115/115	-
38	DGD	1	318	-	-	27/43/83/95	0/2/2/2
43	A86	17	316	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	KC1	14	313	27	-	9/15/71/71	-
45	KC2	0	310	26	-	9/15/71/71	-
37	LMG	W	201	-	-	25/43/63/70	0/1/1/1
31	CLA	14	307	-	-	16/39/115/115	-
43	A86	0	306	-	-	7/34/90/90	0/3/3/3
43	A86	6	306	31	-	8/34/90/90	0/3/3/3
37	LMG	Z	102	-	-	10/26/46/70	0/1/1/1
31	CLA	A	403	1	-	10/39/115/115	-
42	KC1	0	315	-	-	4/15/71/71	-
31	CLA	B	610	-	-	9/39/115/115	-
31	CLA	17	315	-	-	6/10/86/115	-
43	A86	12	305	-	-	8/34/90/90	0/3/3/3
45	KC2	8	311	-	-	6/15/71/71	-
43	A86	7	305	-	-	8/34/90/90	0/3/3/3
43	A86	3	306	-	-	8/34/90/90	0/3/3/3
45	KC2	1	311	-	-	4/15/71/71	-
31	CLA	8	308	-	-	10/35/111/115	-
31	CLA	p	608	16	-	7/23/99/115	-
36	LHG	a	410	1	-	17/41/41/53	-
31	CLA	6	308	-	-	7/12/88/115	-
31	CLA	D	406	-	-	13/39/115/115	-
31	CLA	11	310	-	-	7/21/97/115	-
31	CLA	1	316	43	-	5/12/88/115	-
33	BCR	h	101	-	-	10/29/63/63	0/2/2/2
43	A86	19	303	-	-	7/34/90/90	0/3/3/3
37	LMG	10	319	-	-	8/26/46/70	0/1/1/1
31	CLA	c	504	31	-	23/39/115/115	-
33	BCR	C	516	-	-	9/29/63/63	0/2/2/2
31	CLA	C	508	-	-	16/39/115/115	-
37	LMG	b	621	-	-	26/46/66/70	0/1/1/1
43	A86	10	304	-	-	6/34/90/90	0/3/3/3
37	LMG	f	102	-	-	14/41/61/70	0/1/1/1
43	A86	16	306	31	-	8/34/90/90	0/3/3/3
43	A86	13	306	43	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	D	405	4	-	12/39/115/115	-
43	A86	8	306	-	-	8/34/90/90	0/3/3/3
31	CLA	4	307	-	-	16/39/115/115	-
37	LMG	D	404	4	-	22/35/55/70	0/1/1/1
43	A86	12	301	-	-	8/34/90/90	0/3/3/3
42	KC1	16	314	27	-	1/15/71/71	-
42	KC1	P	609	-	-	8/15/71/71	-
36	LHG	b	623	-	-	15/47/47/53	-
43	A86	4	305	-	-	8/34/90/90	0/3/3/3
31	CLA	9	312	43	-	6/39/115/115	-
45	KC2	15	308	-	-	7/15/71/71	-
31	CLA	14	311	-	-	10/17/93/115	-
38	DGD	H	102	-	-	29/51/91/95	0/2/2/2
31	CLA	B	608	-	-	16/39/115/115	-
33	BCR	y	101	-	-	13/29/63/63	0/2/2/2
43	A86	6	301	43	-	9/34/90/90	0/3/3/3
43	A86	15	301	31	-	6/34/90/90	0/3/3/3
45	KC2	17	309	-	-	10/15/71/71	-
43	A86	1	306	-	-	8/34/90/90	0/3/3/3
37	LMG	w	201	-	-	25/43/63/70	0/1/1/1
31	CLA	10	317	-	-	6/19/95/115	-
31	CLA	15	306	-	-	6/12/88/115	-
31	CLA	15	312	-	-	8/18/94/115	-
42	KC1	1	314	-	-	7/15/71/71	-
31	CLA	2	311	-	-	7/15/91/115	-
31	CLA	z	103	-	-	5/19/95/115	-
31	CLA	9	311	43	-	8/17/93/115	-
43	A86	11	319	-	-	6/34/90/90	0/3/3/3
31	CLA	19	310	-	-	15/39/115/115	-
37	LMG	M	101	-	-	18/35/55/70	0/1/1/1
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
31	CLA	p	605	16	-	5/10/86/115	-
45	KC2	2	308	-	-	10/15/71/71	-
45	KC2	6	310	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	D	408	-	-	28/53/53/53	-
36	LHG	18	316	-	-	23/34/34/53	-
43	A86	18	301	-	-	5/34/90/90	0/3/3/3
42	KC1	12	314	-	-	3/15/71/71	-
36	LHG	z	102	-	-	16/29/29/53	-
41	HEM	e	101	5,6	-	5/14/54/54	-
43	A86	5	301	31	-	6/34/90/90	0/3/3/3
36	LHG	15	316	-	-	15/29/29/53	-
43	A86	2	303	-	-	7/34/90/90	0/3/3/3
43	A86	13	304	-	-	8/34/90/90	0/3/3/3
31	CLA	b	603	2	-	17/39/115/115	-
31	CLA	3	307	-	-	5/12/88/115	-
31	CLA	B	603	2	-	17/39/115/115	-
43	A86	9	306	-	-	8/34/90/90	0/3/3/3
31	CLA	0	314	-	-	7/18/94/115	-
31	CLA	12	308	-	-	17/39/115/115	-
31	CLA	6	314	-	-	5/12/88/115	-
43	A86	14	304	-	-	7/34/90/90	0/3/3/3
31	CLA	9	310	-	-	15/39/115/115	-
41	HEM	E	101	5,6	-	5/14/54/54	-
31	CLA	R	101	-	-	6/18/94/115	-
33	BCR	C	515	-	-	14/29/63/63	0/2/2/2
31	CLA	5	307	-	-	13/39/115/115	-
31	CLA	11	315	-	-	5/10/86/115	-
37	LMG	c	522	-	-	10/26/46/70	0/1/1/1
37	LMG	14	316	-	-	24/44/64/70	0/1/1/1
42	KC1	2	313	27	-	4/15/71/71	-
43	A86	2	301	-	-	10/34/90/90	0/3/3/3
31	CLA	10	308	-	-	10/21/97/115	-
34	SQD	10	320	31	-	24/36/56/69	0/1/1/1
43	A86	0	301	-	-	7/34/90/90	0/3/3/3
34	SQD	i	101	-	-	21/35/55/69	0/1/1/1
42	KC1	7	314	27	-	2/15/71/71	-
45	KC2	12	311	-	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	KC2	7	311	27	-	6/15/71/71	-
33	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	CLA	13	307	-	-	3/12/88/115	-
43	A86	16	303	43	-	8/34/90/90	0/3/3/3
31	CLA	B	616	-	-	14/39/115/115	-
31	CLA	B	604	-	-	14/39/115/115	-
43	A86	11	305	-	-	9/34/90/90	0/3/3/3
31	CLA	c	503	3,31	-	13/39/115/115	-
31	CLA	b	609	-	-	16/39/115/115	-
33	BCR	c	517	-	-	10/29/63/63	0/2/2/2
32	PHO	d	403	-	-	5/37/103/103	0/5/6/6
31	CLA	1	312	-	-	6/17/93/115	-
31	CLA	2	315	43	-	8/17/93/115	-
31	CLA	10	314	-	-	6/18/94/115	-
31	CLA	C	509	3	-	11/39/115/115	-
31	CLA	C	514	-	-	5/20/96/115	-
43	A86	1	303	-	-	8/34/90/90	0/3/3/3
31	CLA	C	513	-	-	18/39/115/115	-
31	CLA	a	406	1	-	5/33/109/115	-
43	A86	1	302	-	-	8/34/90/90	0/3/3/3
37	LMG	d	409	4	-	16/32/52/70	0/1/1/1
43	A86	12	306	-	-	9/34/90/90	0/3/3/3
31	CLA	19	311	43	-	6/17/93/115	-
43	A86	7	306	-	-	7/34/90/90	0/3/3/3
31	CLA	b	617	-	-	15/39/115/115	-
43	A86	2	305	31	-	7/34/90/90	0/3/3/3
31	CLA	14	309	-	-	20/39/115/115	-
31	CLA	16	312	-	-	8/18/94/115	-
31	CLA	13	312	-	-	8/15/91/115	-
33	BCR	b	618	-	-	13/29/63/63	0/2/2/2
43	A86	0	305	-	-	9/34/90/90	0/3/3/3
36	LHG	14	317	-	-	22/38/38/53	-
33	BCR	A	407	-	-	8/29/63/63	0/2/2/2
31	CLA	13	315	-	-	2/13/90/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	602	2	-	17/39/115/115	-
31	CLA	p	604	-	-	5/19/95/115	-
31	CLA	16	308	-	-	15/39/115/115	-
31	CLA	p	610	-	-	2/10/86/115	-
31	CLA	7	315	-	-	6/10/86/115	-
31	CLA	3	315	-	-	6/13/90/115	-
37	LMG	k	101	-	-	23/41/61/70	0/1/1/1
31	CLA	6	309	-	-	15/39/115/115	-
31	CLA	8	315	-	-	4/13/89/115	-
31	CLA	14	315	-	-	9/13/89/115	-
31	CLA	P	605	16	-	5/10/86/115	-
31	CLA	5	311	-	-	5/15/91/115	-
43	A86	5	304	-	-	11/34/90/90	0/3/3/3
31	CLA	15	311	27	-	7/15/91/115	-
45	KC2	4	310	-	-	6/15/71/71	-
31	CLA	C	502	-	-	13/39/115/115	-
43	A86	14	303	-	-	9/34/90/90	0/3/3/3
31	CLA	1	310	-	-	6/21/97/115	-
42	KC1	18	313	27,31	-	3/15/71/71	-
31	CLA	P	610	-	-	2/10/86/115	-
45	KC2	2	310	-	-	8/15/71/71	-
31	CLA	7	307	-	-	4/10/86/115	-
31	CLA	19	315	-	-	3/10/86/115	-
31	CLA	17	308	-	-	3/10/86/115	-
36	LHG	L	101	-	-	22/53/53/53	-
43	A86	3	305	-	-	10/34/90/90	0/3/3/3
31	CLA	2	312	-	-	10/19/95/115	-
31	CLA	w	203	-	-	19/39/115/115	-
31	CLA	12	310	-	-	6/13/89/115	-
43	A86	18	305	-	-	12/34/90/90	0/3/3/3
36	LHG	18	315	-	-	21/43/43/53	-
41	HEM	v	201	21	-	8/14/54/54	-
31	CLA	0	312	26,34	-	7/17/93/115	-
31	CLA	16	310	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	15	305	27	-	6/34/90/90	0/3/3/3
43	A86	9	305	-	-	9/34/90/90	0/3/3/3
31	CLA	10	307	-	-	9/19/95/115	-
43	A86	19	306	-	-	8/34/90/90	0/3/3/3
31	CLA	c	507	-	-	16/39/115/115	-
43	A86	1	305	-	-	10/34/90/90	0/3/3/3
45	KC2	6	312	27	-	6/15/71/71	-
43	A86	0	302	26	-	8/34/90/90	0/3/3/3
31	CLA	C	511	3	-	20/39/115/115	-
43	A86	17	305	-	-	8/34/90/90	0/3/3/3
34	SQD	B	623	-	-	25/49/69/69	0/1/1/1
31	CLA	c	509	3	-	11/39/115/115	-
43	A86	5	302	-	-	8/34/90/90	0/3/3/3
43	A86	14	301	-	-	14/34/90/90	0/3/3/3
45	KC2	7	309	-	-	10/15/71/71	-
43	A86	14	302	43	-	7/34/90/90	0/3/3/3
33	BCR	C	517	-	-	10/29/63/63	0/2/2/2
31	CLA	12	312	-	-	8/15/91/115	-
43	A86	8	305	-	-	8/34/90/90	0/3/3/3
31	CLA	11	313	-	-	14/39/115/115	-
38	DGD	W	203	-	-	28/45/85/95	0/2/2/2
43	A86	16	305	43	-	8/34/90/90	0/3/3/3
43	A86	13	305	-	-	9/34/90/90	0/3/3/3
43	A86	12	303	-	-	5/34/90/90	0/3/3/3
33	BCR	B	617	-	-	13/29/63/63	0/2/2/2
31	CLA	B	611	2	-	12/39/115/115	-
43	A86	13	302	-	-	8/34/90/90	0/3/3/3
45	KC2	11	311	-	-	4/15/71/71	-
31	CLA	2	314	-	-	6/10/86/115	-
31	CLA	11	307	27	-	5/13/89/115	-
31	CLA	13	316	-	-	16/39/115/115	-
31	CLA	15	313	-	-	0/10/86/115	-
31	CLA	b	607	-	-	12/39/115/115	-
37	LMG	c	521	-	-	25/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	10	313	26	-	6/12/88/115	-
31	CLA	10	316	-	-	6/17/93/115	-
31	CLA	B	607	-	-	16/39/115/115	-
43	A86	p	613	31	-	8/34/90/90	1/3/3/3
43	A86	1	320	-	-	8/34/90/90	0/3/3/3
43	A86	6	303	-	-	9/34/90/90	0/3/3/3
31	CLA	B	609	-	-	12/39/115/115	-
37	LMG	5	315	-	-	16/32/52/70	0/1/1/1
35	PL9	D	407	-	-	9/53/73/73	0/1/1/1
42	KC1	6	315	27	-	1/15/71/71	-
43	A86	6	302	-	-	8/34/90/90	0/3/3/3
38	DGD	c	519	-	-	27/51/91/95	0/2/2/2
31	CLA	p	603	-	-	10/21/97/115	-
31	CLA	z	101	-	-	8/23/99/115	-
31	CLA	b	612	2	-	12/39/115/115	-
37	LMG	K	101	-	-	23/41/61/70	0/1/1/1
43	A86	17	301	-	-	10/34/90/90	0/3/3/3
31	CLA	17	313	27	-	6/21/97/115	-
31	CLA	a	403	1	-	10/39/115/115	-
31	CLA	C	505	-	-	10/39/115/115	-
31	CLA	8	312	-	-	9/17/93/115	-
45	KC2	12	309	-	-	6/15/71/71	-
38	DGD	h	102	-	-	29/51/91/95	0/2/2/2
35	PL9	d	407	-	-	9/53/73/73	0/1/1/1
31	CLA	c	513	-	-	18/39/115/115	-
31	CLA	5	312	-	-	6/18/94/115	-
43	A86	0	303	-	-	7/34/90/90	0/3/3/3
31	CLA	W	202	-	-	19/39/115/115	-
45	KC2	5	310	27	-	7/15/71/71	-
31	CLA	P	603	-	-	10/21/97/115	-
31	CLA	7	308	-	-	3/10/86/115	-
37	LMG	C	522	-	-	25/46/66/70	0/1/1/1
31	CLA	16	315	-	-	4/13/89/115	-
31	CLA	2	306	-	-	6/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	4	316	-	-	24/44/64/70	0/1/1/1
37	LMG	5	316	-	-	17/31/51/70	0/1/1/1
44	DD6	p	612	-	-	10/26/80/80	0/3/3/3
37	LMG	D	409	4	-	16/32/52/70	0/1/1/1
31	CLA	18	306	42	-	8/21/97/115	-
31	CLA	8	310	-	-	7/24/100/115	-
31	CLA	9	307	-	-	10/35/111/115	-
43	A86	7	304	-	-	9/34/90/90	0/3/3/3
45	KC2	19	309	28	-	4/15/71/71	-
42	KC1	11	314	-	-	8/15/71/71	-
31	CLA	9	315	-	-	2/10/86/115	-
43	A86	19	304	-	-	7/34/90/90	0/3/3/3
31	CLA	18	314	27	-	9/13/89/115	-
45	KC2	17	311	27	-	6/15/71/71	-
31	CLA	1	315	27	-	3/10/86/115	-
31	CLA	b	602	-	-	22/39/115/115	-
31	CLA	13	313	-	-	16/39/115/115	-
32	PHO	D	403	-	-	5/37/103/103	0/5/6/6
31	CLA	c	510	3	-	8/39/115/115	-
31	CLA	b	606	-	-	12/39/115/115	-
31	CLA	7	313	-	-	7/21/97/115	-
31	CLA	3	313	-	-	19/39/115/115	-
31	CLA	B	615	-	-	9/39/115/115	-
37	LMG	P	614	-	-	11/26/46/70	0/1/1/1
33	BCR	Y	101	-	-	13/29/63/63	0/2/2/2
43	A86	13	303	-	-	6/34/90/90	0/3/3/3
45	KC2	13	311	-	-	7/15/71/71	-
31	CLA	P	606	-	-	8/13/89/115	-
34	SQD	a	408	38	-	23/49/69/69	0/1/1/1
42	KC1	5	313	-	-	3/15/71/71	-
43	A86	10	306	-	-	8/34/90/90	0/3/3/3
42	KC1	3	314	27	-	1/15/71/71	-
31	CLA	A	404	-	-	6/20/96/115	-
37	LMG	N	101	14	-	6/23/43/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	6	305	43	-	8/34/90/90	0/3/3/3
31	CLA	P	604	-	-	5/19/95/115	-
36	LHG	w	202	-	-	20/44/44/53	-
42	KC1	15	317	27	-	0/15/71/71	-
45	KC2	14	308	27	-	7/15/71/71	-
31	CLA	c	502	-	-	13/39/115/115	-
31	CLA	A	406	1	-	5/33/109/115	-
31	CLA	0	309	-	-	15/32/108/115	-
43	A86	15	303	-	-	8/34/90/90	0/3/3/3
31	CLA	0	316	-	-	7/17/93/115	-
31	CLA	9	313	-	-	12/39/115/115	-
43	A86	10	303	-	-	7/34/90/90	0/3/3/3
33	BCR	f	101	-	-	19/29/63/63	0/2/2/2
43	A86	12	304	-	-	7/34/90/90	0/3/3/3
43	A86	17	306	-	-	8/34/90/90	0/3/3/3
31	CLA	D	402	-	-	9/39/115/115	-
31	CLA	3	308	-	-	4/13/89/115	-
31	CLA	6	316	-	-	4/13/89/115	-
31	CLA	1	313	-	-	16/39/115/115	-
31	CLA	4	309	-	-	20/39/115/115	-
43	A86	7	302	-	-	10/34/90/90	0/3/3/3
31	CLA	5	314	-	-	1/10/86/115	-
37	LMG	d	404	-	-	17/35/55/70	0/1/1/1
42	KC1	19	314	-	-	5/15/71/71	-
37	LMG	B	620	-	-	26/46/66/70	0/1/1/1
33	BCR	B	619	-	-	12/29/63/63	0/2/2/2
43	A86	6	304	-	-	7/34/90/90	0/3/3/3
36	LHG	B	622	-	-	15/47/47/53	-
45	KC2	13	309	-	-	10/15/71/71	-
31	CLA	b	610	-	-	12/39/115/115	-
43	A86	17	303	-	-	10/34/90/90	0/3/3/3
38	DGD	C	518	-	-	22/44/84/95	0/2/2/2
37	LMG	0	317	-	-	7/26/46/70	0/1/1/1
38	DGD	C	520	34	-	32/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	A86	17	304	-	-	8/34/90/90	0/3/3/3
31	CLA	14	306	-	-	15/35/111/115	-
38	DGD	w	204	-	-	28/45/85/95	0/2/2/2
45	KC2	9	309	28	-	5/15/71/71	-
43	A86	11	306	-	-	8/34/90/90	0/3/3/3
33	BCR	c	516	-	-	9/29/63/63	0/2/2/2
31	CLA	16	313	-	-	5/12/88/115	-
43	A86	10	301	-	-	7/34/90/90	0/3/3/3
45	KC2	15	310	27	-	7/15/71/71	-
31	CLA	B	614	2	-	20/39/115/115	-
43	A86	P	611	-	-	7/34/90/90	1/3/3/3
45	KC2	18	308	-	-	10/15/71/71	-
37	LMG	m	101	-	-	19/35/55/70	0/1/1/1
45	KC2	5	308	-	-	7/15/71/71	-
31	CLA	C	512	3	-	8/39/115/115	-
31	CLA	11	312	27	-	7/17/93/115	-
37	LMG	p	614	-	-	11/26/46/70	0/1/1/1
42	KC1	13	314	-	-	4/15/71/71	-
31	CLA	5	306	-	-	5/12/88/115	-
31	CLA	C	504	31	-	23/39/115/115	-
34	SQD	b	601	38	-	25/49/69/69	0/1/1/1
31	CLA	10	312	26,34	-	6/17/93/115	-
42	KC1	p	609	-	-	8/15/71/71	-
43	A86	11	303	-	-	9/34/90/90	0/3/3/3
43	A86	4	304	-	-	9/34/90/90	0/3/3/3
45	KC2	1	309	-	-	9/15/71/71	-
43	A86	5	303	-	-	8/34/90/90	0/3/3/3
43	A86	11	302	-	-	6/34/90/90	0/3/3/3
43	A86	12	302	-	-	7/34/90/90	0/3/3/3
31	CLA	19	308	-	-	15/39/115/115	-
43	A86	15	302	-	-	9/34/90/90	1/3/3/3
43	A86	10	302	-	-	7/34/90/90	0/3/3/3
31	CLA	1	308	-	-	15/39/115/115	-
36	LHG	A	410	1	-	17/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	p	607	43	-	5/13/89/115	-
43	A86	P	613	31	-	8/34/90/90	1/3/3/3
37	LMG	j	101	-	-	29/45/65/70	0/1/1/1
31	CLA	0	313	-	-	4/12/88/115	-
31	CLA	B	612	2	-	16/39/115/115	-
31	CLA	C	503	3,31	-	13/39/115/115	-
43	A86	7	303	-	-	8/34/90/90	0/3/3/3
31	CLA	18	311	27	-	8/17/93/115	-
43	A86	17	302	-	-	6/34/90/90	0/3/3/3
31	CLA	b	613	2	-	16/39/115/115	-
33	BCR	a	407	-	-	8/29/63/63	0/2/2/2
42	KC1	17	314	27	-	2/15/71/71	-
31	CLA	P	601	16	-	24/39/115/115	-
45	KC2	16	311	-	-	6/15/71/71	-
43	A86	4	306	-	-	7/34/90/90	1/3/3/3
43	A86	14	305	-	-	6/34/90/90	1/3/3/3
31	CLA	b	615	2	-	21/39/115/115	-
31	CLA	c	505	-	-	10/39/115/115	-
31	CLA	p	606	-	-	8/13/89/115	-
43	A86	16	304	-	-	7/34/90/90	0/3/3/3
38	DGD	b	622	34	-	28/44/84/95	0/2/2/2
42	KC1	9	314	-	-	5/15/71/71	-
37	LMG	11	317	-	-	24/40/60/70	0/1/1/1
43	A86	11	320	-	-	8/34/90/90	0/3/3/3
31	CLA	13	308	-	-	4/13/89/115	-
31	CLA	c	511	3	-	20/39/115/115	-
31	CLA	B	613	2	-	10/39/115/115	-
34	SQD	A	408	38	-	23/49/69/69	0/1/1/1
31	CLA	C	510	3	-	8/39/115/115	-
43	A86	8	302	-	-	11/34/90/90	0/3/3/3
31	CLA	0	307	-	-	6/19/95/115	-
35	PL9	a	409	-	-	15/27/47/73	0/1/1/1
36	LHG	P	615	-	-	14/31/31/53	-
34	SQD	l	101	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	d	405	4	-	12/39/115/115	-
42	KC1	10	315	-	-	4/15/71/71	-
43	A86	3	302	-	-	6/34/90/90	0/3/3/3
31	CLA	19	313	-	-	13/39/115/115	-
31	CLA	4	315	-	-	9/13/89/115	-
42	KC1	4	313	-	-	9/15/71/71	-
33	BCR	H	101	-	-	10/29/63/63	0/2/2/2
43	A86	1	304	31	-	6/34/90/90	0/3/3/3
31	CLA	19	307	-	-	10/35/111/115	-
31	CLA	7	312	-	-	10/18/94/115	-
31	CLA	5	309	-	-	11/27/103/115	-
31	CLA	14	312	-	-	10/23/99/115	-
43	A86	3	301	-	-	10/34/90/90	0/3/3/3
45	KC2	8	309	-	-	10/15/71/71	-
31	CLA	17	310	-	-	6/15/91/115	-
31	CLA	c	508	-	-	16/39/115/115	-
45	KC2	10	310	26	-	7/15/71/71	-
31	CLA	12	307	-	-	3/12/88/115	-
43	A86	7	301	-	-	6/34/90/90	0/3/3/3
31	CLA	B	606	-	-	12/39/115/115	-
43	A86	8	303	-	-	8/34/90/90	0/3/3/3
43	A86	19	301	-	-	8/34/90/90	0/3/3/3
31	CLA	b	608	-	-	17/39/115/115	-
31	CLA	3	312	-	-	6/15/91/115	-
42	KC1	8	314	31,43	-	3/15/71/71	-
31	CLA	18	312	27	-	10/27/103/115	-
43	A86	16	302	-	-	8/34/90/90	0/3/3/3
33	BCR	b	620	-	-	12/29/63/63	0/2/2/2
43	A86	3	303	-	-	9/34/90/90	0/3/3/3
31	CLA	P	607	43	-	5/13/89/115	-
36	LHG	l	102	-	-	22/53/53/53	-
31	CLA	c	512	3	-	8/39/115/115	-
31	CLA	3	310	-	-	3/10/86/115	-
45	KC2	14	310	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	1	301	-	-	14/31/51/70	0/1/1/1
43	A86	p	611	-	-	7/34/90/90	1/3/3/3
33	BCR	F	101	-	-	19/29/63/63	0/2/2/2
31	CLA	a	404	-	-	6/20/96/115	-
35	PL9	A	409	-	-	16/27/47/73	0/1/1/1
43	A86	9	302	-	-	6/34/90/90	0/3/3/3
31	CLA	15	307	-	-	17/39/115/115	-
31	CLA	17	312	-	-	7/18/94/115	-
36	LHG	Z	103	-	-	16/29/29/53	-
43	A86	11	304	31	-	8/34/90/90	0/3/3/3
36	LHG	p	615	-	-	14/31/31/53	-
36	LHG	4	317	-	-	18/38/38/53	-
31	CLA	C	506	-	-	12/39/115/115	-
37	LMG	F	102	-	-	14/41/61/70	0/1/1/1
33	BCR	c	515	-	-	14/29/63/63	0/2/2/2
43	A86	4	301	-	-	8/34/90/90	0/3/3/3
43	A86	9	301	-	-	8/34/90/90	0/3/3/3
31	CLA	10	309	-	-	16/32/108/115	-
31	CLA	14	314	-	-	7/13/89/115	-
44	DD6	P	612	-	-	7/26/80/80	0/3/3/3
31	CLA	17	307	-	-	4/10/86/115	-
38	DGD	c	518	-	-	22/44/84/95	0/2/2/2
45	KC2	3	311	-	-	6/15/71/71	-
31	CLA	c	514	-	-	5/20/96/115	-
31	CLA	P	608	16	-	7/23/99/115	-
31	CLA	b	611	-	-	9/39/115/115	-
37	LMG	11	301	-	-	14/31/51/70	0/1/1/1
38	DGD	c	520	34	-	32/51/91/95	0/2/2/2
31	CLA	b	614	2	-	10/39/115/115	-
31	CLA	B	601	-	-	22/39/115/115	-
31	CLA	4	312	27	-	11/23/99/115	-
43	A86	18	303	-	-	12/34/90/90	0/3/3/3
37	LMG	n	701	14	-	6/23/43/70	0/1/1/1
31	CLA	1	321	-	-	15/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	307	-	-	17/39/115/115	-
32	PHO	a	405	-	-	14/37/103/103	0/5/6/6
31	CLA	11	316	43	-	0/10/86/115	-
31	CLA	12	316	-	-	5/17/93/115	-
31	CLA	b	604	2	-	16/39/115/115	-
43	A86	2	304	-	-	6/34/90/90	1/3/3/3
43	A86	4	303	-	-	12/34/90/90	0/3/3/3
31	CLA	p	601	16	-	24/39/115/115	-
31	CLA	13	310	-	-	4/10/86/115	-
43	A86	9	303	-	-	8/34/90/90	0/3/3/3
43	A86	5	305	-	-	6/34/90/90	0/3/3/3
45	KC2	11	309	-	-	10/15/71/71	-
43	A86	4	302	-	-	7/34/90/90	0/3/3/3
31	CLA	0	311	-	-	6/27/103/115	-
37	LMG	15	314	-	-	17/32/52/70	0/1/1/1
31	CLA	2	309	-	-	6/13/89/115	-
36	LHG	C	521	-	-	20/44/44/53	-
43	A86	0	304	-	-	6/34/90/90	0/3/3/3
38	DGD	11	318	-	-	33/49/89/95	0/2/2/2
36	LHG	5	317	-	-	15/29/29/53	-
31	CLA	11	308	-	-	22/39/115/115	-
43	A86	15	304	-	-	10/34/90/90	1/3/3/3
43	A86	19	305	-	-	9/34/90/90	0/3/3/3
43	A86	5	318	42	-	10/34/90/90	0/3/3/3
34	SQD	L	102	-	-	22/49/69/69	0/1/1/1
31	CLA	18	309	-	-	7/24/100/115	-
31	CLA	d	402	-	-	9/39/115/115	-
45	KC2	4	308	27	-	5/15/71/71	-
31	CLA	15	309	-	-	13/27/103/115	-
45	KC2	16	309	-	-	10/15/71/71	-
31	CLA	d	406	-	-	13/39/115/115	-
31	CLA	12	313	-	-	10/19/95/115	-
43	A86	6	307	-	-	13/34/90/90	0/3/3/3
45	KC2	3	309	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	507	-	-	16/39/115/115	-
31	CLA	8	307	42	-	7/21/97/115	-
43	A86	10	305	-	-	9/34/90/90	0/3/3/3
31	CLA	6	313	-	-	8/18/94/115	-
31	CLA	16	307	-	-	5/12/88/115	-
41	HEM	V	201	21	-	8/14/54/54	-
43	A86	8	304	-	-	9/34/90/90	0/3/3/3
31	CLA	3	316	-	-	17/39/115/115	-
31	CLA	6	311	-	-	3/10/86/115	-
31	CLA	4	314	-	-	7/13/89/115	-
31	CLA	0	308	-	-	10/21/97/115	-
31	CLA	b	605	-	-	14/39/115/115	-
43	A86	2	302	-	-	10/34/90/90	0/3/3/3
31	CLA	P	602	-	-	15/39/115/115	-
37	LMG	1	317	-	-	26/40/60/70	0/1/1/1
43	A86	10	318	-	-	8/34/90/90	0/3/3/3
34	SQD	A	411	-	-	22/35/55/69	0/1/1/1
36	LHG	8	316	-	-	23/43/43/53	-
31	CLA	19	312	43	-	8/39/115/115	-
43	A86	3	304	-	-	6/34/90/90	0/3/3/3
31	CLA	r	101	-	-	6/18/94/115	-
31	CLA	10	311	-	-	6/27/103/115	-
43	A86	1	319	-	-	8/34/90/90	0/3/3/3
31	CLA	1	307	-	-	4/13/89/115	-
43	A86	19	302	-	-	8/34/90/90	0/3/3/3
38	DGD	B	621	-	-	31/43/83/95	0/2/2/2
45	KC2	18	310	27	-	7/15/71/71	-
32	PHO	A	405	-	-	14/37/103/103	0/5/6/6
31	CLA	c	506	-	-	12/39/115/115	-
43	A86	16	301	43	-	10/34/90/90	0/3/3/3
43	A86	13	301	-	-	6/34/90/90	0/3/3/3
31	CLA	Z	101	-	-	8/23/99/115	-
31	CLA	8	313	-	-	12/27/103/115	-
38	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	9	308	-	-	18/39/115/115	-
36	LHG	d	408	-	-	28/53/53/53	-
31	CLA	7	310	-	-	6/15/91/115	-
34	SQD	8	301	31	-	22/36/56/69	0/1/1/1
31	CLA	18	307	-	-	11/35/111/115	-
37	LMG	J	101	-	-	29/45/65/70	0/1/1/1
36	LHG	8	317	-	-	20/34/34/53	-
31	CLA	b	616	-	-	9/39/115/115	-
37	LMG	15	315	-	-	18/31/51/70	0/1/1/1
43	A86	18	304	-	-	6/34/90/90	0/3/3/3
31	CLA	B	605	-	-	12/39/115/115	-
31	CLA	4	311	-	-	8/17/93/115	-
43	A86	9	304	-	-	7/34/90/90	0/3/3/3

All (4566) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	p	612	DD6	C29-C27	-8.80	1.25	1.42
44	P	612	DD6	C29-C27	-8.78	1.25	1.42
32	D	403	PHO	C1B-C2B	8.37	1.48	1.39
32	d	403	PHO	C1B-C2B	8.33	1.48	1.39
32	A	405	PHO	C1B-C2B	8.29	1.48	1.39
32	a	405	PHO	C1B-C2B	8.25	1.48	1.39
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
45	13	311	KC2	C4C-NC	7.88	1.49	1.37
45	1	309	KC2	C4C-NC	7.85	1.49	1.37
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
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	311	KC2	C4C-NC	7.70	1.49	1.37
45	2	308	KC2	C4C-NC	7.69	1.49	1.37
45	17	309	KC2	C4C-NC	7.68	1.49	1.37
45	6	312	KC2	C4C-NC	7.68	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
45	19	309	KC2	C4C-NC	7.62	1.49	1.37
45	7	309	KC2	C4C-NC	7.62	1.49	1.37
45	3	311	KC2	C4C-NC	7.62	1.49	1.37
42	15	317	KC1	C4C-NC	7.62	1.49	1.37
42	19	314	KC1	C4C-NC	7.61	1.49	1.37
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
45	3	309	KC2	C4C-NC	7.53	1.49	1.37
42	13	314	KC1	C4C-NC	7.50	1.49	1.37
45	13	309	KC2	C4C-NC	7.49	1.49	1.37
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	309	KC2	C4C-NC	7.48	1.49	1.37
45	15	310	KC2	C4C-NC	7.47	1.49	1.37
42	5	313	KC1	C4C-NC	7.47	1.49	1.37
45	5	310	KC2	C4C-NC	7.47	1.49	1.37
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
45	8	311	KC2	C4C-NC	7.43	1.48	1.37
42	16	314	KC1	C4C-NC	7.40	1.48	1.37
42	12	314	KC1	C4C-NC	7.38	1.48	1.37
45	12	309	KC2	C4C-NC	7.36	1.48	1.37
45	8	309	KC2	C4C-NC	7.34	1.48	1.37
45	11	309	KC2	C4C-NC	7.34	1.48	1.37
32	d	403	PHO	C3B-C4B	7.34	1.49	1.41
32	D	403	PHO	C3B-C4B	7.32	1.49	1.41
42	2	313	KC1	C4C-NC	7.27	1.48	1.37
45	10	310	KC2	C4C-NC	7.26	1.48	1.37
45	0	310	KC2	C4C-NC	7.26	1.48	1.37
45	18	308	KC2	C4C-NC	7.25	1.48	1.37
42	10	315	KC1	C4C-NC	7.25	1.48	1.37
45	14	310	KC2	C4C-NC	7.22	1.48	1.37
45	11	311	KC2	C4C-NC	7.20	1.48	1.37
45	4	310	KC2	C4C-NC	7.17	1.48	1.37
35	D	407	PL9	C3-C4	-7.14	1.37	1.49
42	6	315	KC1	C4C-NC	7.13	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	407	PL9	C3-C4	-7.12	1.37	1.49
45	1	311	KC2	C4C-NC	7.10	1.48	1.37
32	a	405	PHO	C3B-C4B	7.06	1.49	1.41
42	0	315	KC1	C4C-NC	7.05	1.48	1.37
42	17	314	KC1	C4C-NC	7.01	1.48	1.37
42	7	314	KC1	C4C-NC	7.01	1.48	1.37
32	A	405	PHO	C3B-C4B	7.00	1.49	1.41
42	18	313	KC1	C4C-NC	6.93	1.48	1.37
42	3	314	KC1	C4C-NC	6.92	1.48	1.37
42	P	609	KC1	C4C-NC	6.83	1.48	1.37
42	p	609	KC1	C4C-NC	6.80	1.48	1.37
43	8	302	A86	O4-C38	6.31	1.49	1.35
42	3	314	KC1	C2A-C3A	6.25	1.49	1.37
42	16	314	KC1	C2A-C3A	6.25	1.49	1.37
45	17	311	KC2	C1A-NA	6.24	1.50	1.38
42	7	314	KC1	C2A-C3A	6.21	1.49	1.37
42	2	313	KC1	C2A-C3A	6.15	1.49	1.37
42	16	314	KC1	C1A-NA	6.12	1.50	1.38
45	13	311	KC2	C3C-C2C	6.10	1.49	1.37
42	10	315	KC1	C1A-NA	6.09	1.49	1.38
43	11	306	A86	O1-C20	-6.08	1.37	1.46
42	8	314	KC1	C4C-NC	6.07	1.46	1.37
45	18	310	KC2	C1A-NA	6.02	1.49	1.38
42	5	313	KC1	C1A-NA	6.02	1.49	1.38
42	17	314	KC1	C2A-C3A	6.00	1.49	1.37
42	6	315	KC1	C2A-C3A	5.97	1.49	1.37
45	2	308	KC2	CHD-C4C	5.97	1.50	1.38
45	12	311	KC2	C1A-NA	5.95	1.49	1.38
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	2	308	KC2	C3C-C2C	5.91	1.49	1.37
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	2	310	KC2	C1A-NA	5.87	1.49	1.38
45	3	309	KC2	CHD-C4C	5.87	1.50	1.38
42	2	313	KC1	C1A-NA	5.86	1.49	1.38
45	16	309	KC2	CHD-C4C	5.85	1.50	1.38
42	15	317	KC1	C1A-NA	5.85	1.49	1.38
45	17	309	KC2	CHD-C4C	5.85	1.50	1.38
45	7	309	KC2	CHD-C4C	5.84	1.50	1.38
45	19	309	KC2	C3C-C2C	5.83	1.49	1.37
43	3	304	A86	O4-C38	5.83	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	8	314	KC1	C2A-C3A	5.82	1.49	1.37
45	13	311	KC2	CHD-C4C	5.82	1.50	1.38
45	6	310	KC2	CHD-C4C	5.82	1.50	1.38
42	18	313	KC1	C2A-C3A	5.82	1.49	1.37
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	311	KC2	C1A-NA	5.80	1.49	1.38
45	3	311	KC2	C2A-C3A	5.79	1.49	1.37
42	19	314	KC1	C2A-C3A	5.79	1.49	1.37
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
42	1	314	KC1	C2A-C3A	5.77	1.49	1.37
45	5	308	KC2	CHD-C4C	5.77	1.50	1.38
45	2	310	KC2	CHD-C4C	5.76	1.50	1.38
45	12	311	KC2	C3C-C2C	5.76	1.48	1.37
45	17	309	KC2	C3C-C2C	5.76	1.48	1.37
45	7	309	KC2	C2A-C3A	5.75	1.48	1.37
45	15	308	KC2	CHD-C4C	5.75	1.50	1.38
45	18	308	KC2	CHD-C4C	5.73	1.50	1.38
45	16	309	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	311	KC2	C2A-C3A	5.72	1.48	1.37
45	16	311	KC2	C1A-NA	5.72	1.49	1.38
45	6	312	KC2	CHD-C4C	5.72	1.50	1.38
45	14	308	KC2	C3C-C2C	5.71	1.48	1.37
45	1	309	KC2	CHD-C4C	5.71	1.50	1.38
45	9	309	KC2	C3C-C2C	5.71	1.48	1.37
45	16	311	KC2	CHD-C4C	5.70	1.50	1.38
45	16	311	KC2	C3C-C2C	5.70	1.48	1.37
45	4	308	KC2	CHD-C4C	5.70	1.50	1.38
43	11	302	A86	O4-C38	5.70	1.48	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
45	5	310	KC2	CHD-C4C	5.69	1.50	1.38
42	3	314	KC1	C1A-NA	5.69	1.49	1.38
45	4	310	KC2	C3C-C2C	5.68	1.48	1.37
45	6	312	KC2	C3C-C2C	5.68	1.48	1.37
35	d	407	PL9	C7-C3	-5.67	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
45	4	310	KC2	CHD-C4C	5.66	1.50	1.38
42	12	314	KC1	C1A-NA	5.66	1.49	1.38
42	13	314	KC1	C1A-NA	5.65	1.49	1.38
45	9	309	KC2	C1A-NA	5.65	1.49	1.38
45	15	310	KC2	CHD-C4C	5.65	1.50	1.38
45	3	311	KC2	C3C-C2C	5.65	1.48	1.37
45	14	308	KC2	CHD-C4C	5.65	1.50	1.38
45	12	309	KC2	CHD-C4C	5.65	1.50	1.38
45	8	309	KC2	CHD-C4C	5.65	1.50	1.38
43	11	320	A86	O4-C38	5.64	1.48	1.35
45	9	309	KC2	CHD-C4C	5.64	1.50	1.38
45	13	309	KC2	C3C-C2C	5.64	1.48	1.37
45	12	311	KC2	C2A-C3A	5.63	1.48	1.37
45	19	309	KC2	CHD-C4C	5.63	1.49	1.38
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
43	10	306	A86	O4-C38	5.61	1.47	1.35
45	14	310	KC2	CHD-C4C	5.60	1.49	1.38
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
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	407	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
45	6	310	KC2	C2A-C3A	5.58	1.48	1.37
42	15	317	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	309	KC2	C2A-C3A	5.57	1.48	1.37
45	12	311	KC2	CHD-C4C	5.57	1.49	1.38
42	7	314	KC1	C1A-NA	5.57	1.48	1.38
45	9	309	KC2	C2A-C3A	5.56	1.48	1.37
41	e	101	HEM	FE-ND	5.56	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	11	311	KC2	C1A-NA	5.56	1.48	1.38
41	E	101	HEM	FE-ND	5.56	2.12	1.94
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
45	7	311	KC2	CHD-C4C	5.54	1.49	1.38
43	7	305	A86	O4-C38	5.53	1.47	1.35
45	7	311	KC2	C2A-C3A	5.53	1.48	1.37
45	13	309	KC2	CHD-C4C	5.52	1.49	1.38
42	0	315	KC1	CHD-C4C	5.52	1.49	1.38
45	1	309	KC2	C3C-C2C	5.52	1.48	1.37
45	17	311	KC2	CHD-C4C	5.51	1.49	1.38
42	15	317	KC1	CHD-C4C	5.51	1.49	1.38
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	309	KC2	C2A-C3A	5.50	1.48	1.37
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
45	11	311	KC2	CHD-C4C	5.48	1.49	1.38
42	9	314	KC1	C3C-C2C	5.47	1.48	1.36
45	11	309	KC2	CHD-C4C	5.47	1.49	1.38
45	10	310	KC2	C1A-NA	5.47	1.48	1.38
45	0	310	KC2	C2A-C3A	5.47	1.48	1.37
45	3	311	KC2	CHD-C4C	5.47	1.49	1.38
43	12	301	A86	O4-C38	5.47	1.47	1.35
45	5	310	KC2	C3C-C2C	5.47	1.48	1.37
42	19	314	KC1	CHD-C4C	5.47	1.49	1.38
42	9	314	KC1	CHD-C4C	5.46	1.49	1.38
43	2	305	A86	O4-C38	5.46	1.47	1.35
45	8	311	KC2	C2A-C3A	5.46	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	13	306	A86	O4-C38	5.45	1.47	1.35
42	1	314	KC1	CHD-C4C	5.45	1.49	1.38
45	5	308	KC2	C3C-C2C	5.44	1.48	1.37
45	15	308	KC2	C2A-C3A	5.44	1.48	1.37
42	19	314	KC1	C3C-C2C	5.44	1.48	1.36
42	16	314	KC1	CHD-C4C	5.44	1.49	1.38
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	15	317	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	CHD-C4C	5.42	1.49	1.38
42	5	313	KC1	C3C-C2C	5.42	1.48	1.36
42	4	313	KC1	CHD-C4C	5.42	1.49	1.38
45	8	311	KC2	CHD-C4C	5.42	1.49	1.38
43	14	305	A86	O4-C38	5.42	1.47	1.35
42	11	314	KC1	CHD-C4C	5.41	1.49	1.38
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	306	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	311	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
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	4	313	KC1	C2A-C3A	5.37	1.48	1.37
42	14	313	KC1	CHD-C4C	5.37	1.49	1.38
42	9	314	KC1	C3B-C2B	5.36	1.48	1.37
43	0	301	A86	O4-C38	5.36	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	314	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
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	p	609	KC1	CHD-C4C	5.34	1.49	1.38
42	12	314	KC1	C2A-C3A	5.33	1.48	1.37
45	18	310	KC2	CHD-C4C	5.33	1.49	1.38
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
45	17	311	KC2	C2A-C3A	5.31	1.48	1.37
45	5	308	KC2	C2A-C3A	5.31	1.48	1.37
45	1	311	KC2	CHD-C4C	5.31	1.49	1.38
43	6	305	A86	O1-C20	-5.30	1.38	1.46
42	3	314	KC1	C3B-C2B	5.30	1.48	1.37
43	16	305	A86	O4-C38	5.30	1.47	1.35
42	P	609	KC1	CHD-C4C	5.30	1.49	1.38
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	309	KC2	C3C-C2C	5.27	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	1	311	KC2	C2A-C3A	5.27	1.47	1.37
42	2	313	KC1	CHD-C4C	5.26	1.49	1.38
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	16	314	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
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	10	310	KC2	CHD-C4C	5.22	1.49	1.38
45	19	309	KC2	C3B-C2B	5.22	1.47	1.37
43	17	305	A86	O4-C38	5.21	1.47	1.35
42	12	314	KC1	CHD-C4C	5.21	1.49	1.38
42	7	314	KC1	CHD-C4C	5.20	1.49	1.38
43	P	613	A86	O4-C38	5.19	1.46	1.35
43	16	305	A86	O1-C20	-5.19	1.38	1.46
42	18	313	KC1	C3C-C2C	5.19	1.47	1.36
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	311	KC2	O2D-CGD	5.19	1.45	1.33
45	3	311	KC2	O2D-CGD	5.18	1.45	1.33
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
43	7	303	A86	O4-C38	5.17	1.46	1.35
42	18	313	KC1	C3B-C2B	5.17	1.47	1.37
43	11	304	A86	O4-C38	5.17	1.46	1.35
45	16	309	KC2	O2D-CGD	5.16	1.45	1.33
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
43	16	306	A86	O4-C38	5.15	1.46	1.35
45	0	310	KC2	CHD-C4C	5.15	1.49	1.38
45	2	308	KC2	O2D-CGD	5.15	1.45	1.33
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	18	313	KC1	CHD-C4C	5.14	1.49	1.38
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	3	311	KC2	C3B-C2B	5.12	1.47	1.37
45	16	309	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	10	315	KC1	CHD-C4C	5.11	1.48	1.38
42	7	314	KC1	O2D-CGD	5.11	1.45	1.33
42	6	315	KC1	CHD-C4C	5.11	1.48	1.38
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	309	KC2	C3B-C2B	5.10	1.47	1.37
35	D	407	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	314	KC1	C3C-C2C	5.09	1.47	1.36
45	15	310	KC2	C2A-C3A	5.09	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	14	304	A86	O4-C38	5.09	1.46	1.35
42	19	314	KC1	O2D-CGD	5.09	1.45	1.33
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
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	314	KC1	C1A-NA	5.07	1.47	1.38
35	d	407	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	314	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	15	317	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	13	314	KC1	CHD-C4C	5.04	1.48	1.38
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	311	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	305	A86	O4-C38	5.03	1.46	1.35
42	17	314	KC1	C3B-C2B	5.03	1.47	1.37
42	17	314	KC1	CHD-C4C	5.03	1.48	1.38
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	302	A86	C32-C31	5.02	1.62	1.54
43	16	302	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	311	KC2	O2D-CGD	5.00	1.45	1.33
42	11	314	KC1	C3B-C2B	4.99	1.47	1.37
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
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	314	KC1	C3B-C2B	4.94	1.47	1.37
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	309	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	1	311	KC2	O2D-CGD	4.90	1.45	1.33
43	16	302	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
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	17	311	KC2	C3B-C2B	4.89	1.47	1.37
43	1	305	A86	O4-C38	4.89	1.46	1.35
45	7	309	KC2	CHC-C4B	4.88	1.47	1.38
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	314	KC1	O2D-CGD	4.86	1.45	1.33
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	11	311	KC2	O2D-CGD	4.85	1.45	1.33
43	8	304	A86	O4-C38	4.85	1.46	1.35
42	1	314	KC1	C3B-C2B	4.85	1.47	1.37
43	7	306	A86	O4-C38	4.84	1.46	1.35
43	18	305	A86	O4-C38	4.84	1.46	1.35
43	1	303	A86	O1-C20	-4.84	1.39	1.46
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
42	5	313	KC1	O2D-CGD	4.82	1.45	1.33
45	16	309	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
45	5	308	KC2	C3B-C2B	4.81	1.47	1.37
42	p	609	KC1	C3B-C2B	4.81	1.47	1.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	16	314	KC1	O2D-CGD	4.81	1.44	1.33
45	3	309	KC2	CHC-C4B	4.81	1.47	1.38
43	16	301	A86	O4-C38	4.81	1.46	1.35
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
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	313	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	13	314	KC1	CHC-C4B	4.78	1.47	1.38
42	11	314	KC1	CHC-C4B	4.78	1.47	1.38
45	8	309	KC2	C3B-C2B	4.78	1.47	1.37
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	309	KC2	C1A-NA	4.77	1.47	1.38
45	13	311	KC2	CHB-C1B	4.77	1.47	1.38
42	17	314	KC1	CHB-C1B	4.77	1.47	1.38
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	311	KC2	CHB-C1B	4.76	1.47	1.38
43	13	302	A86	O4-C38	4.76	1.45	1.35
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	311	KC2	C3B-C2B	4.75	1.46	1.37
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
43	p	613	A86	O1-C20	-4.74	1.39	1.46
43	18	302	A86	O4-C38	4.74	1.45	1.35
42	6	315	KC1	O2D-CGD	4.73	1.44	1.33
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
42	6	315	KC1	CHD-C1D	4.71	1.50	1.39
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
31	C	503	CLA	CHC-C4B	-4.70	1.28	1.39
45	4	310	KC2	CHB-C1B	4.70	1.47	1.38
45	15	310	KC2	O2D-CGD	4.69	1.44	1.33
45	16	309	KC2	CHB-C1B	4.69	1.47	1.38
45	4	308	KC2	CHB-C1B	4.68	1.47	1.38
42	15	317	KC1	O2D-CGD	4.68	1.44	1.33
43	18	303	A86	O4-C38	4.68	1.45	1.35
43	0	304	A86	O4-C38	4.68	1.45	1.35
43	3	306	A86	O4-C38	4.67	1.45	1.35
31	c	503	CLA	CHC-C4B	-4.67	1.28	1.39
42	3	314	KC1	CHD-C4C	4.67	1.48	1.38
45	9	309	KC2	CHC-C4B	4.67	1.47	1.38
45	13	309	KC2	CHC-C4B	4.67	1.47	1.38
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	15	317	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
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	304	A86	O4-C38	4.64	1.45	1.35
37	0	317	LMG	C4-C5	4.63	1.62	1.53
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
43	6	304	A86	O4-C38	4.63	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1	319	A86	O1-C20	-4.62	1.39	1.46
45	8	309	KC2	CHC-C4B	4.62	1.47	1.38
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
42	14	313	KC1	CHC-C4B	4.60	1.47	1.38
43	17	316	A86	O1-C20	-4.60	1.39	1.46
42	4	313	KC1	CHC-C4B	4.59	1.47	1.38
43	8	303	A86	O4-C38	4.59	1.45	1.35
45	17	311	KC2	CHC-C4B	4.58	1.47	1.38
45	16	311	KC2	CHC-C4B	4.58	1.47	1.38
43	0	305	A86	O4-C38	4.58	1.45	1.35
42	15	317	KC1	CHB-C1B	4.57	1.47	1.38
43	5	303	A86	O4-C38	4.57	1.45	1.35
42	16	314	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
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	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
37	10	319	LMG	C4-C5	4.54	1.62	1.53
42	5	313	KC1	CHC-C4B	4.53	1.47	1.38
45	0	310	KC2	C3B-C2B	4.53	1.46	1.37
43	12	302	A86	O1-C20	-4.52	1.39	1.46
43	13	302	A86	O1-C20	-4.52	1.39	1.46
43	8	305	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
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
42	17	314	KC1	CHC-C4B	4.50	1.47	1.38
42	8	314	KC1	CHC-C4B	4.49	1.47	1.38
43	8	303	A86	O1-C20	-4.49	1.39	1.46
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
42	18	313	KC1	O2D-CGD	4.47	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1	319	A86	O4-C38	4.47	1.45	1.35
43	3	303	A86	O4-C38	4.47	1.45	1.35
45	3	309	KC2	CHB-C1B	4.46	1.47	1.38
45	10	310	KC2	C3B-C2B	4.46	1.46	1.37
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	311	KC2	CHB-C1B	4.44	1.47	1.38
43	10	305	A86	O1-C20	-4.44	1.39	1.46
45	0	310	KC2	CHC-C4B	4.43	1.47	1.38
43	3	303	A86	O1-C20	-4.43	1.39	1.46
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	309	KC2	CBC-CAC	4.42	1.52	1.30
45	7	309	KC2	CBC-CAC	4.41	1.52	1.30
45	17	309	KC2	CBC-CAC	4.41	1.52	1.30
45	13	311	KC2	CBC-CAC	4.40	1.52	1.30
45	3	309	KC2	CBC-CAC	4.39	1.52	1.30
45	2	310	KC2	CHB-C1B	4.39	1.46	1.38
45	15	308	KC2	CBC-CAC	4.39	1.52	1.30
42	5	313	KC1	CHB-C1B	4.39	1.46	1.38
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	311	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
41	V	201	HEM	FE-NC	4.37	2.09	1.95
41	v	201	HEM	FE-NC	4.37	2.09	1.95
43	0	306	A86	C30-C29	-4.37	1.24	1.32
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	12	313	CLA	C4B-NB	4.34	1.43	1.37
45	3	311	KC2	CBC-CAC	4.34	1.51	1.30
43	4	306	A86	O4-C38	4.34	1.45	1.35
31	17	313	CLA	C4B-NB	4.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	8	309	KC2	CHB-C1B	4.33	1.46	1.38
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
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
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	311	KC2	CBC-CAC	4.31	1.51	1.30
45	8	309	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
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	311	KC2	CBC-CAC	4.29	1.51	1.30
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	6	312	KC2	CBC-CAC	4.28	1.51	1.30
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	0	310	KC2	CHB-C1B	4.26	1.46	1.38
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
45	15	310	KC2	CHC-C4B	4.22	1.46	1.38
31	b	605	CLA	C4D-ND	-4.22	1.31	1.37
31	2	315	CLA	C4B-NB	4.21	1.43	1.37
43	P	611	A86	O4-C38	4.21	1.44	1.35
45	5	310	KC2	CHC-C4B	4.21	1.46	1.38
31	12	313	CLA	C3B-C4B	4.20	1.52	1.42
31	2	312	CLA	C4B-NB	4.19	1.42	1.37
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
43	13	304	A86	O4-C38	4.18	1.44	1.35
31	12	316	CLA	C1D-ND	4.17	1.42	1.37
43	15	303	A86	O1-C20	-4.17	1.40	1.46
42	16	314	KC1	CHD-C1D	4.17	1.48	1.39
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
42	5	313	KC1	OBD-CAD	4.16	1.29	1.22
31	C	503	CLA	C1B-C2B	4.16	1.53	1.43
31	2	312	CLA	C3B-C4B	4.16	1.52	1.42
31	B	605	CLA	C4D-ND	-4.15	1.32	1.37
31	19	311	CLA	C1D-ND	4.15	1.42	1.37
31	c	503	CLA	C1B-C2B	4.13	1.53	1.43
31	b	606	CLA	C4D-ND	-4.13	1.32	1.37
31	D	405	CLA	C4D-ND	-4.12	1.32	1.37
31	7	313	CLA	C4B-NB	4.12	1.42	1.37
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	18	313	KC1	CHD-C1D	4.11	1.48	1.39
42	P	609	KC1	CHC-C4B	4.11	1.46	1.38
43	7	302	A86	O1-C20	-4.11	1.40	1.46
42	13	314	KC1	OBD-CAD	4.11	1.29	1.22
31	3	315	CLA	C1D-ND	4.11	1.42	1.37
31	5	306	CLA	C1D-ND	4.10	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	6	315	KC1	OBD-CAD	4.10	1.29	1.22
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
42	8	314	KC1	CHD-C1D	4.07	1.48	1.39
31	p	602	CLA	C4D-ND	-4.07	1.32	1.37
43	8	306	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	405	CLA	C4D-ND	-4.06	1.32	1.37
31	16	315	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
31	15	311	CLA	CMB-C2B	-4.05	1.42	1.50
43	13	302	A86	C30-C29	-4.05	1.25	1.32
31	13	315	CLA	C1D-ND	4.04	1.42	1.37
31	14	306	CLA	C1B-NB	-4.04	1.32	1.37
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	15	313	CLA	C1D-ND	4.01	1.42	1.37
31	13	313	CLA	C4B-NB	4.01	1.42	1.37
31	2	315	CLA	C3B-C4B	4.01	1.52	1.42
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	14	306	CLA	C3B-C4B	4.00	1.52	1.42
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
43	14	301	A86	C30-C29	-3.98	1.25	1.32
31	P	604	CLA	C4D-ND	-3.98	1.32	1.37
43	16	303	A86	O1-C20	-3.97	1.40	1.46
43	7	304	A86	O4-C38	3.96	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	6	315	KC1	C4D-ND	3.95	1.43	1.37
31	12	307	CLA	C1D-ND	3.95	1.42	1.37
45	2	308	KC2	CHD-C1D	3.94	1.48	1.39
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
45	13	311	KC2	CHD-C1D	3.93	1.48	1.39
31	A	404	CLA	C4D-ND	-3.93	1.32	1.37
42	16	314	KC1	OBD-CAD	3.93	1.29	1.22
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
31	16	307	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	314	KC1	CHB-C4A	3.92	1.48	1.39
31	11	316	CLA	C4B-NB	3.91	1.42	1.37
42	8	314	KC1	CHD-C4C	3.91	1.46	1.38
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
31	C	513	CLA	C4D-ND	-3.89	1.32	1.37
31	6	308	CLA	C1D-ND	3.89	1.42	1.37
31	13	313	CLA	C3B-C4B	3.89	1.51	1.42
37	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
31	B	613	CLA	C4D-ND	-3.88	1.32	1.37
31	9	310	CLA	C1D-ND	3.88	1.42	1.37
45	2	310	KC2	CHD-C1D	3.87	1.48	1.39
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	302	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	304	A86	C30-C29	-3.85	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	614	CLA	C4D-ND	-3.85	1.32	1.37
45	3	309	KC2	CHD-C1D	3.85	1.48	1.39
31	4	312	CLA	MG-NB	-3.85	1.98	2.05
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
45	7	309	KC2	CHD-C1D	3.85	1.48	1.39
43	10	302	A86	O1-C20	-3.85	1.40	1.46
43	16	305	A86	C19-C20	3.84	1.57	1.52
43	10	318	A86	O1-C20	-3.84	1.40	1.46
45	17	309	KC2	CHD-C1D	3.84	1.48	1.39
31	3	313	CLA	C4B-NB	3.84	1.42	1.37
43	3	305	A86	C19-C20	3.84	1.57	1.52
43	2	305	A86	O1-C20	-3.84	1.40	1.46
45	6	312	KC2	CHD-C1D	3.83	1.48	1.39
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
42	7	314	KC1	OBD-CAD	3.82	1.29	1.22
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
42	13	314	KC1	CHD-C1D	3.81	1.48	1.39
31	11	316	CLA	C3B-C4B	3.81	1.51	1.42
31	16	313	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
31	1	316	CLA	C1D-ND	3.80	1.42	1.37
45	5	310	KC2	CHD-C1D	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	15	301	A86	C33-C34	3.80	1.58	1.51
45	16	309	KC2	CHD-C1D	3.80	1.47	1.39
42	11	314	KC1	CHB-C4A	3.79	1.47	1.39
45	17	311	KC2	OBD-CAD	3.79	1.29	1.22
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
45	7	311	KC2	OBD-CAD	3.78	1.29	1.22
31	14	312	CLA	C4D-ND	-3.78	1.32	1.37
45	6	310	KC2	CHD-C1D	3.78	1.47	1.39
42	9	314	KC1	OBD-CAD	3.77	1.29	1.22
45	16	311	KC2	CHD-C1D	3.77	1.47	1.39
43	16	303	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
45	15	310	KC2	CHD-C1D	3.77	1.47	1.39
31	17	313	CLA	CMD-C2D	-3.77	1.42	1.50
31	c	504	CLA	C4D-ND	-3.77	1.32	1.37
45	1	309	KC2	CHD-C1D	3.77	1.47	1.39
45	19	309	KC2	CHD-C1D	3.77	1.47	1.39
43	18	304	A86	C30-C29	-3.77	1.25	1.32
42	7	314	KC1	CHD-C1D	3.76	1.47	1.39
31	B	604	CLA	CMB-C2B	-3.76	1.42	1.50
45	16	311	KC2	CHB-C4A	3.76	1.47	1.39
31	3	313	CLA	MG-NB	-3.76	1.98	2.05
43	3	305	A86	C40-C32	-3.76	1.46	1.53
45	12	311	KC2	CHD-C1D	3.76	1.47	1.39
31	D	402	CLA	C4D-ND	-3.76	1.32	1.37
45	12	309	KC2	CHD-C1D	3.76	1.47	1.39
31	3	308	CLA	C4D-ND	-3.76	1.32	1.37
45	5	308	KC2	CHD-C1D	3.75	1.47	1.39
43	11	305	A86	C30-C29	-3.75	1.25	1.32
45	3	309	KC2	OBD-CAD	3.75	1.28	1.22
45	15	308	KC2	CHD-C1D	3.75	1.47	1.39
42	19	314	KC1	OBD-CAD	3.75	1.28	1.22
31	C	510	CLA	C4D-ND	-3.75	1.32	1.37
43	6	307	A86	C30-C29	-3.75	1.25	1.32
45	17	311	KC2	CHD-C1D	3.75	1.47	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	12	316	CLA	C4B-NB	3.74	1.42	1.37
45	3	311	KC2	OBD-CAD	3.74	1.28	1.22
31	2	309	CLA	C1D-ND	3.74	1.42	1.37
42	3	314	KC1	CHD-C1D	3.74	1.47	1.39
45	17	309	KC2	CHB-C4A	3.74	1.47	1.39
43	8	305	A86	C30-C29	-3.74	1.25	1.32
31	c	510	CLA	C4D-ND	-3.74	1.32	1.37
45	4	308	KC2	CHD-C1D	3.73	1.47	1.39
45	3	311	KC2	CHB-C4A	3.73	1.47	1.39
31	b	605	CLA	CMB-C2B	-3.73	1.42	1.50
45	18	308	KC2	CHD-C1D	3.73	1.47	1.39
42	17	314	KC1	CHD-C1D	3.73	1.47	1.39
43	1	305	A86	C30-C29	-3.73	1.25	1.32
42	8	314	KC1	CHB-C1B	3.73	1.45	1.38
31	12	316	CLA	C3B-C4B	3.73	1.51	1.42
31	16	310	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
31	16	313	CLA	MG-NB	-3.72	1.98	2.05
42	17	314	KC1	CHB-C4A	3.72	1.47	1.39
31	B	615	CLA	C4D-ND	-3.72	1.32	1.37
45	12	309	KC2	OBD-CAD	3.71	1.28	1.22
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	304	A86	O1-C20	-3.71	1.40	1.46
31	13	310	CLA	C1D-ND	3.71	1.42	1.37
31	d	402	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	0	313	CLA	C1D-ND	3.70	1.42	1.37
45	13	309	KC2	OBD-CAD	3.70	1.28	1.22
31	18	307	CLA	C4D-ND	-3.70	1.32	1.37
31	15	311	CLA	C4D-ND	-3.70	1.32	1.37
43	16	303	A86	O1-C15	-3.70	1.39	1.45
45	13	311	KC2	OBD-CAD	3.70	1.28	1.22
31	12	310	CLA	C1D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	9	309	KC2	CHD-C1D	3.70	1.47	1.39
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
42	1	314	KC1	OBD-CAD	3.68	1.28	1.22
45	13	311	KC2	CHC-C1C	3.68	1.47	1.39
31	7	313	CLA	C3B-C4B	3.68	1.51	1.42
45	8	309	KC2	CHD-C1D	3.68	1.47	1.39
31	C	504	CLA	C4D-ND	-3.68	1.32	1.37
45	7	309	KC2	CHB-C4A	3.68	1.47	1.39
45	14	308	KC2	CHD-C1D	3.67	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
42	1	314	KC1	CHD-C1D	3.66	1.47	1.39
35	a	409	PL9	C3-C4	-3.66	1.43	1.49
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	308	CLA	C4D-ND	-3.66	1.32	1.37
42	9	314	KC1	CHB-C4A	3.66	1.47	1.39
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
45	14	310	KC2	OBD-CAD	3.65	1.28	1.22
31	5	314	CLA	C3B-C4B	3.65	1.51	1.42
31	6	314	CLA	CMB-C2B	-3.65	1.43	1.50
31	3	312	CLA	C4B-NB	3.65	1.42	1.37
43	16	306	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
42	0	315	KC1	CHD-C1D	3.65	1.47	1.39
31	8	313	CLA	CMD-C2D	-3.64	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	10	314	CLA	C1D-ND	3.64	1.42	1.37
42	3	314	KC1	OBD-CAD	3.64	1.28	1.22
31	w	203	CLA	C4D-ND	-3.64	1.32	1.37
42	19	314	KC1	CHD-C1D	3.64	1.47	1.39
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	13	315	CLA	C4B-NB	3.63	1.42	1.37
45	7	311	KC2	CHD-C1D	3.63	1.47	1.39
31	b	604	CLA	C4D-ND	-3.63	1.32	1.37
31	14	312	CLA	MG-NB	-3.63	1.98	2.05
43	6	305	A86	C30-C29	-3.63	1.25	1.32
45	8	311	KC2	CHD-C1D	3.63	1.47	1.39
42	5	313	KC1	CHD-C1D	3.62	1.47	1.39
43	15	302	A86	O1-C20	-3.62	1.41	1.46
43	2	304	A86	C35-C34	3.62	1.58	1.51
42	2	313	KC1	OBD-CAD	3.62	1.28	1.22
33	Y	101	BCR	C30-C25	-3.62	1.48	1.53
42	15	317	KC1	OBD-CAD	3.62	1.28	1.22
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
31	15	311	CLA	C4B-NB	3.62	1.42	1.37
43	16	306	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
43	5	318	A86	O1-C20	-3.62	1.41	1.46
38	b	622	DGD	O3G-C1D	3.61	1.46	1.40
42	9	314	KC1	CHD-C1D	3.61	1.47	1.39
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
31	13	315	CLA	C3B-C4B	3.60	1.51	1.42
45	3	311	KC2	CHD-C1D	3.60	1.47	1.39
31	17	313	CLA	C3B-C4B	3.60	1.51	1.42
43	3	302	A86	C30-C29	-3.60	1.26	1.32
42	12	314	KC1	OBD-CAD	3.59	1.28	1.22
43	9	306	A86	O1-C20	-3.59	1.41	1.46
43	9	305	A86	C19-C20	3.59	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	18	310	KC2	CHD-C1D	3.59	1.47	1.39
31	15	313	CLA	C3B-C4B	3.59	1.51	1.42
45	13	309	KC2	CHD-C1D	3.59	1.47	1.39
31	2	307	CLA	C4D-ND	-3.59	1.32	1.37
45	4	310	KC2	OBD-CAD	3.59	1.28	1.22
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	303	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	315	CLA	C4B-NB	3.58	1.42	1.37
31	0	316	CLA	C1D-ND	3.58	1.42	1.37
31	C	512	CLA	C4D-ND	-3.58	1.32	1.37
31	10	313	CLA	C4B-NB	3.58	1.42	1.37
45	12	311	KC2	OBD-CAD	3.58	1.28	1.22
43	13	305	A86	O1-C20	-3.58	1.41	1.46
38	B	621	DGD	C4D-C5D	3.58	1.60	1.53
31	3	316	CLA	C4D-ND	-3.57	1.32	1.37
42	15	317	KC1	CHB-C4A	3.57	1.47	1.39
31	4	312	CLA	MG-ND	-3.57	1.98	2.05
45	2	308	KC2	OBD-CAD	3.57	1.28	1.22
31	b	615	CLA	C4D-ND	-3.57	1.32	1.37
31	P	608	CLA	C4D-ND	-3.57	1.32	1.37
31	4	315	CLA	C4B-NB	3.57	1.42	1.37
31	P	603	CLA	C4D-ND	-3.57	1.32	1.37
43	16	301	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	406	CLA	C4D-ND	-3.56	1.32	1.37
31	d	406	CLA	C4D-ND	-3.56	1.32	1.37
45	11	309	KC2	OBD-CAD	3.56	1.28	1.22
31	8	313	CLA	C4D-ND	-3.56	1.32	1.37
31	2	312	CLA	CMB-C2B	-3.56	1.43	1.50
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	11	303	A86	C30-C29	-3.56	1.26	1.32
45	16	311	KC2	OBD-CAD	3.56	1.28	1.22
43	7	304	A86	C19-C20	3.55	1.57	1.52
31	0	314	CLA	C4D-ND	-3.55	1.32	1.37
37	K	101	LMG	O7-C8	-3.55	1.37	1.46
37	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
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	5	308	KC2	OBD-CAD	3.54	1.28	1.22
45	2	310	KC2	CHB-C4A	3.54	1.47	1.39
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	c	511	CLA	C4D-ND	-3.53	1.32	1.37
31	4	312	CLA	C1B-NB	-3.53	1.33	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
45	6	312	KC2	OBD-CAD	3.53	1.28	1.22
38	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
42	14	313	KC1	CHD-C1D	3.52	1.47	1.39
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	4	310	KC2	CHD-C1D	3.52	1.47	1.39
45	7	309	KC2	CHC-C1C	3.52	1.47	1.39
31	6	314	CLA	MG-NB	-3.52	1.98	2.05
38	c	520	DGD	O5D-C6D	-3.51	1.37	1.43
43	2	304	A86	C37-C36	3.51	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	604	CLA	CHC-C4B	-3.51	1.31	1.39
31	p	608	CLA	C1D-ND	3.51	1.42	1.37
31	d	405	CLA	C3B-C4B	3.51	1.51	1.42
43	2	305	A86	C30-C29	-3.51	1.26	1.32
45	18	308	KC2	C1D-ND	-3.51	1.33	1.37
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	8	309	KC2	C1D-ND	-3.50	1.33	1.37
31	b	605	CLA	CHC-C4B	-3.50	1.31	1.39
45	17	309	KC2	CHC-C1C	3.50	1.47	1.39
31	18	306	CLA	C1D-ND	3.50	1.42	1.37
32	D	403	PHO	C1D-C2D	3.50	1.43	1.39
31	B	614	CLA	C4D-ND	-3.50	1.32	1.37
43	1	305	A86	C13-C11	-3.50	1.42	1.49
31	14	312	CLA	C1B-NB	-3.50	1.33	1.37
43	14	303	A86	O1-C20	-3.50	1.41	1.46
45	8	311	KC2	OBD-CAD	3.50	1.28	1.22
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
32	d	403	PHO	C1D-C2D	3.49	1.43	1.39
42	8	314	KC1	OBD-CAD	3.49	1.28	1.22
31	B	606	CLA	C4D-ND	-3.49	1.32	1.37
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	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
37	1	301	LMG	C4-C5	3.48	1.60	1.53
42	4	313	KC1	CHD-C1D	3.48	1.47	1.39
31	6	314	CLA	C4D-ND	-3.48	1.32	1.37
43	0	301	A86	C30-C29	-3.48	1.26	1.32
38	B	621	DGD	O3G-C1D	3.48	1.46	1.40
31	7	312	CLA	C4B-NB	3.48	1.42	1.37
31	Z	101	CLA	C4D-ND	-3.48	1.32	1.37
31	D	405	CLA	C3B-C4B	3.48	1.50	1.42
42	13	314	KC1	CHC-C1C	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	1	311	KC2	OBD-CAD	3.48	1.28	1.22
45	2	310	KC2	OBD-CAD	3.48	1.28	1.22
42	9	314	KC1	CHC-C1C	3.48	1.47	1.39
45	11	309	KC2	CHC-C1C	3.48	1.47	1.39
45	16	309	KC2	CHB-C4A	3.48	1.47	1.39
45	15	308	KC2	OBD-CAD	3.48	1.28	1.22
31	17	312	CLA	C1D-ND	3.48	1.42	1.37
43	6	307	A86	C2-C1	-3.47	1.31	1.35
31	16	313	CLA	C4D-ND	-3.47	1.32	1.37
43	12	305	A86	O1-C20	-3.47	1.41	1.46
31	4	312	CLA	C3B-C4B	3.47	1.50	1.42
43	3	304	A86	C30-C29	-3.47	1.26	1.32
42	18	313	KC1	OBD-CAD	3.47	1.28	1.22
31	A	404	CLA	C1D-ND	3.47	1.42	1.37
37	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	16	309	KC2	OBD-CAD	3.46	1.28	1.22
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	308	CLA	C4D-ND	-3.46	1.32	1.37
45	11	311	KC2	OBD-CAD	3.46	1.28	1.22
45	11	309	KC2	CHD-C1D	3.46	1.47	1.39
42	15	317	KC1	CHD-C1D	3.45	1.47	1.39
43	1	304	A86	C30-C29	-3.45	1.26	1.32
43	4	306	A86	C30-C29	-3.45	1.26	1.32
42	18	313	KC1	CHB-C4A	3.45	1.47	1.39
31	1	310	CLA	C1D-ND	3.45	1.42	1.37
43	4	305	A86	O1-C20	-3.45	1.41	1.46
31	16	313	CLA	CMB-C2B	-3.44	1.43	1.50
45	1	309	KC2	OBD-CAD	3.44	1.28	1.22
42	2	313	KC1	CHD-C1D	3.44	1.47	1.39
43	19	303	A86	O1-C20	-3.44	1.41	1.46
31	P	608	CLA	C1D-ND	3.44	1.42	1.37
31	14	312	CLA	C4B-NB	3.44	1.42	1.37
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	17	312	CLA	C4B-NB	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
31	14	306	CLA	MG-NB	-3.43	1.99	2.05
42	7	314	KC1	C4D-ND	3.42	1.42	1.37
45	14	308	KC2	CHB-C4A	3.42	1.47	1.39
45	14	310	KC2	CHD-C1D	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
31	11	312	CLA	C4B-NB	3.42	1.42	1.37
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	2	312	CLA	MG-NB	-3.42	1.99	2.05
33	Y	101	BCR	C1-C6	-3.42	1.49	1.53
31	12	308	CLA	C3B-C4B	3.41	1.50	1.42
31	15	312	CLA	CMB-C2B	-3.41	1.43	1.50
31	W	202	CLA	C1D-ND	3.41	1.42	1.37
31	6	309	CLA	C4D-ND	-3.41	1.33	1.37
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	b	607	CLA	C4D-ND	-3.41	1.33	1.37
45	18	310	KC2	OBD-CAD	3.40	1.28	1.22
31	8	315	CLA	C1D-ND	3.40	1.42	1.37
43	0	301	A86	O1-C15	-3.40	1.39	1.45
43	18	304	A86	C32-C31	-3.40	1.48	1.54
31	0	307	CLA	C4D-ND	-3.40	1.33	1.37
31	B	609	CLA	C4D-ND	-3.40	1.33	1.37
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	310	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
38	B	621	DGD	C4E-C5E	3.39	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	611	CLA	C4D-ND	-3.39	1.33	1.37
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
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	309	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	6	313	CLA	C1D-ND	3.39	1.41	1.37
31	12	313	CLA	C4D-ND	-3.39	1.33	1.37
45	8	311	KC2	CHB-C4A	3.38	1.47	1.39
31	8	307	CLA	C1D-ND	3.38	1.41	1.37
31	7	313	CLA	MG-NB	-3.38	1.99	2.05
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	4	308	KC2	OBD-CAD	3.38	1.28	1.22
31	1	315	CLA	C4B-NB	3.38	1.41	1.37
37	5	316	LMG	C4-C5	3.38	1.60	1.53
37	5	316	LMG	O1-C7	-3.37	1.37	1.43
43	6	307	A86	C26-C27	-3.37	1.31	1.35
31	18	312	CLA	C4B-NB	3.37	1.41	1.37
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	6	314	CLA	MG-ND	-3.37	1.99	2.05
31	5	309	CLA	C1D-ND	3.37	1.41	1.37
45	14	308	KC2	OBD-CAD	3.37	1.28	1.22
31	8	315	CLA	C4D-ND	-3.37	1.33	1.37
33	b	620	BCR	C1-C6	-3.37	1.49	1.53
31	11	312	CLA	C3B-C4B	3.36	1.50	1.42
45	17	311	KC2	CHB-C4A	3.36	1.46	1.39
31	10	313	CLA	C1D-ND	3.36	1.41	1.37
42	11	314	KC1	CHD-C1D	3.36	1.46	1.39
43	p	611	A86	C19-C20	3.36	1.56	1.52
31	2	312	CLA	C4D-ND	-3.36	1.33	1.37
45	18	308	KC2	OBD-CAD	3.36	1.28	1.22
31	1	321	CLA	MG-NB	-3.36	1.99	2.05
31	3	316	CLA	C1D-ND	3.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	16	307	CLA	C4B-NB	3.36	1.41	1.37
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
45	6	310	KC2	OBD-CAD	3.35	1.28	1.22
31	c	511	CLA	C1D-ND	3.35	1.41	1.37
31	6	314	CLA	C4B-NB	3.35	1.41	1.37
45	10	310	KC2	OBD-CAD	3.35	1.28	1.22
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
42	12	314	KC1	CHD-C1D	3.35	1.46	1.39
31	19	310	CLA	C4B-NB	3.35	1.41	1.37
43	0	303	A86	C30-C29	-3.34	1.26	1.32
42	P	609	KC1	C1B-NB	-3.34	1.33	1.37
45	0	310	KC2	OBD-CAD	3.34	1.28	1.22
42	1	314	KC1	CHC-C1C	3.34	1.46	1.39
31	1	308	CLA	C3B-C4B	3.34	1.50	1.42
43	17	305	A86	C33-C34	3.34	1.57	1.51
45	14	308	KC2	CHC-C1C	3.34	1.46	1.39
42	p	609	KC1	CHD-C1D	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	10	310	KC2	CHD-C1D	3.33	1.46	1.39
31	9	311	CLA	C4B-NB	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
31	3	308	CLA	C3B-C4B	3.33	1.50	1.42
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
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
31	14	306	CLA	C4B-NB	3.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	11	311	KC2	CHB-C4A	3.32	1.46	1.39
31	12	315	CLA	C4B-NB	3.32	1.41	1.37
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	13	307	CLA	C4B-NB	3.32	1.41	1.37
42	P	609	KC1	CHD-C1D	3.32	1.46	1.39
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
42	3	314	KC1	C4D-ND	3.32	1.42	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
45	5	310	KC2	OBD-CAD	3.31	1.28	1.22
45	15	310	KC2	OBD-CAD	3.31	1.28	1.22
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
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	312	CLA	C1D-ND	3.30	1.41	1.37
42	12	314	KC1	CHC-C1C	3.30	1.46	1.39
31	B	611	CLA	CMB-C2B	-3.30	1.43	1.50
31	6	316	CLA	C3B-C4B	3.30	1.50	1.42
43	16	304	A86	O1-C20	-3.30	1.41	1.46
31	5	311	CLA	C4D-ND	-3.30	1.33	1.37
31	A	406	CLA	C4D-ND	-3.30	1.33	1.37
45	15	308	KC2	CHC-C1C	3.30	1.46	1.39
31	17	312	CLA	C4D-ND	-3.30	1.33	1.37
31	B	604	CLA	C1B-NB	-3.30	1.33	1.37
31	b	605	CLA	C1B-NB	-3.30	1.33	1.37
31	5	314	CLA	C4B-NB	3.30	1.41	1.37
31	8	313	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
31	P	606	CLA	C3B-C4B	3.30	1.50	1.42
38	b	622	DGD	C4D-C5D	3.30	1.60	1.53
31	0	312	CLA	C4D-ND	-3.30	1.33	1.37
31	2	311	CLA	C4B-NB	3.30	1.41	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	19	315	CLA	C4B-NB	3.29	1.41	1.37
31	P	604	CLA	C1D-ND	3.29	1.41	1.37
42	15	317	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
45	17	309	KC2	OBD-CAD	3.28	1.28	1.22
45	7	309	KC2	OBD-CAD	3.28	1.28	1.22
31	12	307	CLA	C3B-C4B	3.28	1.50	1.42
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
31	11	315	CLA	C3B-C4B	3.28	1.50	1.42
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	1	313	CLA	C4B-NB	3.27	1.41	1.37
31	b	612	CLA	CMB-C2B	-3.27	1.43	1.50
31	14	312	CLA	C3B-C4B	3.27	1.50	1.42
31	10	317	CLA	C1D-ND	3.27	1.41	1.37
31	9	315	CLA	C4B-NB	3.27	1.41	1.37
31	6	316	CLA	C4B-NB	3.27	1.41	1.37
33	C	517	BCR	C1-C6	-3.27	1.49	1.53
31	16	315	CLA	C3B-C4B	3.27	1.50	1.42
31	19	313	CLA	C3B-C4B	3.27	1.50	1.42
31	c	504	CLA	C1D-ND	3.27	1.41	1.37
31	16	312	CLA	C4B-NB	3.27	1.41	1.37
45	8	309	KC2	OBD-CAD	3.26	1.28	1.22
42	17	314	KC1	OBD-CAD	3.26	1.28	1.22
45	1	311	KC2	CHB-C4A	3.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	316	CLA	C4D-ND	-3.26	1.33	1.37
42	8	314	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	18	314	CLA	C4D-ND	-3.26	1.33	1.37
31	5	312	CLA	MG-NB	-3.26	1.99	2.05
43	10	303	A86	C30-C29	-3.26	1.26	1.32
31	B	607	CLA	C1D-ND	3.26	1.41	1.37
31	15	312	CLA	C4B-NB	3.26	1.41	1.37
31	p	606	CLA	C3B-C4B	3.26	1.50	1.42
31	5	311	CLA	C1B-C2B	3.26	1.50	1.43
35	A	409	PL9	C7-C3	-3.25	1.48	1.51
42	10	315	KC1	C1B-NB	-3.25	1.33	1.37
42	8	314	KC1	C4D-ND	3.25	1.42	1.37
45	11	311	KC2	CHD-C1D	3.25	1.46	1.39
31	B	606	CLA	C1D-ND	3.25	1.41	1.37
31	18	314	CLA	C1D-ND	3.25	1.41	1.37
45	0	310	KC2	CHD-C1D	3.25	1.46	1.39
31	8	307	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	z	101	CLA	C1D-ND	3.25	1.41	1.37
31	7	312	CLA	C4D-ND	-3.25	1.33	1.37
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
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	6	313	CLA	C4B-NB	3.24	1.41	1.37
31	10	316	CLA	C4D-ND	-3.24	1.33	1.37
31	C	507	CLA	CMB-C2B	-3.24	1.43	1.50
31	C	512	CLA	MG-NB	-3.24	1.99	2.05
31	c	512	CLA	MG-NB	-3.24	1.99	2.05
35	a	409	PL9	C7-C3	-3.24	1.48	1.51
31	11	313	CLA	C4B-NB	3.24	1.41	1.37
45	11	309	KC2	C1B-NB	-3.24	1.33	1.37
42	0	315	KC1	CHB-C4A	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	10	301	A86	O1-C15	-3.24	1.40	1.45
31	0	316	CLA	C4D-ND	-3.23	1.33	1.37
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	9	313	CLA	C3B-C4B	3.23	1.50	1.42
33	c	517	BCR	C1-C6	-3.23	1.49	1.53
31	P	606	CLA	C1D-ND	3.23	1.41	1.37
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	13	308	CLA	C3B-C4B	3.23	1.50	1.42
31	19	307	CLA	C4B-NB	3.22	1.41	1.37
31	1	310	CLA	C4D-ND	-3.22	1.33	1.37
31	10	312	CLA	C4D-ND	-3.22	1.33	1.37
31	19	311	CLA	C4B-NB	3.22	1.41	1.37
45	10	310	KC2	CHB-C4A	3.22	1.46	1.39
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	11	308	CLA	C3B-C4B	3.22	1.50	1.42
45	1	311	KC2	CHD-C1D	3.22	1.46	1.39
31	8	313	CLA	MG-NB	-3.21	1.99	2.05
31	14	314	CLA	C4D-ND	-3.21	1.33	1.37
31	3	313	CLA	C3B-C4B	3.21	1.50	1.42
43	9	306	A86	O3-C36	-3.21	1.37	1.43
31	9	310	CLA	C4B-NB	3.21	1.41	1.37
31	7	315	CLA	C3B-C4B	3.21	1.50	1.42
43	16	303	A86	C30-C29	-3.20	1.26	1.32
31	9	308	CLA	C4D-ND	-3.20	1.33	1.37
31	16	310	CLA	C4D-ND	-3.20	1.33	1.37
31	0	313	CLA	C4B-NB	3.20	1.41	1.37
42	16	314	KC1	CHC-C1C	3.20	1.46	1.39
31	8	313	CLA	CMB-C2B	-3.20	1.44	1.50
31	c	507	CLA	CMB-C2B	-3.20	1.44	1.50
31	13	312	CLA	C4B-NB	3.20	1.41	1.37
43	11	304	A86	O1-C20	-3.20	1.41	1.46
45	7	311	KC2	CHC-C1C	3.20	1.46	1.39
43	15	303	A86	C30-C29	-3.20	1.26	1.32
43	10	303	A86	C13-C11	-3.19	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	306	CLA	C4D-ND	-3.19	1.33	1.37
42	16	314	KC1	C4D-ND	3.19	1.42	1.37
31	1	321	CLA	C1B-NB	-3.19	1.33	1.37
43	16	305	A86	C30-C29	-3.19	1.26	1.32
31	18	312	CLA	CMB-C2B	-3.19	1.44	1.50
31	r	101	CLA	C1D-ND	3.19	1.41	1.37
31	19	311	CLA	C3B-C4B	3.19	1.50	1.42
31	19	312	CLA	C1D-ND	3.19	1.41	1.37
31	17	315	CLA	C3B-C4B	3.19	1.50	1.42
31	b	616	CLA	CMC-C2C	-3.18	1.44	1.50
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	312	CLA	CMD-C2D	-3.18	1.44	1.50
31	14	314	CLA	C4B-NB	3.18	1.41	1.37
45	1	311	KC2	CHC-C1C	3.18	1.46	1.39
43	15	301	A86	O1-C20	-3.18	1.41	1.46
31	3	315	CLA	C3B-C4B	3.18	1.50	1.42
31	2	307	CLA	C3B-C4B	3.17	1.50	1.42
31	B	613	CLA	C1D-ND	3.17	1.41	1.37
31	6	313	CLA	C4D-ND	-3.17	1.33	1.37
42	18	313	KC1	C4D-ND	3.17	1.42	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
31	9	312	CLA	C4B-NB	3.17	1.41	1.37
42	4	313	KC1	CHB-C4A	3.17	1.46	1.39
43	16	301	A86	O1-C20	-3.17	1.41	1.46
31	C	512	CLA	CMD-C2D	-3.17	1.44	1.50
45	6	310	KC2	C1D-ND	-3.17	1.33	1.37
32	A	405	PHO	C4D-ND	-3.17	1.34	1.38
31	14	311	CLA	C1D-ND	3.17	1.41	1.37
31	6	311	CLA	C4D-ND	-3.17	1.33	1.37
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	3	315	CLA	C4B-NB	3.16	1.41	1.37
31	0	316	CLA	C3B-C4B	3.16	1.50	1.42
31	15	312	CLA	C4D-ND	-3.16	1.33	1.37
31	8	310	CLA	C1D-ND	3.16	1.41	1.37
31	15	313	CLA	C4B-NB	3.16	1.41	1.37
31	11	315	CLA	C4B-NB	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	5	313	KC1	CHC-C1C	3.16	1.46	1.39
31	1	315	CLA	C3B-C4B	3.16	1.50	1.42
31	16	315	CLA	C4B-NB	3.16	1.41	1.37
42	8	314	KC1	C1D-ND	-3.16	1.33	1.37
44	p	612	DD6	C13-C11	3.16	1.52	1.45
37	10	319	LMG	C4-C3	3.16	1.60	1.52
31	7	307	CLA	C3B-C4B	3.15	1.50	1.42
43	7	305	A86	C30-C29	-3.15	1.26	1.32
45	9	309	KC2	OBD-CAD	3.15	1.27	1.22
43	1	320	A86	O1-C20	-3.15	1.41	1.46
31	8	312	CLA	C4B-NB	3.15	1.41	1.37
45	16	309	KC2	C1D-ND	-3.15	1.33	1.37
31	3	307	CLA	C4D-ND	-3.15	1.33	1.37
31	7	310	CLA	C4D-ND	-3.15	1.33	1.37
31	0	309	CLA	C3B-C4B	3.15	1.50	1.42
31	11	307	CLA	C3B-C4B	3.14	1.50	1.42
31	B	610	CLA	C1D-ND	3.14	1.41	1.37
31	8	312	CLA	C1D-ND	3.14	1.41	1.37
42	6	315	KC1	CHC-C1C	3.14	1.46	1.39
31	10	309	CLA	C3B-C4B	3.14	1.50	1.42
31	17	307	CLA	C3B-C4B	3.14	1.50	1.42
31	10	308	CLA	C4B-NB	3.14	1.41	1.37
31	19	312	CLA	C4B-NB	3.14	1.41	1.37
31	11	313	CLA	C3B-C4B	3.14	1.50	1.42
31	R	101	CLA	C1D-ND	3.14	1.41	1.37
31	9	311	CLA	C3B-C4B	3.14	1.50	1.42
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	0	307	CLA	C4B-NB	3.14	1.41	1.37
31	2	314	CLA	C3B-C4B	3.14	1.50	1.42
31	10	317	CLA	C4B-NB	3.14	1.41	1.37
31	15	312	CLA	MG-NB	-3.13	1.99	2.05
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	4	312	CLA	C4B-NB	3.13	1.41	1.37
45	17	311	KC2	CHC-C1C	3.13	1.46	1.39
31	17	307	CLA	C4B-NB	3.13	1.41	1.37
43	17	302	A86	C32-C31	-3.13	1.49	1.54
43	17	304	A86	C30-C29	-3.13	1.26	1.32
41	e	101	HEM	CAC-C3C	3.13	1.56	1.47
31	z	103	CLA	C4B-NB	3.13	1.41	1.37
45	3	309	KC2	C1D-ND	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	309	CLA	C4D-ND	-3.13	1.33	1.37
31	14	315	CLA	C3B-C4B	3.13	1.50	1.42
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	309	KC2	CHC-C1C	3.13	1.46	1.39
45	18	310	KC2	CHC-C1C	3.13	1.46	1.39
31	18	306	CLA	C3B-C4B	3.12	1.50	1.42
31	1	316	CLA	C4B-NB	3.12	1.41	1.37
34	8	301	SQD	O48-C23	3.12	1.42	1.33
31	1	312	CLA	C3B-C4B	3.12	1.50	1.42
31	4	315	CLA	C4D-ND	-3.12	1.33	1.37
43	4	302	A86	C13-C11	-3.12	1.43	1.49
31	14	312	CLA	CMB-C2B	-3.12	1.44	1.50
32	a	405	PHO	C4D-ND	-3.12	1.34	1.38
31	8	313	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
45	11	311	KC2	CHC-C1C	3.11	1.46	1.39
31	10	307	CLA	C1D-ND	3.11	1.41	1.37
41	E	101	HEM	CAC-C3C	3.11	1.55	1.47
31	1	313	CLA	CMD-C2D	-3.11	1.44	1.50
45	18	308	KC2	CHC-C1C	3.11	1.46	1.39
38	C	518	DGD	O1G-C1G	-3.11	1.38	1.45
31	16	312	CLA	C4D-ND	-3.11	1.33	1.37
43	14	305	A86	O1-C20	-3.11	1.41	1.46
31	1	321	CLA	C1D-ND	3.11	1.41	1.37
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	311	KC2	CHC-C1C	3.10	1.46	1.39
43	7	301	A86	O1-C20	-3.10	1.41	1.46
31	12	307	CLA	C4B-NB	3.10	1.41	1.37
43	1	306	A86	C32-C31	-3.10	1.49	1.54
31	5	307	CLA	C1D-ND	3.10	1.41	1.37
31	16	313	CLA	C1B-NB	-3.10	1.34	1.37
43	5	305	A86	O1-C20	-3.10	1.41	1.46
43	8	305	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	19	308	CLA	C4D-ND	-3.10	1.33	1.37
45	9	309	KC2	CHC-C1C	3.10	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	16	311	KC2	CHC-C1C	3.10	1.46	1.39
43	17	316	A86	C17-C18	-3.10	1.47	1.52
31	12	313	CLA	CHC-C1C	3.10	1.44	1.38
31	10	314	CLA	C4B-NB	3.09	1.41	1.37
34	i	101	SQD	O48-C23	3.09	1.42	1.33
45	8	309	KC2	CHB-C4A	3.09	1.46	1.39
31	7	307	CLA	C4B-NB	3.09	1.41	1.37
31	B	616	CLA	C1D-ND	3.09	1.41	1.37
31	14	312	CLA	MG-ND	-3.09	1.99	2.05
38	c	518	DGD	O1G-C1G	-3.09	1.38	1.45
42	0	315	KC1	OBD-CAD	3.08	1.27	1.22
43	9	305	A86	C30-C29	-3.08	1.26	1.32
45	19	309	KC2	OBD-CAD	3.08	1.27	1.22
43	13	303	A86	C30-C29	-3.08	1.26	1.32
31	14	315	CLA	C4D-ND	-3.08	1.33	1.37
42	4	313	KC1	CHC-C1C	3.08	1.46	1.39
43	3	302	A86	O1-C20	-3.08	1.41	1.46
31	14	311	CLA	C4B-NB	3.08	1.41	1.37
31	17	313	CLA	C4D-ND	-3.08	1.33	1.37
31	1	313	CLA	C3B-C4B	3.08	1.50	1.42
41	e	101	HEM	CAB-C3B	3.08	1.55	1.47
31	7	315	CLA	C4B-NB	3.08	1.41	1.37
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	16	307	CLA	C3B-C4B	3.08	1.50	1.42
31	11	315	CLA	C4D-ND	-3.08	1.33	1.37
31	10	316	CLA	C3B-C4B	3.08	1.50	1.42
31	5	312	CLA	C4B-NB	3.08	1.41	1.37
35	D	407	PL9	C7-C8	-3.08	1.46	1.50
42	14	313	KC1	CHC-C1C	3.08	1.46	1.39
31	12	310	CLA	C4D-ND	-3.07	1.33	1.37
37	0	317	LMG	C4-C3	3.07	1.60	1.52
31	8	312	CLA	CMD-C2D	-3.07	1.44	1.50
43	1	304	A86	O1-C20	-3.07	1.41	1.46
31	2	314	CLA	C4B-NB	3.07	1.41	1.37
31	16	313	CLA	C4B-NB	3.07	1.41	1.37
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	3	310	CLA	C4D-ND	-3.07	1.33	1.37
31	r	101	CLA	C4D-ND	-3.07	1.33	1.37
45	15	308	KC2	C3C-C4C	3.07	1.51	1.44
31	15	311	CLA	MG-ND	-3.06	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
31	19	312	CLA	C3B-C4B	3.06	1.49	1.42
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	11	312	CLA	C1D-ND	3.06	1.41	1.37
42	P	609	KC1	OBD-CAD	3.06	1.27	1.22
45	14	310	KC2	C1A-CHA	3.06	1.48	1.40
31	12	315	CLA	C3B-C4B	3.06	1.49	1.42
31	C	503	CLA	C1D-ND	3.06	1.41	1.37
31	15	307	CLA	C1D-ND	3.06	1.41	1.37
31	9	311	CLA	C4D-ND	-3.05	1.33	1.37
43	11	305	A86	C13-C11	-3.05	1.43	1.49
31	0	308	CLA	C4B-NB	3.05	1.41	1.37
43	4	303	A86	O1-C20	-3.05	1.41	1.46
31	p	605	CLA	C4B-NB	3.05	1.41	1.37
31	12	313	CLA	CMD-C2D	-3.05	1.44	1.50
31	1	312	CLA	C4B-NB	3.05	1.41	1.37
31	0	312	CLA	C4B-NB	3.05	1.41	1.37
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	10	312	CLA	C4B-NB	3.05	1.41	1.37
31	b	617	CLA	C1D-ND	3.05	1.41	1.37
31	15	306	CLA	C4B-NB	3.05	1.41	1.37
43	6	307	A86	C40-C32	-3.05	1.47	1.53
31	c	512	CLA	MG-ND	-3.05	1.99	2.05
42	p	609	KC1	OBD-CAD	3.05	1.27	1.22
31	9	312	CLA	C3B-C4B	3.05	1.49	1.42
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	314	KC1	CHB-C4A	3.04	1.46	1.39
31	R	101	CLA	C4D-ND	-3.04	1.33	1.37
45	7	309	KC2	C1D-ND	-3.04	1.34	1.37
37	J	101	LMG	O7-C8	-3.04	1.39	1.46
31	D	405	CLA	MG-NB	-3.04	1.99	2.05
31	11	316	CLA	C4D-ND	-3.04	1.33	1.37
31	10	307	CLA	CMB-C2B	-3.04	1.44	1.50
43	7	303	A86	C30-C29	-3.03	1.26	1.32
31	10	307	CLA	MG-NB	-3.03	1.99	2.05
31	c	503	CLA	C1C-NC	-3.03	1.33	1.37
32	A	405	PHO	CMD-C2D	-3.03	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	V	201	HEM	CAB-C3B	3.03	1.55	1.47
31	11	308	CLA	C4B-NB	3.03	1.41	1.37
43	11	302	A86	O1-C15	-3.03	1.40	1.45
31	P	605	CLA	C4B-NB	3.03	1.41	1.37
43	p	611	A86	C13-C11	-3.03	1.43	1.49
31	12	312	CLA	C4B-NB	3.03	1.41	1.37
37	m	101	LMG	O8-C9	-3.03	1.38	1.45
37	j	101	LMG	O7-C8	-3.03	1.39	1.46
31	3	307	CLA	C4B-NB	3.03	1.41	1.37
43	14	305	A86	C13-C11	-3.02	1.43	1.49
37	D	404	LMG	C4-C3	3.02	1.60	1.52
31	3	310	CLA	C4B-NB	3.02	1.41	1.37
34	L	102	SQD	O47-C7	3.02	1.42	1.34
41	v	201	HEM	CAB-C3B	3.02	1.55	1.47
31	4	314	CLA	C4B-NB	3.02	1.41	1.37
34	10	320	SQD	O48-C23	3.02	1.42	1.33
33	a	407	BCR	C1-C6	-3.02	1.49	1.53
35	d	407	PL9	C7-C8	-3.02	1.46	1.50
33	c	516	BCR	C1-C6	-3.02	1.49	1.53
31	b	608	CLA	C4B-NB	3.02	1.41	1.37
31	2	311	CLA	C4D-ND	-3.02	1.33	1.37
31	14	306	CLA	MG-ND	-3.02	1.99	2.05
31	2	312	CLA	CHC-C1C	3.02	1.44	1.38
42	2	313	KC1	C1A-CHA	3.02	1.48	1.40
45	1	309	KC2	C3C-C4C	3.02	1.50	1.44
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	b	604	CLA	CMD-C2D	-3.02	1.44	1.50
31	b	616	CLA	C1D-ND	3.02	1.41	1.37
31	13	316	CLA	C4B-NB	3.02	1.41	1.37
31	4	314	CLA	C3B-C4B	3.02	1.49	1.42
31	3	316	CLA	C4B-NB	3.02	1.41	1.37
31	3	313	CLA	CMD-C2D	-3.02	1.44	1.50
31	d	405	CLA	MG-NB	-3.01	1.99	2.05
31	b	602	CLA	C1D-ND	3.01	1.41	1.37
31	10	314	CLA	C4D-ND	-3.01	1.33	1.37
43	P	611	A86	C13-C11	-3.01	1.43	1.49
31	10	309	CLA	C1D-ND	3.01	1.41	1.37
31	19	310	CLA	C3B-C4B	3.01	1.49	1.42
31	B	603	CLA	CMD-C2D	-3.01	1.44	1.50
31	5	306	CLA	C3B-C4B	3.01	1.49	1.42
31	6	309	CLA	C3B-C4B	3.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B	601	CLA	C1D-ND	3.01	1.41	1.37
35	D	407	PL9	C16-C14	-3.00	1.45	1.51
35	d	407	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	3	307	CLA	C3B-C4B	3.00	1.49	1.42
31	D	405	CLA	C4B-NB	3.00	1.41	1.37
31	d	405	CLA	C4B-NB	3.00	1.41	1.37
31	D	405	CLA	CMD-C2D	-3.00	1.44	1.50
32	a	405	PHO	CMD-C2D	-3.00	1.45	1.51
42	10	315	KC1	C1D-ND	-3.00	1.34	1.37
43	16	304	A86	C30-C29	-3.00	1.27	1.32
31	B	607	CLA	C4B-NB	3.00	1.41	1.37
33	B	619	BCR	C30-C25	-3.00	1.49	1.53
43	11	302	A86	C30-C29	-3.00	1.27	1.32
31	16	308	CLA	C3B-C4B	3.00	1.49	1.42
43	10	302	A86	C30-C29	-3.00	1.27	1.32
38	c	520	DGD	O1G-C1G	-3.00	1.38	1.45
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
31	11	307	CLA	C4B-NB	2.99	1.41	1.37
45	2	310	KC2	CHC-C1C	2.99	1.46	1.39
31	d	405	CLA	CMD-C2D	-2.99	1.44	1.50
31	2	309	CLA	C4D-ND	-2.99	1.33	1.37
31	2	312	CLA	MG-ND	-2.99	1.99	2.05
31	1	308	CLA	C4B-NB	2.99	1.41	1.37
31	4	311	CLA	C4B-NB	2.99	1.41	1.37
31	16	308	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
45	13	311	KC2	C1D-ND	-2.99	1.34	1.37
31	c	502	CLA	CMD-C2D	-2.99	1.44	1.50
32	D	403	PHO	C4D-ND	-2.99	1.34	1.38
31	B	612	CLA	CMD-C2D	-2.99	1.44	1.50
31	14	311	CLA	CMD-C2D	-2.98	1.44	1.50
35	d	407	PL9	C53-C6	-2.98	1.44	1.50
31	5	314	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B	603	CLA	MG-NB	-2.98	1.99	2.05
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
32	D	403	PHO	CMC-C2C	-2.98	1.45	1.50
31	p	603	CLA	MG-NB	-2.98	1.99	2.05
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	15	306	CLA	C3B-C4B	2.98	1.49	1.42
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
31	b	607	CLA	CMD-C2D	-2.98	1.44	1.50
43	5	304	A86	C30-C29	-2.97	1.27	1.32
31	A	403	CLA	MG-NB	-2.97	1.99	2.05
45	17	309	KC2	C1D-ND	-2.97	1.34	1.37
37	d	404	LMG	C4-C3	2.97	1.59	1.52
34	l	101	SQD	O47-C7	2.97	1.42	1.34
38	C	520	DGD	O1G-C1G	-2.97	1.38	1.45
43	12	301	A86	O1-C15	-2.97	1.40	1.45
43	19	302	A86	C30-C29	-2.97	1.27	1.32
31	18	311	CLA	CMD-C2D	-2.97	1.44	1.50
31	2	309	CLA	C4B-NB	2.97	1.41	1.37
31	P	603	CLA	MG-NB	-2.97	1.99	2.05
31	17	315	CLA	C4D-ND	-2.97	1.33	1.37
31	15	311	CLA	MG-NB	-2.97	1.99	2.05
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
31	b	604	CLA	MG-NB	-2.96	1.99	2.05
43	15	302	A86	C40-C32	-2.96	1.47	1.53
31	b	603	CLA	CMC-C2C	-2.96	1.44	1.50
43	15	305	A86	C30-C29	-2.96	1.27	1.32
31	5	312	CLA	CMB-C2B	-2.96	1.44	1.50
35	D	407	PL9	C53-C6	-2.96	1.44	1.50
31	D	406	CLA	C1D-ND	2.95	1.41	1.37
43	2	304	A86	C40-C32	-2.95	1.47	1.53
31	5	311	CLA	C4B-NB	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	315	CLA	C3C-C2C	2.95	1.43	1.36
31	1	313	CLA	MG-ND	-2.95	1.99	2.05
31	a	403	CLA	MG-NB	-2.95	1.99	2.05
31	0	307	CLA	C3B-C4B	2.95	1.49	1.42
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	b	611	CLA	C3B-C4B	2.95	1.49	1.42
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
32	A	405	PHO	C4D-CHA	2.94	1.44	1.39
34	B	623	SQD	O48-C23	2.94	1.41	1.33
31	C	502	CLA	CMD-C2D	-2.94	1.44	1.50
31	B	610	CLA	C3B-C4B	2.94	1.49	1.42
31	p	602	CLA	MG-NB	-2.94	2.00	2.05
31	3	315	CLA	C4D-ND	-2.94	1.33	1.37
31	9	310	CLA	C3B-C4B	2.94	1.49	1.42
31	B	603	CLA	C1B-NB	-2.94	1.34	1.37
31	b	605	CLA	MG-NB	-2.94	2.00	2.05
42	10	315	KC1	CHD-C1D	2.94	1.46	1.39
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	9	307	CLA	C4B-NB	2.94	1.41	1.37
31	b	604	CLA	C1B-NB	-2.94	1.34	1.37
31	19	315	CLA	C3B-C4B	2.94	1.49	1.42
31	C	505	CLA	C1D-ND	2.94	1.41	1.37
31	10	307	CLA	C4B-NB	2.93	1.41	1.37
31	17	310	CLA	C4B-NB	2.93	1.41	1.37
45	2	308	KC2	C1D-ND	-2.93	1.34	1.37
31	13	307	CLA	C4D-ND	-2.93	1.33	1.37
31	14	314	CLA	C3B-C4B	2.93	1.49	1.42
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	P	610	CLA	C1D-ND	2.93	1.41	1.37
45	5	308	KC2	C1B-NB	-2.93	1.34	1.37
32	d	403	PHO	C4D-ND	-2.93	1.34	1.38
43	15	301	A86	C13-C11	-2.93	1.44	1.49
31	B	612	CLA	MG-NB	-2.93	2.00	2.05
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	18	311	CLA	MG-NB	-2.93	2.00	2.05
31	P	601	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	314	KC1	OBD-CAD	2.93	1.27	1.22
31	9	308	CLA	C3B-C4B	2.93	1.49	1.42
31	d	406	CLA	C1D-ND	2.93	1.41	1.37
33	c	516	BCR	C30-C25	-2.93	1.49	1.53
31	B	601	CLA	C4B-NB	2.93	1.41	1.37
31	B	607	CLA	CMB-C2B	-2.93	1.44	1.50
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
45	11	311	KC2	C1D-ND	-2.93	1.34	1.37
31	12	310	CLA	C4B-NB	2.92	1.41	1.37
42	8	314	KC1	CHC-C1C	2.92	1.45	1.39
31	19	313	CLA	C1D-ND	2.92	1.41	1.37
31	4	315	CLA	C3B-C4B	2.92	1.49	1.42
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
45	5	308	KC2	C1D-ND	-2.92	1.34	1.37
32	d	403	PHO	CMC-C2C	-2.92	1.45	1.50
43	9	306	A86	C40-C32	-2.92	1.48	1.53
31	B	615	CLA	C1D-ND	2.92	1.41	1.37
31	17	315	CLA	C4B-NB	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	6	316	CLA	C4D-ND	-2.92	1.33	1.37
33	C	516	BCR	C30-C25	-2.92	1.49	1.53
32	a	405	PHO	C4D-CHA	2.92	1.44	1.39
45	8	309	KC2	C1B-NB	-2.92	1.34	1.37
45	18	310	KC2	C1B-NB	-2.92	1.34	1.37
31	0	314	CLA	C4B-NB	2.92	1.41	1.37
31	19	308	CLA	C3B-C4B	2.92	1.49	1.42
43	16	302	A86	O1-C20	-2.92	1.42	1.46
45	4	308	KC2	C1D-ND	-2.92	1.34	1.37
43	8	302	A86	C33-C34	2.92	1.57	1.51
45	15	308	KC2	C1D-ND	-2.92	1.34	1.37
31	r	101	CLA	C4B-NB	2.92	1.41	1.37
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	17	313	CLA	CHC-C1C	2.92	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	603	CLA	CMD-C2D	-2.91	1.44	1.50
43	8	304	A86	C13-C11	-2.91	1.44	1.49
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	P	609	KC1	C1D-ND	-2.91	1.34	1.37
31	17	313	CLA	MG-NB	-2.91	2.00	2.05
42	6	315	KC1	C1B-NB	-2.91	1.34	1.37
31	7	313	CLA	MG-ND	-2.91	2.00	2.05
31	7	310	CLA	C4B-NB	2.91	1.41	1.37
31	2	306	CLA	C3B-C4B	2.91	1.49	1.42
31	10	308	CLA	C3B-C4B	2.91	1.49	1.42
31	10	313	CLA	C4D-ND	-2.91	1.33	1.37
31	19	315	CLA	C4D-ND	-2.91	1.33	1.37
42	9	314	KC1	C4D-ND	2.91	1.41	1.37
31	19	307	CLA	C3B-C4B	2.90	1.49	1.42
31	2	314	CLA	C4D-ND	-2.90	1.33	1.37
31	14	307	CLA	C3B-C4B	2.90	1.49	1.42
31	b	613	CLA	MG-NB	-2.90	2.00	2.05
31	B	604	CLA	MG-NB	-2.90	2.00	2.05
31	P	602	CLA	MG-NB	-2.90	2.00	2.05
31	7	308	CLA	C3B-C4B	2.90	1.49	1.42
43	p	613	A86	C30-C29	-2.90	1.27	1.32
31	0	313	CLA	CMB-C2B	-2.90	1.44	1.50
43	14	305	A86	C30-C29	-2.90	1.27	1.32
31	0	307	CLA	MG-NB	-2.90	2.00	2.05
34	a	408	SQD	O48-C23	2.90	1.41	1.33
31	13	313	CLA	CHC-C1C	2.90	1.44	1.38
43	9	306	A86	C30-C29	-2.90	1.27	1.32
43	16	302	A86	C13-C11	-2.90	1.44	1.49
31	3	313	CLA	CMB-C2B	-2.90	1.44	1.50
43	10	304	A86	O1-C15	-2.90	1.40	1.45
31	9	315	CLA	C3B-C4B	2.90	1.49	1.42
31	0	313	CLA	C4D-ND	-2.89	1.33	1.37
35	d	407	PL9	C52-C5	-2.89	1.44	1.50
35	a	409	PL9	C6-C1	-2.89	1.43	1.48
31	C	502	CLA	C1D-ND	2.89	1.41	1.37
42	p	609	KC1	C1D-ND	-2.89	1.34	1.37
31	C	506	CLA	C1D-ND	2.89	1.41	1.37
31	b	609	CLA	C1B-NB	-2.89	1.34	1.37
31	b	608	CLA	CMB-C2B	-2.89	1.44	1.50
31	C	509	CLA	C1B-NB	-2.89	1.34	1.37
43	0	304	A86	O1-C15	-2.89	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	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
31	b	617	CLA	C3B-C4B	2.89	1.49	1.42
31	1	313	CLA	MG-NB	-2.89	2.00	2.05
35	D	407	PL9	C52-C5	-2.89	1.44	1.50
31	18	312	CLA	C3B-C4B	2.89	1.49	1.42
31	b	609	CLA	MG-NB	-2.88	2.00	2.05
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	3	310	CLA	C3B-C4B	2.88	1.49	1.42
31	13	316	CLA	C4D-ND	-2.88	1.33	1.37
43	P	613	A86	C30-C29	-2.88	1.27	1.32
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	6	308	CLA	C1B-C2B	2.88	1.50	1.43
31	7	307	CLA	C4D-ND	-2.88	1.33	1.37
38	B	621	DGD	O1G-C1G	-2.88	1.38	1.45
34	l	101	SQD	O48-C23	2.88	1.41	1.33
31	17	308	CLA	C3B-C4B	2.88	1.49	1.42
31	b	606	CLA	C1D-ND	2.88	1.41	1.37
43	11	305	A86	C40-C32	-2.87	1.48	1.53
38	C	518	DGD	O5D-C6D	-2.87	1.38	1.43
38	c	518	DGD	O5D-C6D	-2.87	1.38	1.43
31	B	608	CLA	MG-NB	-2.87	2.00	2.05
43	9	301	A86	O1-C15	-2.87	1.40	1.45
31	B	605	CLA	C1D-ND	2.87	1.41	1.37
31	10	307	CLA	C1B-NB	-2.87	1.34	1.37
43	9	303	A86	C30-C29	-2.87	1.27	1.32
45	1	309	KC2	C1D-ND	-2.87	1.34	1.37
31	P	607	CLA	C3B-C4B	2.87	1.49	1.42
33	h	101	BCR	C1-C6	-2.87	1.49	1.53
43	14	301	A86	C13-C11	-2.87	1.44	1.49
43	19	301	A86	O1-C15	-2.87	1.40	1.45
31	b	604	CLA	C1D-ND	2.87	1.41	1.37
43	3	306	A86	C30-C29	-2.87	1.27	1.32
31	6	314	CLA	C1B-NB	-2.86	1.34	1.37
31	12	308	CLA	C1D-ND	2.86	1.41	1.37
43	17	302	A86	C13-C11	-2.86	1.44	1.49
37	1	301	LMG	C4-C3	2.86	1.59	1.52
31	R	101	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	8	311	KC2	C1B-NB	-2.86	1.34	1.37
45	17	311	KC2	C1A-CHA	2.86	1.48	1.40
33	y	101	BCR	C33-C5	-2.86	1.46	1.50
45	1	311	KC2	C1B-NB	-2.86	1.34	1.37
37	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	616	CLA	C3B-C4B	2.86	1.49	1.42
31	2	307	CLA	CMD-C2D	-2.86	1.44	1.50
31	13	316	CLA	C3B-C4B	2.85	1.49	1.42
36	L	101	LHG	O7-C5	-2.85	1.39	1.46
31	4	307	CLA	C3B-C4B	2.85	1.49	1.42
31	12	316	CLA	C4D-ND	-2.85	1.33	1.37
33	F	101	BCR	C1-C6	-2.85	1.49	1.53
31	1	315	CLA	C1B-C2B	2.85	1.50	1.43
34	L	102	SQD	O48-C23	2.85	1.41	1.33
31	16	313	CLA	C3B-C4B	2.85	1.49	1.42
31	p	601	CLA	C1D-ND	2.85	1.41	1.37
45	15	310	KC2	C1B-NB	-2.85	1.34	1.37
32	A	405	PHO	CMC-C2C	-2.85	1.46	1.50
32	a	405	PHO	CMC-C2C	-2.85	1.46	1.50
31	p	607	CLA	C3B-C4B	2.85	1.49	1.42
31	10	317	CLA	C3B-C4B	2.84	1.49	1.42
31	2	312	CLA	C1B-NB	-2.84	1.34	1.37
31	c	509	CLA	CMB-C2B	-2.84	1.44	1.50
31	17	312	CLA	CMD-C2D	-2.84	1.44	1.50
45	18	308	KC2	C1B-NB	-2.84	1.34	1.37
31	A	403	CLA	C1D-ND	2.84	1.41	1.37
31	19	311	CLA	C4D-ND	-2.84	1.33	1.37
31	17	313	CLA	CMB-C2B	-2.84	1.44	1.50
36	l	102	LHG	O7-C5	-2.84	1.39	1.46
31	c	509	CLA	C1B-NB	-2.84	1.34	1.37
43	13	306	A86	O1-C15	-2.84	1.40	1.45
43	8	304	A86	C26-C27	-2.84	1.32	1.35
35	D	407	PL9	C46-C44	-2.84	1.45	1.51
35	d	407	PL9	C46-C44	-2.84	1.45	1.51
31	10	307	CLA	C3B-C4B	2.84	1.49	1.42
31	10	311	CLA	C1D-ND	2.84	1.41	1.37
42	10	315	KC1	C1A-CHA	2.84	1.48	1.40
31	p	604	CLA	C3B-C4B	2.84	1.49	1.42
31	1	307	CLA	C4B-NB	2.83	1.41	1.37
31	7	312	CLA	CMD-C2D	-2.83	1.44	1.50
31	12	312	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	11	307	CLA	C1B-NB	-2.83	1.34	1.37
31	0	307	CLA	CMB-C2B	-2.83	1.44	1.50
43	13	305	A86	C30-C29	-2.83	1.27	1.32
31	13	313	CLA	MG-NB	-2.83	2.00	2.05
31	7	308	CLA	C4B-NB	2.83	1.41	1.37
42	15	317	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
33	H	101	BCR	C1-C6	-2.83	1.49	1.53
43	17	305	A86	C30-C29	-2.83	1.27	1.32
31	C	509	CLA	CMB-C2B	-2.83	1.44	1.50
31	c	513	CLA	MG-NB	-2.82	2.00	2.05
42	16	314	KC1	C1B-NB	-2.82	1.34	1.37
31	z	101	CLA	C3B-C4B	2.82	1.49	1.42
31	C	513	CLA	MG-NB	-2.82	2.00	2.05
31	4	309	CLA	C3B-C4B	2.82	1.49	1.42
38	C	518	DGD	O4D-C4D	-2.82	1.36	1.43
31	D	406	CLA	C3B-C4B	2.82	1.49	1.42
33	B	617	BCR	C30-C25	-2.82	1.49	1.53
31	C	503	CLA	C1B-NB	-2.82	1.34	1.37
31	c	503	CLA	C1B-NB	-2.82	1.34	1.37
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	308	CLA	CMC-C2C	-2.82	1.44	1.50
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	8	315	CLA	C4B-NB	2.82	1.41	1.37
31	13	310	CLA	C4B-NB	2.82	1.41	1.37
31	8	312	CLA	C4D-ND	-2.82	1.33	1.37
31	C	513	CLA	C1B-NB	-2.82	1.34	1.37
31	c	513	CLA	C1B-NB	-2.82	1.34	1.37
31	b	602	CLA	C4B-NB	2.82	1.41	1.37
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	z	103	CLA	CMB-C2B	-2.81	1.44	1.50
33	b	618	BCR	C30-C25	-2.81	1.49	1.53
42	13	314	KC1	C1D-ND	-2.81	1.34	1.37
31	17	308	CLA	CMD-C2D	-2.81	1.44	1.50
37	N	101	LMG	O2-C2	-2.81	1.36	1.43
34	A	411	SQD	O47-C7	2.81	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C	514	CLA	C3B-C4B	2.81	1.49	1.42
31	C	507	CLA	MG-NB	-2.81	2.00	2.05
31	8	308	CLA	CMD-C2D	-2.81	1.44	1.50
31	p	606	CLA	C4D-ND	-2.80	1.33	1.37
31	z	103	CLA	C3B-C4B	2.80	1.49	1.42
35	D	407	PL9	C11-C9	-2.80	1.45	1.51
35	d	407	PL9	C11-C9	-2.80	1.45	1.51
31	a	403	CLA	C1D-ND	2.80	1.41	1.37
31	18	309	CLA	C3B-C4B	2.80	1.49	1.42
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	8	307	CLA	C1B-NB	-2.80	1.34	1.37
31	8	310	CLA	C3B-C4B	2.80	1.49	1.42
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
31	14	309	CLA	C3B-C4B	2.80	1.49	1.42
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	b	611	CLA	C4B-NB	2.79	1.41	1.37
31	8	307	CLA	MG-NB	-2.79	2.00	2.05
42	10	315	KC1	OBD-CAD	2.79	1.27	1.22
31	11	307	CLA	C4D-ND	-2.79	1.33	1.37
31	16	315	CLA	C4D-ND	-2.79	1.33	1.37
31	d	406	CLA	C3B-C4B	2.79	1.49	1.42
31	B	610	CLA	C4B-NB	2.79	1.41	1.37
31	Z	101	CLA	C4B-NB	2.79	1.41	1.37
31	9	307	CLA	C3B-C4B	2.79	1.49	1.42
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	608	CLA	C1B-NB	-2.79	1.34	1.37
43	1	319	A86	C30-C29	-2.79	1.27	1.32
31	18	307	CLA	MG-NB	-2.79	2.00	2.05
45	16	311	KC2	C4D-ND	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	19	310	CLA	C4D-ND	-2.79	1.33	1.37
31	C	509	CLA	C3B-C4B	2.78	1.49	1.42
31	c	509	CLA	C3B-C4B	2.78	1.49	1.42
31	d	402	CLA	C1D-ND	2.78	1.41	1.37
45	1	309	KC2	C1B-NB	-2.78	1.34	1.37
31	13	307	CLA	C3B-C4B	2.78	1.49	1.42
42	1	314	KC1	C4D-ND	2.78	1.41	1.37
31	P	606	CLA	C4D-ND	-2.78	1.33	1.37
31	8	307	CLA	CMB-C2B	-2.78	1.44	1.50
31	19	308	CLA	C4B-NB	2.78	1.41	1.37
31	P	604	CLA	C3B-C4B	2.78	1.49	1.42
31	p	608	CLA	C4B-NB	2.78	1.41	1.37
31	c	514	CLA	C3B-C4B	2.78	1.49	1.42
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	b	612	CLA	C1B-NB	-2.78	1.34	1.37
42	19	314	KC1	C4D-ND	2.78	1.41	1.37
31	8	313	CLA	C4B-NB	2.78	1.41	1.37
31	2	311	CLA	CMD-C2D	-2.77	1.44	1.50
31	10	314	CLA	C3B-C4B	2.77	1.49	1.42
41	v	201	HEM	CAC-C3C	2.77	1.55	1.47
31	17	308	CLA	C4B-NB	2.77	1.41	1.37
42	0	315	KC1	C1D-ND	-2.77	1.34	1.37
31	B	616	CLA	C4B-NB	2.77	1.41	1.37
31	B	608	CLA	CMD-C2D	-2.77	1.44	1.50
31	3	312	CLA	CMD-C2D	-2.77	1.44	1.50
31	B	604	CLA	CAC-C3C	-2.77	1.44	1.51
38	c	518	DGD	O2G-C2G	-2.77	1.39	1.46
35	D	407	PL9	C36-C34	-2.77	1.45	1.51
35	d	407	PL9	C36-C34	-2.77	1.45	1.51
31	6	311	CLA	C1B-C2B	2.77	1.49	1.43
38	C	518	DGD	O2G-C2G	-2.77	1.39	1.46
31	c	503	CLA	CMB-C2B	-2.77	1.44	1.50
31	7	313	CLA	CMB-C2B	-2.77	1.44	1.50
31	16	313	CLA	C1D-ND	2.77	1.41	1.37
43	10	305	A86	C30-C29	-2.77	1.27	1.32
31	0	311	CLA	C3B-C4B	2.77	1.49	1.42
43	11	302	A86	C32-C31	2.77	1.59	1.54
38	c	518	DGD	O4D-C4D	-2.77	1.36	1.43
32	A	405	PHO	C1D-C2D	2.76	1.42	1.39
31	1	316	CLA	CMB-C2B	-2.76	1.44	1.50
31	10	311	CLA	MG-NB	-2.76	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	E	101	HEM	FE-NC	2.76	2.04	1.95
38	w	204	DGD	O2G-C2G	-2.76	1.39	1.46
32	a	405	PHO	C1D-C2D	2.76	1.42	1.39
31	7	310	CLA	C3B-C4B	2.76	1.49	1.42
41	V	201	HEM	CAC-C3C	2.76	1.55	1.47
31	8	307	CLA	C4B-NB	2.76	1.41	1.37
31	b	605	CLA	CAC-C3C	-2.76	1.44	1.51
31	P	605	CLA	C1B-C2B	2.76	1.49	1.43
43	p	611	A86	C35-C34	2.76	1.56	1.51
37	k	101	LMG	O6-C5	-2.76	1.37	1.44
31	9	307	CLA	C1B-C2B	2.76	1.49	1.43
31	c	507	CLA	MG-NB	-2.76	2.00	2.05
41	e	101	HEM	FE-NC	2.76	2.04	1.95
45	11	311	KC2	C4D-ND	2.76	1.41	1.37
31	9	308	CLA	C4B-NB	2.76	1.41	1.37
31	13	308	CLA	C4B-NB	2.76	1.41	1.37
45	12	311	KC2	C1B-NB	-2.76	1.34	1.37
31	6	309	CLA	C1D-ND	2.76	1.41	1.37
37	F	102	LMG	O7-C8	-2.76	1.39	1.46
37	K	101	LMG	O6-C5	-2.76	1.37	1.44
31	w	203	CLA	C3B-C4B	2.75	1.49	1.42
31	Z	101	CLA	C3B-C4B	2.75	1.49	1.42
37	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	17	310	CLA	C3B-C4B	2.75	1.49	1.42
43	6	302	A86	C13-C11	-2.75	1.44	1.49
31	12	313	CLA	MG-NB	-2.75	2.00	2.05
31	0	309	CLA	C1D-ND	2.75	1.41	1.37
31	5	306	CLA	C4B-NB	2.75	1.41	1.37
31	18	314	CLA	C4B-NB	2.75	1.41	1.37
31	5	307	CLA	C3B-C4B	2.75	1.49	1.42
43	11	320	A86	O1-C20	-2.75	1.42	1.46
31	p	601	CLA	C4B-NB	2.75	1.41	1.37
31	w	203	CLA	C4B-NB	2.75	1.41	1.37
45	14	310	KC2	C1B-NB	-2.75	1.34	1.37
31	8	313	CLA	C3B-C4B	2.75	1.49	1.42
31	B	605	CLA	C1B-C2B	2.75	1.49	1.43
38	W	203	DGD	O2G-C2G	-2.75	1.39	1.46
45	14	308	KC2	C1D-ND	-2.75	1.34	1.37
31	1	321	CLA	C3B-C4B	2.75	1.49	1.42
31	P	608	CLA	C4B-NB	2.74	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	606	CLA	C1B-C2B	2.74	1.49	1.43
31	B	603	CLA	CMB-C2B	-2.74	1.45	1.50
31	B	616	CLA	CMC-C2C	-2.74	1.45	1.50
43	12	306	A86	C13-C11	-2.74	1.44	1.49
31	16	310	CLA	C4B-NB	2.74	1.41	1.37
31	18	307	CLA	CMB-C2B	-2.74	1.45	1.50
31	C	514	CLA	C1D-ND	2.74	1.41	1.37
31	16	310	CLA	C1B-C2B	2.74	1.49	1.43
43	17	302	A86	C37-C36	-2.74	1.48	1.52
45	1	309	KC2	C4D-ND	2.74	1.41	1.37
31	z	101	CLA	C4B-NB	2.74	1.41	1.37
45	6	312	KC2	C4D-ND	2.74	1.41	1.37
31	D	402	CLA	C1D-ND	2.74	1.41	1.37
31	17	312	CLA	C3B-C4B	2.74	1.49	1.42
31	c	504	CLA	C3B-C4B	2.74	1.49	1.42
43	11	320	A86	C30-C29	-2.74	1.27	1.32
31	17	307	CLA	C4D-ND	-2.74	1.33	1.37
31	2	306	CLA	C4B-NB	2.74	1.41	1.37
43	8	305	A86	C33-C34	2.74	1.56	1.51
31	p	605	CLA	C1B-C2B	2.74	1.49	1.43
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
43	16	304	A86	C13-C11	-2.74	1.44	1.49
31	b	604	CLA	CMB-C2B	-2.74	1.45	1.50
43	5	303	A86	C30-C29	-2.73	1.27	1.32
31	C	503	CLA	CMB-C2B	-2.73	1.45	1.50
31	W	202	CLA	C3B-C4B	2.73	1.49	1.42
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	C	509	CLA	MG-NB	-2.73	2.00	2.05
31	c	509	CLA	MG-NB	-2.73	2.00	2.05
31	P	601	CLA	C4B-NB	2.73	1.41	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	A	406	CLA	C1D-ND	2.73	1.41	1.37
43	10	306	A86	C13-C11	-2.73	1.44	1.49
31	b	617	CLA	C4B-NB	2.73	1.41	1.37
37	n	701	LMG	O2-C2	-2.73	1.36	1.43
38	W	203	DGD	C1E-C2E	2.73	1.60	1.52
43	6	304	A86	C13-C11	-2.73	1.44	1.49
42	5	313	KC1	C1D-ND	-2.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
38	C	518	DGD	O2D-C2D	-2.73	1.36	1.43
31	B	611	CLA	C1B-NB	-2.73	1.34	1.37
45	3	311	KC2	C1A-CHA	2.73	1.47	1.40
34	B	623	SQD	O47-C7	2.73	1.42	1.34
38	c	518	DGD	O2D-C2D	-2.73	1.36	1.43
31	C	504	CLA	C3B-C4B	2.73	1.49	1.42
31	9	307	CLA	C4D-ND	-2.72	1.33	1.37
31	C	511	CLA	CMD-C2D	-2.72	1.45	1.50
34	b	601	SQD	O47-C7	2.72	1.42	1.34
37	Z	102	LMG	C4-C5	2.72	1.58	1.53
31	19	312	CLA	C4D-ND	-2.72	1.33	1.37
31	12	308	CLA	C4B-NB	2.72	1.41	1.37
31	17	313	CLA	C1B-NB	-2.72	1.34	1.37
34	8	301	SQD	O47-C7	2.72	1.42	1.34
37	f	102	LMG	O7-C8	-2.72	1.39	1.46
31	z	103	CLA	MG-NB	-2.72	2.00	2.05
31	8	315	CLA	C3B-C4B	2.72	1.49	1.42
31	B	604	CLA	MG-ND	-2.72	2.00	2.05
31	b	605	CLA	MG-ND	-2.72	2.00	2.05
38	C	519	DGD	O4E-C4E	-2.72	1.36	1.43
31	P	602	CLA	C3B-C4B	2.71	1.49	1.42
38	w	204	DGD	C1E-C2E	2.71	1.60	1.52
31	C	513	CLA	C1D-ND	2.71	1.41	1.37
45	3	309	KC2	C3C-C4C	2.71	1.50	1.44
31	19	307	CLA	C1B-C2B	2.71	1.49	1.43
45	3	309	KC2	C1A-CHA	2.71	1.47	1.40
43	3	301	A86	O1-C20	-2.71	1.42	1.46
31	5	311	CLA	CMB-C2B	-2.71	1.45	1.50
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	C	504	CLA	C4B-NB	2.71	1.41	1.37
31	2	315	CLA	CHC-C1C	2.71	1.44	1.38
31	0	308	CLA	C3B-C4B	2.71	1.49	1.42
31	4	311	CLA	C3B-C4B	2.71	1.49	1.42
31	8	307	CLA	C3B-C4B	2.71	1.49	1.42
31	4	312	CLA	CMB-C2B	-2.70	1.45	1.50
31	9	312	CLA	C1B-C2B	2.70	1.49	1.43
43	1	305	A86	O1-C20	-2.70	1.42	1.46
31	p	606	CLA	MG-NA	-2.70	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	10	317	CLA	MG-NB	-2.70	2.00	2.05
31	B	602	CLA	C1B-NB	-2.70	1.34	1.37
31	3	308	CLA	C1D-ND	2.70	1.41	1.37
31	15	311	CLA	CMD-C2D	-2.70	1.45	1.50
31	c	502	CLA	MG-NB	-2.70	2.00	2.05
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	a	406	CLA	MG-NB	-2.70	2.00	2.05
31	b	603	CLA	C1B-NB	-2.70	1.34	1.37
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	609	CLA	CMB-C2B	-2.70	1.45	1.50
31	0	311	CLA	MG-NB	-2.70	2.00	2.05
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	B	609	CLA	C4B-NB	2.69	1.41	1.37
31	12	310	CLA	C3B-C4B	2.69	1.49	1.42
31	17	308	CLA	MG-NB	-2.69	2.00	2.05
45	4	308	KC2	C1B-NB	-2.69	1.34	1.37
31	19	312	CLA	C1B-C2B	2.69	1.49	1.43
31	10	311	CLA	C3B-C4B	2.69	1.49	1.42
31	4	307	CLA	C4B-NB	2.69	1.41	1.37
31	6	309	CLA	C4B-NB	2.69	1.41	1.37
31	14	311	CLA	C3B-C4B	2.69	1.49	1.42
43	14	303	A86	C30-C29	-2.69	1.27	1.32
31	11	307	CLA	MG-NB	-2.69	2.00	2.05
33	c	517	BCR	C30-C25	-2.69	1.50	1.53
42	2	313	KC1	C4D-ND	2.69	1.41	1.37
38	W	203	DGD	O5D-C1E	2.69	1.44	1.40
31	18	307	CLA	C3B-C4B	2.69	1.49	1.42
38	w	204	DGD	O5D-C1E	2.69	1.44	1.40
43	6	305	A86	C14-C13	2.69	1.54	1.51
31	10	309	CLA	C4B-NB	2.69	1.41	1.37
31	6	309	CLA	CMD-C2D	-2.69	1.45	1.50
43	0	302	A86	C30-C29	-2.69	1.27	1.32
31	p	610	CLA	C4B-NB	2.69	1.41	1.37
31	P	610	CLA	C4B-NB	2.68	1.41	1.37
31	1	316	CLA	C1B-C2B	2.68	1.49	1.43
45	13	309	KC2	C1A-CHA	2.68	1.47	1.40
31	13	312	CLA	C3B-C4B	2.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	511	CLA	CMD-C2D	-2.68	1.45	1.50
31	15	312	CLA	C1A-CHA	-2.68	1.32	1.43
31	W	202	CLA	C4B-NB	2.68	1.41	1.37
31	8	312	CLA	MG-NB	-2.68	2.00	2.05
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	D	402	CLA	C1B-NB	-2.68	1.34	1.37
31	2	307	CLA	C4B-NB	2.68	1.41	1.37
31	14	307	CLA	C4B-NB	2.68	1.41	1.37
43	8	303	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	311	CLA	C4B-NB	2.68	1.41	1.37
32	a	405	PHO	CAC-C3C	-2.68	1.46	1.51
31	7	312	CLA	C3B-C4B	2.68	1.49	1.42
43	6	302	A86	C33-C34	2.68	1.56	1.51
38	c	519	DGD	O4E-C4E	-2.68	1.36	1.43
43	1	302	A86	C30-C29	-2.68	1.27	1.32
45	1	311	KC2	C4D-ND	2.68	1.41	1.37
31	8	308	CLA	C3B-C4B	2.68	1.49	1.42
45	18	310	KC2	C1A-CHA	2.68	1.47	1.40
43	12	304	A86	C30-C29	-2.67	1.27	1.32
31	A	406	CLA	MG-NB	-2.67	2.00	2.05
31	c	504	CLA	C4B-NB	2.67	1.41	1.37
42	17	314	KC1	C1A-CHA	2.67	1.47	1.40
31	0	314	CLA	C3B-C4B	2.67	1.49	1.42
33	h	101	BCR	C30-C25	-2.67	1.50	1.53
31	p	602	CLA	C4B-NB	2.67	1.41	1.37
38	b	622	DGD	O1G-C1G	-2.67	1.39	1.45
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	0	308	CLA	C4D-ND	-2.67	1.34	1.37
31	6	308	CLA	C4D-ND	-2.67	1.34	1.37
31	7	308	CLA	MG-NB	-2.67	2.00	2.05
31	8	310	CLA	C4B-NB	2.67	1.41	1.37
31	C	502	CLA	MG-NB	-2.67	2.00	2.05
32	A	405	PHO	CAC-C3C	-2.67	1.46	1.51
42	3	314	KC1	C1A-CHA	2.67	1.47	1.40
31	d	402	CLA	CMB-C2B	-2.67	1.45	1.50
31	13	312	CLA	C1B-C2B	2.67	1.49	1.43
31	b	617	CLA	CMC-C2C	-2.67	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	513	CLA	C1D-ND	2.67	1.41	1.37
31	C	507	CLA	C1B-NB	-2.66	1.34	1.37
31	c	507	CLA	C1B-NB	-2.66	1.34	1.37
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	C	507	CLA	C4B-NB	2.66	1.41	1.37
31	1	307	CLA	MG-NB	-2.66	2.00	2.05
31	11	313	CLA	MG-NB	-2.66	2.00	2.05
31	11	313	CLA	MG-ND	-2.66	2.00	2.05
31	3	313	CLA	MG-ND	-2.66	2.00	2.05
31	b	608	CLA	MG-NB	-2.66	2.00	2.05
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	B	608	CLA	CMB-C2B	-2.66	1.45	1.50
45	2	310	KC2	C1A-CHA	2.66	1.47	1.40
31	0	309	CLA	C4B-NB	2.66	1.41	1.37
31	p	602	CLA	C3B-C4B	2.66	1.49	1.42
31	B	611	CLA	MG-NB	-2.66	2.00	2.05
31	a	404	CLA	MG-NB	-2.66	2.00	2.05
31	p	606	CLA	C1C-NC	-2.66	1.33	1.37
31	0	312	CLA	CMD-C2D	-2.66	1.45	1.50
38	c	520	DGD	O2G-C2G	-2.65	1.40	1.46
31	c	507	CLA	C4B-NB	2.65	1.41	1.37
45	5	310	KC2	C1D-ND	-2.65	1.34	1.37
43	18	304	A86	C33-C34	2.65	1.56	1.51
31	P	610	CLA	C3B-C4B	2.65	1.49	1.42
31	B	613	CLA	MG-NB	-2.65	2.00	2.05
31	3	308	CLA	CHC-C1C	2.65	1.43	1.38
43	19	304	A86	O1-C15	-2.65	1.41	1.45
31	p	603	CLA	C3B-C4B	2.65	1.49	1.42
42	0	315	KC1	C1B-NB	-2.65	1.34	1.37
31	15	309	CLA	C3B-C4B	2.65	1.49	1.42
43	17	302	A86	O3-C36	2.65	1.47	1.43
31	d	402	CLA	C1B-NB	-2.65	1.34	1.37
45	12	309	KC2	C4D-ND	2.65	1.41	1.37
42	15	317	KC1	C1A-CHA	2.65	1.47	1.40
32	A	405	PHO	CMB-C2B	-2.65	1.46	1.51
31	17	308	CLA	C1D-ND	2.64	1.41	1.37
38	C	520	DGD	O2G-C2G	-2.64	1.40	1.46
45	17	309	KC2	C3C-C4C	2.64	1.50	1.44
31	1	312	CLA	CMD-C2D	-2.64	1.45	1.50
31	B	611	CLA	C4B-NB	2.64	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	313	CLA	C3D-C2D	-2.64	1.31	1.39
38	C	520	DGD	O2E-C2E	-2.64	1.36	1.43
31	15	307	CLA	C3B-C4B	2.64	1.48	1.42
31	16	312	CLA	C1B-C2B	2.64	1.49	1.43
43	11	304	A86	C13-C11	-2.64	1.44	1.49
31	p	601	CLA	C3B-C4B	2.64	1.48	1.42
31	2	315	CLA	CMC-C2C	-2.64	1.45	1.50
31	p	608	CLA	C3B-C4B	2.64	1.48	1.42
42	5	313	KC1	C1B-NB	-2.64	1.34	1.37
31	p	610	CLA	C3B-C4B	2.64	1.48	1.42
31	D	405	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
31	6	308	CLA	C4B-NB	2.63	1.41	1.37
31	P	603	CLA	C3B-C4B	2.63	1.48	1.42
43	4	305	A86	C40-C32	-2.63	1.48	1.53
31	A	404	CLA	MG-NB	-2.63	2.00	2.05
31	2	309	CLA	C1B-C2B	2.63	1.49	1.43
31	7	313	CLA	CHC-C1C	2.63	1.43	1.38
45	7	311	KC2	C1A-CHA	2.63	1.47	1.40
31	b	610	CLA	C3B-C4B	2.63	1.48	1.42
31	b	612	CLA	MG-NB	-2.63	2.00	2.05
43	18	301	A86	C30-C29	-2.63	1.27	1.32
31	15	307	CLA	MG-NB	-2.63	2.00	2.05
37	c	522	LMG	C4-C5	2.63	1.58	1.53
31	18	306	CLA	C4B-NB	2.63	1.41	1.37
31	1	313	CLA	CMB-C2B	-2.63	1.45	1.50
33	c	515	BCR	C1-C6	-2.63	1.50	1.53
31	0	313	CLA	C1B-C2B	2.63	1.49	1.43
31	p	602	CLA	C1D-ND	2.62	1.41	1.37
31	P	604	CLA	MG-NB	-2.62	2.00	2.05
43	17	302	A86	C33-C34	2.62	1.56	1.51
31	w	203	CLA	CMC-C2C	-2.62	1.45	1.50
31	b	610	CLA	C4B-NB	2.62	1.41	1.37
31	P	601	CLA	C3B-C4B	2.62	1.48	1.42
31	B	607	CLA	MG-NB	-2.62	2.00	2.05
43	4	305	A86	C13-C11	-2.62	1.44	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	608	CLA	C3B-C4B	2.62	1.48	1.42
31	10	317	CLA	CMB-C2B	-2.62	1.45	1.50
45	4	308	KC2	C1A-CHA	2.62	1.47	1.40
31	15	312	CLA	C3B-C4B	2.62	1.48	1.42
31	C	505	CLA	C4B-NB	2.62	1.41	1.37
31	b	612	CLA	C4B-NB	2.62	1.41	1.37
31	c	505	CLA	C4B-NB	2.62	1.41	1.37
31	P	605	CLA	C3B-C4B	2.62	1.48	1.42
31	13	310	CLA	C3B-C4B	2.62	1.48	1.42
31	b	605	CLA	CMD-C2D	-2.62	1.45	1.50
31	d	402	CLA	MG-NB	-2.62	2.00	2.05
31	B	605	CLA	CMD-C2D	-2.62	1.45	1.50
31	13	312	CLA	C4D-ND	-2.62	1.34	1.37
33	C	517	BCR	C30-C25	-2.62	1.50	1.53
37	J	101	LMG	C4-C5	2.62	1.58	1.53
31	16	308	CLA	C4B-NB	2.62	1.41	1.37
31	2	311	CLA	C3B-C4B	2.62	1.48	1.42
31	16	315	CLA	C1B-C2B	2.61	1.49	1.43
31	10	312	CLA	CMD-C2D	-2.61	1.45	1.50
31	a	403	CLA	C1B-NB	-2.61	1.34	1.37
36	d	408	LHG	O7-C5	-2.61	1.40	1.46
43	18	305	A86	C13-C11	-2.61	1.44	1.49
32	D	403	PHO	CMD-C2D	-2.61	1.46	1.51
31	8	313	CLA	C1B-NB	-2.61	1.34	1.37
31	10	311	CLA	C4B-NB	2.61	1.41	1.37
31	5	307	CLA	MG-NB	-2.61	2.00	2.05
32	d	403	PHO	CMD-C2D	-2.61	1.46	1.51
36	D	408	LHG	O7-C5	-2.61	1.40	1.46
31	B	612	CLA	MG-ND	-2.61	2.00	2.05
31	b	614	CLA	MG-NB	-2.61	2.00	2.05
31	p	604	CLA	MG-NB	-2.61	2.00	2.05
31	18	311	CLA	C4B-NB	2.61	1.41	1.37
31	18	311	CLA	MG-ND	-2.61	2.00	2.05
31	c	505	CLA	CMD-C2D	-2.61	1.45	1.50
37	1	317	LMG	C4-C5	2.61	1.58	1.53
45	8	309	KC2	C3C-C4C	2.61	1.50	1.44
31	18	314	CLA	C3B-C4B	2.61	1.48	1.42
43	5	318	A86	C30-C29	-2.61	1.27	1.32
31	19	311	CLA	C1B-C2B	2.61	1.49	1.43
31	11	312	CLA	CMD-C2D	-2.61	1.45	1.50
31	D	402	CLA	MG-NB	-2.60	2.00	2.05
31	6	313	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	12	301	A86	C33-C34	2.60	1.56	1.51
31	P	608	CLA	C3B-C4B	2.60	1.48	1.42
31	b	609	CLA	C3B-C4B	2.60	1.48	1.42
43	19	303	A86	C30-C29	-2.60	1.27	1.32
31	0	312	CLA	C3B-C4B	2.60	1.48	1.42
38	c	520	DGD	O2E-C2E	-2.60	1.36	1.43
31	p	602	CLA	CMB-C2B	-2.60	1.45	1.50
31	11	313	CLA	CHC-C1C	2.60	1.43	1.38
31	b	609	CLA	C1D-ND	2.60	1.41	1.37
43	3	301	A86	C40-C32	-2.60	1.48	1.53
31	P	602	CLA	C4B-NB	2.60	1.41	1.37
45	7	309	KC2	C3C-C4C	2.60	1.50	1.44
45	3	311	KC2	C4D-ND	2.60	1.41	1.37
31	B	601	CLA	C3B-C4B	2.60	1.48	1.42
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	p	605	CLA	C3B-C4B	2.60	1.48	1.42
31	d	405	CLA	CMC-C2C	-2.60	1.45	1.50
37	j	101	LMG	C4-C5	2.60	1.58	1.53
31	18	307	CLA	C1B-NB	-2.60	1.34	1.37
31	16	307	CLA	C4D-ND	-2.59	1.34	1.37
31	B	609	CLA	C3B-C4B	2.59	1.48	1.42
31	D	402	CLA	CMB-C2B	-2.59	1.45	1.50
31	0	309	CLA	MG-NB	-2.59	2.00	2.05
37	k	101	LMG	O8-C9	-2.59	1.39	1.45
31	B	614	CLA	MG-NB	-2.59	2.00	2.05
31	b	608	CLA	C1B-NB	-2.59	1.34	1.37
31	B	604	CLA	C1B-C2B	2.59	1.49	1.43
31	10	313	CLA	C1B-C2B	2.59	1.49	1.43
43	16	305	A86	C14-C13	2.59	1.54	1.51
31	9	311	CLA	C1B-C2B	2.59	1.49	1.43
37	5	316	LMG	C4-C3	2.59	1.58	1.52
31	b	613	CLA	MG-ND	-2.59	2.00	2.05
31	R	101	CLA	C3B-C4B	2.59	1.48	1.42
31	12	312	CLA	C3B-C4B	2.59	1.48	1.42
31	C	505	CLA	CMD-C2D	-2.58	1.45	1.50
31	10	313	CLA	CMD-C2D	-2.58	1.45	1.50
31	10	313	CLA	C3B-C4B	2.58	1.48	1.42
31	8	308	CLA	MG-NB	-2.58	2.00	2.05
43	8	305	A86	C13-C11	-2.58	1.44	1.49
31	P	606	CLA	CMD-C2D	-2.58	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	14	309	CLA	C1B-C2B	2.58	1.49	1.43
31	p	606	CLA	CMD-C2D	-2.58	1.45	1.50
31	C	511	CLA	C3B-C4B	2.58	1.48	1.42
31	19	310	CLA	C1B-C2B	2.58	1.49	1.43
31	c	511	CLA	C3B-C4B	2.58	1.48	1.42
42	9	314	KC1	C1A-CHA	2.58	1.47	1.40
31	A	403	CLA	CMB-C2B	-2.58	1.45	1.50
32	a	405	PHO	CMB-C2B	-2.58	1.46	1.51
31	r	101	CLA	C3B-C4B	2.58	1.48	1.42
38	C	519	DGD	O1G-C1G	-2.58	1.39	1.45
38	c	519	DGD	O1G-C1G	-2.58	1.39	1.45
31	9	310	CLA	C1B-C2B	2.58	1.49	1.43
45	16	309	KC2	C1B-NB	-2.58	1.34	1.37
45	2	308	KC2	C3C-C4C	2.58	1.50	1.44
45	14	308	KC2	C1A-CHA	2.58	1.47	1.40
31	C	512	CLA	C1B-NB	-2.58	1.34	1.37
31	c	512	CLA	C1B-NB	-2.58	1.34	1.37
37	K	101	LMG	O8-C9	-2.58	1.39	1.45
31	5	311	CLA	CMD-C2D	-2.58	1.45	1.50
31	3	308	CLA	C4B-NB	2.58	1.41	1.37
31	b	606	CLA	CMD-C2D	-2.57	1.45	1.50
42	3	314	KC1	C1B-NB	-2.57	1.34	1.37
31	3	312	CLA	C1B-C2B	2.57	1.49	1.43
31	0	311	CLA	C4B-NB	2.57	1.40	1.37
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
31	5	309	CLA	C3B-C4B	2.57	1.48	1.42
31	b	602	CLA	C3B-C4B	2.57	1.48	1.42
45	16	309	KC2	C3C-C4C	2.57	1.50	1.44
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	615	CLA	MG-NB	-2.56	2.00	2.05
42	1	314	KC1	C1D-ND	-2.56	1.34	1.37
31	a	403	CLA	CMB-C2B	-2.56	1.45	1.50
31	B	609	CLA	MG-NB	-2.56	2.00	2.05
31	2	309	CLA	C3B-C4B	2.56	1.48	1.42
31	b	612	CLA	C1D-ND	2.56	1.40	1.37
31	10	312	CLA	C1B-C2B	2.56	1.49	1.43
31	b	616	CLA	C4B-NB	2.56	1.40	1.37
31	18	307	CLA	MG-ND	-2.56	2.00	2.05
31	3	313	CLA	C1D-ND	2.56	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	309	CLA	C4B-NB	2.56	1.40	1.37
31	17	310	CLA	C1B-C2B	2.56	1.49	1.43
31	16	312	CLA	C3B-C4B	2.56	1.48	1.42
45	12	309	KC2	C1A-CHA	2.56	1.47	1.40
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	302	A86	C33-C34	2.56	1.56	1.51
31	D	406	CLA	MG-NB	-2.56	2.00	2.05
31	C	506	CLA	C3B-C4B	2.56	1.48	1.42
31	c	507	CLA	C3B-C4B	2.56	1.48	1.42
31	b	605	CLA	C1B-C2B	2.56	1.49	1.43
43	17	303	A86	C19-C20	2.56	1.55	1.52
31	7	310	CLA	C1B-C2B	2.55	1.49	1.43
43	13	302	A86	C13-C11	-2.55	1.44	1.49
31	0	308	CLA	C1B-C2B	2.55	1.49	1.43
31	5	306	CLA	C1B-C2B	2.55	1.49	1.43
31	1	308	CLA	CHC-C1C	2.55	1.43	1.38
42	6	315	KC1	C4C-C3C	2.55	1.49	1.45
31	18	311	CLA	C3B-C4B	2.55	1.48	1.42
31	B	607	CLA	C1B-NB	-2.55	1.34	1.37
31	B	612	CLA	C1B-NB	-2.55	1.34	1.37
45	15	310	KC2	C1D-ND	-2.55	1.34	1.37
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	b	609	CLA	C4B-NB	2.55	1.40	1.37
31	4	312	CLA	CMD-C2D	-2.55	1.45	1.50
31	9	315	CLA	C1B-C2B	2.55	1.49	1.43
33	Y	101	BCR	C38-C26	-2.55	1.46	1.50
31	c	506	CLA	C3B-C4B	2.55	1.48	1.42
43	13	306	A86	C13-C11	-2.55	1.44	1.49
43	16	305	A86	C33-C34	2.55	1.56	1.51
31	1	312	CLA	MG-NB	-2.55	2.00	2.05
31	18	312	CLA	MG-NB	-2.55	2.00	2.05
31	4	307	CLA	C1D-ND	2.55	1.40	1.37
31	1	313	CLA	CHC-C1C	2.55	1.43	1.38
45	6	310	KC2	C1B-NB	-2.55	1.34	1.37
31	3	312	CLA	C3B-C4B	2.55	1.48	1.42
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
31	12	310	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	304	A86	O1-C15	-2.54	1.41	1.45
45	3	309	KC2	C1B-NB	-2.54	1.34	1.37
31	16	307	CLA	C1B-C2B	2.54	1.49	1.43
31	15	306	CLA	C1B-C2B	2.54	1.49	1.43
31	C	505	CLA	C3B-C4B	2.54	1.48	1.42
31	D	402	CLA	CMD-C2D	-2.54	1.45	1.50
31	r	101	CLA	C1B-C2B	2.54	1.49	1.43
31	b	602	CLA	MG-NB	-2.54	2.00	2.05
45	16	309	KC2	C1A-CHA	2.54	1.47	1.40
31	C	508	CLA	CMB-C2B	-2.54	1.45	1.50
37	c	521	LMG	C4-C5	2.54	1.58	1.53
31	4	307	CLA	MG-NB	-2.54	2.00	2.05
31	b	603	CLA	CMB-C2B	-2.54	1.45	1.50
31	B	610	CLA	MG-NB	-2.54	2.00	2.05
31	C	504	CLA	MG-NB	-2.54	2.00	2.05
31	5	312	CLA	CMD-C2D	-2.54	1.45	1.50
31	c	505	CLA	C3B-C4B	2.54	1.48	1.42
31	c	508	CLA	C1B-NB	-2.54	1.34	1.37
31	8	312	CLA	C3B-C4B	2.54	1.48	1.42
31	1	307	CLA	C3B-C4B	2.54	1.48	1.42
31	B	614	CLA	C3B-C4B	2.54	1.48	1.42
31	6	313	CLA	C3B-C4B	2.54	1.48	1.42
31	A	403	CLA	C1B-NB	-2.53	1.34	1.37
31	d	402	CLA	CMD-C2D	-2.53	1.45	1.50
45	7	309	KC2	C4D-ND	2.53	1.41	1.37
31	P	601	CLA	C1B-C2B	2.53	1.49	1.43
31	11	310	CLA	C4B-NB	2.53	1.40	1.37
33	C	515	BCR	C1-C6	-2.53	1.50	1.53
31	b	610	CLA	MG-NB	-2.53	2.00	2.05
31	p	607	CLA	MG-NB	-2.53	2.00	2.05
45	1	311	KC2	C1D-ND	-2.53	1.34	1.37
31	A	406	CLA	CMD-C2D	-2.53	1.45	1.50
31	b	605	CLA	C1D-ND	2.53	1.40	1.37
31	17	308	CLA	CHC-C1C	2.53	1.43	1.38
34	a	408	SQD	O2-C2	-2.53	1.37	1.43
31	P	602	CLA	CMB-C2B	-2.53	1.45	1.50
31	6	316	CLA	C1B-C2B	2.53	1.49	1.43
43	9	306	A86	C41-C32	2.53	1.58	1.53
43	3	301	A86	C26-C27	-2.53	1.32	1.35
45	10	310	KC2	C1D-ND	-2.53	1.34	1.37
31	P	601	CLA	MG-NB	-2.53	2.00	2.05
31	3	313	CLA	CHC-C1C	2.53	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	312	CLA	C1B-C2B	2.53	1.49	1.43
45	0	310	KC2	C1D-ND	-2.53	1.34	1.37
31	c	504	CLA	MG-NB	-2.53	2.00	2.05
31	6	313	CLA	MG-NB	-2.53	2.00	2.05
31	B	601	CLA	MG-NB	-2.53	2.00	2.05
43	10	302	A86	C13-C11	-2.53	1.44	1.49
43	15	305	A86	O1-C20	-2.53	1.42	1.46
37	15	315	LMG	O8-C9	-2.53	1.39	1.45
31	C	506	CLA	C4B-NB	2.52	1.40	1.37
31	c	506	CLA	C4B-NB	2.52	1.40	1.37
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	6	314	CLA	C3B-C4B	2.52	1.48	1.42
31	C	508	CLA	MG-NB	-2.52	2.00	2.05
31	c	508	CLA	MG-NB	-2.52	2.00	2.05
31	C	514	CLA	MG-NB	-2.52	2.00	2.05
31	12	315	CLA	C1B-C2B	2.52	1.49	1.43
34	A	408	SQD	O2-C2	-2.52	1.37	1.43
31	3	316	CLA	C1B-C2B	2.52	1.49	1.43
37	15	315	LMG	C4-C3	2.52	1.58	1.52
31	B	615	CLA	C4B-NB	2.52	1.40	1.37
31	p	601	CLA	C1B-C2B	2.52	1.49	1.43
31	B	608	CLA	C4B-NB	2.52	1.40	1.37
31	5	311	CLA	MG-NB	-2.52	2.00	2.05
38	C	518	DGD	O3G-C3G	-2.52	1.39	1.43
38	h	102	DGD	C3G-C2G	2.52	1.58	1.50
31	12	308	CLA	CMB-C2B	-2.52	1.45	1.50
31	A	406	CLA	C3B-C4B	2.52	1.48	1.42
31	c	508	CLA	CMB-C2B	-2.52	1.45	1.50
31	B	602	CLA	CMB-C2B	-2.52	1.45	1.50
31	16	312	CLA	MG-NB	-2.52	2.00	2.05
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
31	7	308	CLA	C1D-ND	2.52	1.40	1.37
31	C	507	CLA	C3B-C4B	2.52	1.48	1.42
31	11	312	CLA	CMB-C2B	-2.52	1.45	1.50
43	2	303	A86	C13-C11	-2.52	1.44	1.49
31	4	309	CLA	C1B-C2B	2.52	1.49	1.43
43	10	318	A86	C32-C31	-2.52	1.50	1.54
31	14	312	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	13	314	KC1	C4D-ND	2.52	1.41	1.37
43	4	301	A86	C13-C11	-2.51	1.44	1.49
31	D	406	CLA	C4B-NB	2.51	1.40	1.37
31	b	615	CLA	C3B-C4B	2.51	1.48	1.42
43	19	304	A86	C13-C11	-2.51	1.44	1.49
45	6	310	KC2	C1A-CHA	2.51	1.47	1.40
43	10	304	A86	C30-C29	-2.51	1.27	1.32
31	14	307	CLA	MG-NB	-2.51	2.00	2.05
31	8	308	CLA	C1D-ND	2.51	1.40	1.37
38	H	102	DGD	C3G-C2G	2.51	1.58	1.50
43	3	303	A86	C13-C11	-2.51	1.44	1.49
31	C	509	CLA	CMD-C2D	-2.51	1.45	1.50
45	17	309	KC2	C4D-ND	2.51	1.41	1.37
31	C	509	CLA	C4B-NB	2.51	1.40	1.37
43	3	302	A86	C13-C11	-2.51	1.44	1.49
42	16	314	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	d	405	CLA	C1B-NB	-2.51	1.34	1.37
31	d	406	CLA	C4B-NB	2.51	1.40	1.37
45	14	310	KC2	C1D-ND	-2.51	1.34	1.37
31	R	101	CLA	C1B-C2B	2.51	1.49	1.43
42	19	314	KC1	C1A-CHA	2.51	1.47	1.40
31	11	308	CLA	MG-NB	-2.51	2.00	2.05
31	B	606	CLA	CMC-C2C	-2.51	1.45	1.50
45	1	311	KC2	C1A-CHA	2.51	1.47	1.40
45	2	308	KC2	C1A-CHA	2.51	1.47	1.40
43	11	303	A86	C13-C11	-2.51	1.44	1.49
42	p	609	KC1	C4B-NB	-2.51	1.34	1.37
31	7	308	CLA	CHC-C1C	2.51	1.43	1.38
43	14	304	A86	C35-C34	2.50	1.56	1.51
45	13	309	KC2	C1D-ND	-2.50	1.34	1.37
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	D	405	CLA	C1B-NB	-2.50	1.34	1.37
31	10	312	CLA	C3B-C4B	2.50	1.48	1.42
31	14	314	CLA	CHC-C1C	2.50	1.43	1.38
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	p	601	CLA	MG-NB	-2.50	2.00	2.05
31	P	608	CLA	CMC-C2C	-2.50	1.45	1.50
31	0	309	CLA	CHC-C1C	2.50	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	12	308	CLA	MG-NB	-2.50	2.00	2.05
31	c	514	CLA	MG-NB	-2.50	2.00	2.05
31	12	313	CLA	CMB-C2B	-2.50	1.45	1.50
45	2	310	KC2	C3C-C4C	2.50	1.49	1.44
33	y	101	BCR	C38-C26	-2.50	1.46	1.50
31	15	307	CLA	CMB-C2B	-2.50	1.45	1.50
43	13	301	A86	C13-C11	-2.50	1.44	1.49
31	p	603	CLA	C4B-NB	2.50	1.40	1.37
31	P	607	CLA	C1D-ND	2.50	1.40	1.37
31	b	613	CLA	C1B-NB	-2.49	1.34	1.37
45	7	311	KC2	C4D-ND	2.49	1.41	1.37
31	19	315	CLA	C1B-C2B	2.49	1.49	1.43
43	8	302	A86	C2-C1	-2.49	1.32	1.35
31	2	307	CLA	MG-NB	-2.49	2.00	2.05
31	B	605	CLA	MG-NB	-2.49	2.00	2.05
31	P	607	CLA	MG-NB	-2.49	2.00	2.05
31	b	606	CLA	MG-NB	-2.49	2.00	2.05
31	12	307	CLA	C4D-ND	-2.49	1.34	1.37
42	16	314	KC1	C1D-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
31	p	604	CLA	C4B-NB	2.49	1.40	1.37
42	17	314	KC1	C1B-NB	-2.49	1.34	1.37
42	16	314	KC1	C4A-C3A	2.49	1.49	1.44
37	C	522	LMG	C4-C5	2.49	1.58	1.53
31	b	611	CLA	MG-NB	-2.49	2.00	2.05
31	a	406	CLA	C3B-C4B	2.49	1.48	1.42
31	c	514	CLA	CMC-C2C	-2.49	1.45	1.50
45	13	311	KC2	C1A-CHA	2.49	1.47	1.40
31	9	308	CLA	C1B-C2B	2.49	1.49	1.43
31	14	306	CLA	C1D-ND	2.49	1.40	1.37
43	12	304	A86	O1-C15	-2.49	1.41	1.45
31	d	406	CLA	MG-NB	-2.49	2.00	2.05
43	3	302	A86	C33-C34	2.49	1.56	1.51
31	p	607	CLA	C4B-NB	2.49	1.40	1.37
36	P	615	LHG	O7-C5	-2.49	1.40	1.46
31	18	309	CLA	C4B-NB	2.49	1.40	1.37
38	c	518	DGD	O3G-C3G	-2.49	1.39	1.43
43	7	301	A86	C33-C34	2.48	1.56	1.51
31	C	511	CLA	C4B-NB	2.48	1.40	1.37
31	c	511	CLA	C4B-NB	2.48	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	510	CLA	CMC-C2C	-2.48	1.45	1.50
31	0	316	CLA	C4B-NB	2.48	1.40	1.37
43	8	303	A86	C17-C18	-2.48	1.48	1.52
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	0	307	CLA	C1B-NB	-2.48	1.34	1.37
31	c	505	CLA	CAC-C3C	-2.48	1.44	1.51
31	3	315	CLA	C1B-C2B	2.48	1.49	1.43
31	2	311	CLA	MG-NB	-2.48	2.00	2.05
31	B	616	CLA	CMB-C2B	-2.48	1.45	1.50
43	18	305	A86	C32-C31	-2.48	1.50	1.54
45	0	310	KC2	C4B-NB	-2.48	1.34	1.37
45	16	311	KC2	C1A-CHA	2.48	1.47	1.40
37	1	301	LMG	O7-C8	-2.48	1.40	1.46
31	2	314	CLA	C1B-C2B	2.48	1.49	1.43
31	c	509	CLA	CMD-C2D	-2.48	1.45	1.50
43	14	304	A86	C13-C11	-2.48	1.44	1.49
31	18	314	CLA	MG-NB	-2.48	2.00	2.05
35	D	407	PL9	C31-C29	-2.48	1.46	1.51
35	d	407	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	0	310	KC2	C1A-CHA	2.48	1.47	1.40
31	C	502	CLA	C3B-C4B	2.48	1.48	1.42
31	c	502	CLA	C3B-C4B	2.48	1.48	1.42
31	5	307	CLA	CMD-C2D	-2.48	1.45	1.50
45	15	310	KC2	C4B-NB	-2.48	1.34	1.37
31	0	316	CLA	MG-NB	-2.48	2.00	2.05
31	5	311	CLA	MG-ND	-2.48	2.00	2.05
31	11	308	CLA	CHC-C1C	2.48	1.43	1.38
31	0	312	CLA	C1B-C2B	2.47	1.49	1.43
45	17	309	KC2	C1A-CHA	2.47	1.47	1.40
31	c	503	CLA	CMD-C2D	-2.47	1.45	1.50
31	C	514	CLA	C4B-NB	2.47	1.40	1.37
31	c	514	CLA	C4B-NB	2.47	1.40	1.37
43	16	303	A86	C13-C11	-2.47	1.44	1.49
45	7	309	KC2	C1A-CHA	2.47	1.47	1.40
31	b	616	CLA	C1B-C2B	2.47	1.49	1.43
45	12	311	KC2	C1A-CHA	2.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	604	CLA	C4B-NB	2.47	1.40	1.37
37	11	301	LMG	O7-C8	-2.47	1.40	1.46
31	3	316	CLA	C3B-C4B	2.47	1.48	1.42
43	5	302	A86	C13-C11	-2.47	1.45	1.49
31	Z	101	CLA	MG-NB	-2.47	2.00	2.05
31	10	309	CLA	CHC-C1C	2.47	1.43	1.38
31	2	306	CLA	C4D-ND	-2.47	1.34	1.37
42	8	314	KC1	C1A-CHA	2.47	1.47	1.40
31	d	405	CLA	CMB-C2B	-2.47	1.45	1.50
31	p	608	CLA	CMC-C2C	-2.47	1.45	1.50
31	10	308	CLA	C1B-C2B	2.47	1.49	1.43
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
31	P	607	CLA	C4B-NB	2.47	1.40	1.37
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	2	306	CLA	C1B-C2B	2.46	1.49	1.43
31	A	404	CLA	C3B-C4B	2.46	1.48	1.42
31	a	404	CLA	C3B-C4B	2.46	1.48	1.42
31	B	612	CLA	CMC-C2C	-2.46	1.45	1.50
38	w	204	DGD	O4D-C4D	-2.46	1.37	1.43
45	9	309	KC2	C1B-NB	-2.46	1.34	1.37
38	W	203	DGD	O4D-C4D	-2.46	1.37	1.43
31	C	508	CLA	C1B-NB	-2.46	1.34	1.37
43	5	305	A86	C32-C31	-2.46	1.50	1.54
31	18	306	CLA	MG-NB	-2.46	2.00	2.05
38	11	318	DGD	C4E-C3E	2.46	1.58	1.52
31	b	608	CLA	C3B-C4B	2.46	1.48	1.42
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
31	c	513	CLA	C3B-C4B	2.46	1.48	1.42
31	11	316	CLA	C1B-C2B	2.46	1.49	1.43
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
42	15	317	KC1	C1D-ND	-2.46	1.34	1.37
31	11	315	CLA	C3C-C2C	2.46	1.41	1.36
42	3	314	KC1	C4A-C3A	2.46	1.49	1.44
38	c	520	DGD	O6D-C5D	-2.46	1.38	1.44
43	3	301	A86	C2-C1	-2.46	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	307	CLA	C1B-NB	-2.45	1.34	1.37
31	B	607	CLA	C3B-C4B	2.45	1.48	1.42
31	D	405	CLA	CMB-C2B	-2.45	1.45	1.50
31	a	404	CLA	CMB-C2B	-2.45	1.45	1.50
31	b	617	CLA	CMB-C2B	-2.45	1.45	1.50
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	2	315	CLA	C1B-C2B	2.45	1.49	1.43
31	p	610	CLA	CMD-C2D	-2.45	1.45	1.50
43	7	302	A86	C26-C27	-2.45	1.32	1.35
45	11	311	KC2	C1A-CHA	2.45	1.47	1.40
31	16	310	CLA	C3B-C4B	2.45	1.48	1.42
42	7	314	KC1	C1A-CHA	2.45	1.47	1.40
43	6	301	A86	C30-C29	-2.45	1.27	1.32
31	8	315	CLA	MG-NB	-2.45	2.00	2.05
45	18	308	KC2	C4B-NB	-2.45	1.34	1.37
43	10	301	A86	C33-C34	2.45	1.56	1.51
31	p	607	CLA	CMD-C2D	-2.45	1.45	1.50
31	8	312	CLA	MG-ND	-2.45	2.00	2.05
42	7	314	KC1	C1D-ND	-2.45	1.34	1.37
45	6	312	KC2	C1A-CHA	2.45	1.47	1.40
31	d	405	CLA	MG-ND	-2.45	2.00	2.05
31	C	508	CLA	C1D-ND	2.45	1.40	1.37
31	c	508	CLA	C1D-ND	2.45	1.40	1.37
31	10	316	CLA	C4B-NB	2.45	1.40	1.37
31	C	513	CLA	C3B-C4B	2.45	1.48	1.42
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	5	309	CLA	MG-NB	-2.44	2.00	2.05
31	B	615	CLA	C1B-C2B	2.44	1.49	1.43
31	z	101	CLA	MG-NB	-2.44	2.00	2.05
45	8	311	KC2	C1A-CHA	2.44	1.47	1.40
38	H	102	DGD	O1G-C1G	-2.44	1.39	1.45
31	17	308	CLA	MG-ND	-2.44	2.00	2.05
31	A	403	CLA	C3B-C4B	2.44	1.48	1.42
43	P	611	A86	C37-C36	2.44	1.56	1.52
31	4	312	CLA	CHC-C1C	2.44	1.43	1.38
31	C	508	CLA	CMC-C2C	-2.44	1.45	1.50
31	1	310	CLA	C1B-C2B	2.44	1.49	1.43
31	10	316	CLA	MG-NB	-2.44	2.00	2.05
43	11	319	A86	O1-C20	-2.44	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	19	308	CLA	C1B-C2B	2.44	1.49	1.43
31	4	311	CLA	C1B-C2B	2.44	1.49	1.43
37	N	101	LMG	C7-C8	2.44	1.58	1.50
31	A	404	CLA	CMB-C2B	-2.44	1.45	1.50
31	17	312	CLA	C1B-C2B	2.44	1.49	1.43
31	B	604	CLA	C1D-ND	2.44	1.40	1.37
31	4	315	CLA	C1B-C2B	2.44	1.49	1.43
31	18	314	CLA	C1B-C2B	2.44	1.49	1.43
31	C	503	CLA	CMD-C2D	-2.43	1.45	1.50
31	c	508	CLA	C4B-NB	2.43	1.40	1.37
31	7	308	CLA	MG-ND	-2.43	2.01	2.05
31	C	511	CLA	MG-NB	-2.43	2.01	2.05
43	12	304	A86	O4-C34	-2.43	1.40	1.46
31	C	506	CLA	MG-NB	-2.43	2.01	2.05
31	11	312	CLA	MG-NB	-2.43	2.01	2.05
31	c	509	CLA	C4B-NB	2.43	1.40	1.37
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
42	3	314	KC1	C1D-ND	-2.43	1.34	1.37
31	3	308	CLA	CMC-C2C	-2.43	1.45	1.50
31	B	611	CLA	C3B-C4B	2.43	1.48	1.42
31	18	312	CLA	CMD-C2D	-2.43	1.45	1.50
31	15	307	CLA	C4B-NB	2.43	1.40	1.37
31	5	307	CLA	MG-ND	-2.43	2.01	2.05
43	0	306	A86	O3-C36	2.43	1.47	1.43
31	13	308	CLA	CMB-C2B	-2.43	1.45	1.50
31	14	315	CLA	C1D-ND	2.43	1.40	1.37
31	8	310	CLA	MG-NB	-2.43	2.01	2.05
31	C	503	CLA	CAC-C3C	-2.43	1.44	1.51
31	18	312	CLA	CHC-C1C	2.43	1.43	1.38
31	B	609	CLA	CMB-C2B	-2.43	1.45	1.50
31	10	313	CLA	CMC-C2C	-2.43	1.45	1.50
31	11	313	CLA	CMB-C2B	-2.43	1.45	1.50
31	B	604	CLA	CMC-C2C	-2.43	1.45	1.50
31	p	608	CLA	CMD-C2D	-2.42	1.45	1.50
31	13	313	CLA	C1D-ND	2.42	1.40	1.37
31	C	512	CLA	CMB-C2B	-2.42	1.45	1.50
42	13	314	KC1	C4B-NB	-2.42	1.34	1.37
42	18	313	KC1	C1D-ND	-2.42	1.34	1.37
43	19	303	A86	C13-C11	-2.42	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	14	307	CLA	CMD-C2D	-2.42	1.45	1.50
32	D	403	PHO	C4D-CHA	2.42	1.43	1.39
32	d	403	PHO	C4D-CHA	2.42	1.43	1.39
31	14	306	CLA	CHB-C4A	-2.42	1.31	1.37
31	p	603	CLA	MG-ND	-2.42	2.01	2.05
45	16	311	KC2	C1B-NB	-2.42	1.34	1.37
31	b	610	CLA	CMB-C2B	-2.42	1.45	1.50
31	14	311	CLA	C1B-C2B	2.42	1.49	1.43
31	18	309	CLA	MG-NB	-2.42	2.01	2.05
31	12	316	CLA	C1B-C2B	2.42	1.49	1.43
31	9	312	CLA	MG-NB	-2.42	2.01	2.05
31	19	312	CLA	MG-NB	-2.42	2.01	2.05
31	15	311	CLA	C1B-NB	-2.42	1.34	1.37
31	12	312	CLA	C1B-C2B	2.42	1.48	1.43
31	C	510	CLA	CMD-C2D	-2.42	1.45	1.50
31	8	308	CLA	CMB-C2B	-2.41	1.45	1.50
31	P	603	CLA	C4B-NB	2.41	1.40	1.37
45	18	310	KC2	C1D-ND	-2.41	1.34	1.37
45	18	308	KC2	C1A-CHA	2.41	1.47	1.40
43	15	304	A86	C13-C11	-2.41	1.45	1.49
31	a	403	CLA	C3B-C4B	2.41	1.48	1.42
31	1	313	CLA	C1B-NB	-2.41	1.34	1.37
31	b	612	CLA	C3B-C4B	2.41	1.48	1.42
31	D	405	CLA	CHC-C1C	2.41	1.43	1.38
31	13	316	CLA	C1B-C2B	2.41	1.48	1.43
31	B	615	CLA	MG-NB	-2.41	2.01	2.05
43	8	304	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	5	312	CLA	C3B-C4B	2.41	1.48	1.42
31	c	503	CLA	CAC-C3C	-2.41	1.44	1.51
45	19	309	KC2	C4A-C3A	2.41	1.49	1.44
32	D	403	PHO	CMB-C2B	-2.41	1.46	1.51
37	M	101	LMG	O8-C9	-2.41	1.39	1.45
31	5	309	CLA	C4B-NB	2.41	1.40	1.37
45	13	311	KC2	C1B-NB	-2.41	1.34	1.37
31	12	313	CLA	MG-ND	-2.41	2.01	2.05
45	15	308	KC2	C4D-ND	2.41	1.41	1.37
31	15	307	CLA	C1B-C2B	2.41	1.48	1.43
31	P	603	CLA	MG-ND	-2.41	2.01	2.05
38	h	102	DGD	O2D-C2D	-2.41	1.37	1.43
43	0	306	A86	C28-C27	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	10	301	A86	C13-C11	-2.41	1.45	1.49
31	1	308	CLA	MG-NB	-2.41	2.01	2.05
31	B	615	CLA	C3B-C4B	2.41	1.48	1.42
31	c	512	CLA	CMB-C2B	-2.41	1.45	1.50
43	10	304	A86	C13-C11	-2.41	1.45	1.49
43	11	306	A86	C13-C11	-2.41	1.45	1.49
45	8	311	KC2	C1D-ND	-2.41	1.34	1.37
31	p	610	CLA	MG-NB	-2.41	2.01	2.05
43	0	304	A86	C13-C11	-2.40	1.45	1.49
31	D	405	CLA	MG-ND	-2.40	2.01	2.05
43	7	306	A86	C13-C11	-2.40	1.45	1.49
43	4	303	A86	C13-C11	-2.40	1.45	1.49
31	b	606	CLA	CMC-C2C	-2.40	1.45	1.50
31	z	103	CLA	C1B-NB	-2.40	1.34	1.37
38	c	519	DGD	O5D-C6D	-2.40	1.39	1.43
31	4	307	CLA	CMB-C2B	-2.40	1.45	1.50
31	b	616	CLA	C3B-C4B	2.40	1.48	1.42
45	15	308	KC2	C1A-CHA	2.40	1.47	1.40
31	b	605	CLA	CMC-C2C	-2.40	1.45	1.50
31	c	511	CLA	MG-NB	-2.40	2.01	2.05
31	3	310	CLA	C1B-C2B	2.40	1.48	1.43
31	3	308	CLA	CMD-C2D	-2.40	1.45	1.50
31	b	617	CLA	C1B-NB	-2.40	1.34	1.37
31	4	309	CLA	C4B-NB	2.40	1.40	1.37
31	17	315	CLA	C1B-C2B	2.40	1.48	1.43
38	C	520	DGD	O6D-C5D	-2.40	1.38	1.44
31	1	312	CLA	C1B-C2B	2.40	1.48	1.43
31	10	309	CLA	MG-NB	-2.40	2.01	2.05
31	C	508	CLA	C4B-NB	2.40	1.40	1.37
45	2	308	KC2	C4D-ND	2.40	1.40	1.37
31	c	510	CLA	CMD-C2D	-2.40	1.45	1.50
31	b	607	CLA	CMB-C2B	-2.40	1.45	1.50
31	c	510	CLA	MG-NB	-2.40	2.01	2.05
31	9	311	CLA	CHC-C1C	2.40	1.43	1.38
31	0	309	CLA	CMD-C2D	-2.40	1.45	1.50
43	16	305	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	11	309	KC2	C1D-ND	-2.39	1.34	1.37
31	B	606	CLA	CMB-C2B	-2.39	1.45	1.50
45	17	311	KC2	C1B-NB	-2.39	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	611	CLA	C1B-NB	-2.39	1.34	1.37
31	c	506	CLA	MG-NB	-2.39	2.01	2.05
37	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
31	P	610	CLA	MG-NB	-2.39	2.01	2.05
33	b	620	BCR	C38-C26	-2.39	1.47	1.50
45	2	310	KC2	C4D-ND	2.39	1.40	1.37
31	5	312	CLA	CMA-C3A	-2.39	1.48	1.53
43	4	302	A86	C33-C34	2.39	1.56	1.51
38	1	318	DGD	C4E-C3E	2.39	1.58	1.52
37	1	301	LMG	C3-C2	2.39	1.58	1.52
31	6	309	CLA	MG-NB	-2.39	2.01	2.05
31	15	307	CLA	MG-ND	-2.39	2.01	2.05
43	8	302	A86	C13-C11	-2.39	1.45	1.49
38	h	102	DGD	O1G-C1G	-2.39	1.39	1.45
31	13	308	CLA	MG-NB	-2.39	2.01	2.05
31	d	405	CLA	CHC-C1C	2.38	1.43	1.38
43	p	611	A86	C30-C29	-2.38	1.28	1.32
43	10	303	A86	C5-C6	-2.38	1.32	1.35
31	1	316	CLA	MG-NB	-2.38	2.01	2.05
31	13	310	CLA	MG-NB	-2.38	2.01	2.05
43	4	306	A86	C33-C34	2.38	1.56	1.51
31	12	308	CLA	CMD-C2D	-2.38	1.45	1.50
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
45	17	309	KC2	C1D-C2D	2.38	1.48	1.43
31	B	613	CLA	C4B-NB	2.38	1.40	1.37
31	13	307	CLA	C1B-C2B	2.38	1.48	1.43
31	11	315	CLA	C1B-C2B	2.38	1.48	1.43
45	4	310	KC2	C1D-ND	-2.38	1.34	1.37
31	P	608	CLA	CMD-C2D	-2.38	1.45	1.50
31	z	103	CLA	CMD-C2D	-2.38	1.45	1.50
45	8	309	KC2	C1A-CHA	2.38	1.46	1.40
31	4	314	CLA	CHC-C1C	2.38	1.43	1.38
31	C	514	CLA	C1B-C2B	2.38	1.48	1.43
45	5	308	KC2	C1A-CHA	2.38	1.46	1.40
31	a	403	CLA	CMC-C2C	-2.38	1.45	1.50
37	W	201	LMG	O1-C1	2.38	1.44	1.40
31	C	510	CLA	C3B-C4B	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	7	302	A86	C2-C1	-2.38	1.32	1.35
31	P	601	CLA	C1B-NB	-2.38	1.34	1.37
45	2	308	KC2	C1D-C2D	2.38	1.48	1.43
31	14	306	CLA	CHC-C1C	2.38	1.43	1.38
31	11	307	CLA	CMD-C2D	-2.38	1.45	1.50
45	2	308	KC2	C1B-NB	-2.38	1.34	1.37
37	w	201	LMG	O1-C1	2.38	1.44	1.40
31	15	312	CLA	CMA-C3A	-2.38	1.48	1.53
45	17	311	KC2	C4D-ND	2.37	1.40	1.37
38	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
31	11	310	CLA	C1B-C2B	2.37	1.48	1.43
42	18	313	KC1	C4B-NB	-2.37	1.34	1.37
31	15	313	CLA	CMD-C2D	-2.37	1.45	1.50
31	3	307	CLA	C1B-C2B	2.37	1.48	1.43
31	3	308	CLA	MG-NB	-2.37	2.01	2.05
31	14	315	CLA	C1B-C2B	2.37	1.48	1.43
31	12	307	CLA	MG-NB	-2.37	2.01	2.05
32	d	403	PHO	CMB-C2B	-2.37	1.46	1.51
31	c	510	CLA	C1B-NB	-2.37	1.34	1.37
31	2	311	CLA	C1B-C2B	2.37	1.48	1.43
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	4	315	CLA	CMB-C2B	-2.37	1.45	1.50
31	13	308	CLA	CMC-C2C	-2.37	1.45	1.50
31	p	601	CLA	C1B-NB	-2.37	1.34	1.37
31	P	608	CLA	C1B-C2B	2.37	1.48	1.43
31	15	309	CLA	MG-NB	-2.37	2.01	2.05
31	15	312	CLA	CHC-C1C	2.37	1.43	1.38
31	1	310	CLA	C4B-NB	2.37	1.40	1.37
31	b	617	CLA	CMD-C2D	-2.36	1.45	1.50
31	11	313	CLA	CMD-C2D	-2.36	1.45	1.50
31	b	607	CLA	MG-NB	-2.36	2.01	2.05
38	C	519	DGD	O5D-C6D	-2.36	1.39	1.43
31	b	615	CLA	CMD-C2D	-2.36	1.45	1.50
31	B	609	CLA	CMD-C2D	-2.36	1.45	1.50
31	5	314	CLA	C1B-C2B	2.36	1.48	1.43
45	8	309	KC2	C4B-NB	-2.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	p	611	A86	C5-C6	-2.36	1.32	1.35
31	B	610	CLA	C1B-NB	-2.36	1.34	1.37
37	d	404	LMG	C3-C2	2.36	1.58	1.52
45	9	309	KC2	C1A-CHA	2.36	1.46	1.40
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	14	309	CLA	C4B-NB	2.36	1.40	1.37
31	3	316	CLA	MG-NB	-2.36	2.01	2.05
31	b	611	CLA	CMD-C2D	-2.36	1.45	1.50
31	C	510	CLA	MG-NB	-2.36	2.01	2.05
31	a	403	CLA	MG-ND	-2.36	2.01	2.05
31	p	608	CLA	C1B-C2B	2.36	1.48	1.43
37	1	317	LMG	C9-C8	2.36	1.57	1.50
45	7	309	KC2	C1D-C2D	2.36	1.48	1.43
43	2	302	A86	C33-C34	2.36	1.56	1.51
31	b	616	CLA	MG-NB	-2.36	2.01	2.05
31	6	308	CLA	C3B-C4B	2.36	1.48	1.42
31	p	607	CLA	CMC-C2C	-2.36	1.45	1.50
31	16	308	CLA	CMD-C2D	-2.36	1.45	1.50
31	z	101	CLA	CMD-C2D	-2.36	1.45	1.50
31	B	616	CLA	C1B-NB	-2.35	1.34	1.37
35	A	409	PL9	C10-C9	-2.35	1.44	1.50
43	6	306	A86	C33-C34	2.35	1.56	1.51
31	D	406	CLA	CMD-C2D	-2.35	1.45	1.50
43	5	318	A86	C13-C11	-2.35	1.45	1.49
31	C	513	CLA	CMC-C2C	-2.35	1.45	1.50
31	p	610	CLA	C1B-C2B	2.35	1.48	1.43
42	13	314	KC1	C1A-CHA	2.35	1.46	1.40
31	5	307	CLA	C1B-C2B	2.35	1.48	1.43
42	P	609	KC1	C1A-CHA	2.35	1.46	1.40
31	c	514	CLA	C1B-C2B	2.35	1.48	1.43
45	3	309	KC2	C1D-C2D	2.35	1.48	1.43
32	D	403	PHO	CAC-C3C	-2.35	1.47	1.51
31	w	203	CLA	CMD-C2D	-2.35	1.45	1.50
31	8	308	CLA	MG-ND	-2.35	2.01	2.05
42	5	313	KC1	C1A-CHA	2.35	1.46	1.40
45	15	310	KC2	C3C-C4C	2.35	1.49	1.44
31	b	612	CLA	MG-ND	-2.35	2.01	2.05
31	c	507	CLA	MG-ND	-2.35	2.01	2.05
31	B	605	CLA	C4B-NB	2.35	1.40	1.37
42	p	609	KC1	C4D-ND	2.35	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	0	304	A86	C30-C29	-2.35	1.28	1.32
43	6	305	A86	C14-C15	2.35	1.57	1.52
43	3	305	A86	C13-C11	-2.35	1.45	1.49
37	D	409	LMG	O8-C9	-2.35	1.39	1.45
31	C	510	CLA	C1B-NB	-2.35	1.34	1.37
31	b	610	CLA	CMD-C2D	-2.35	1.45	1.50
31	10	314	CLA	C1B-C2B	2.35	1.48	1.43
31	B	613	CLA	CMC-C2C	-2.35	1.45	1.50
31	0	307	CLA	MG-ND	-2.35	2.01	2.05
31	c	504	CLA	C1B-NB	-2.35	1.34	1.37
45	7	309	KC2	C1B-NB	-2.35	1.34	1.37
31	11	310	CLA	C3B-C4B	2.35	1.48	1.42
43	17	306	A86	C33-C34	2.35	1.56	1.51
43	0	301	A86	C13-C11	-2.35	1.45	1.49
42	p	609	KC1	C1A-CHA	2.35	1.46	1.40
31	B	605	CLA	CMC-C2C	-2.35	1.45	1.50
31	8	315	CLA	C1B-C2B	2.34	1.48	1.43
43	7	306	A86	C30-C29	-2.34	1.28	1.32
31	7	315	CLA	C1B-C2B	2.34	1.48	1.43
45	6	312	KC2	C1B-NB	-2.34	1.34	1.37
31	b	614	CLA	C1B-C2B	2.34	1.48	1.43
31	c	510	CLA	C3B-C4B	2.34	1.48	1.42
31	c	507	CLA	CMC-C2C	-2.34	1.45	1.50
31	8	312	CLA	C1B-C2B	2.34	1.48	1.43
45	16	309	KC2	C1D-C2D	2.34	1.48	1.43
31	P	601	CLA	MG-ND	-2.34	2.01	2.05
31	b	614	CLA	C3B-C4B	2.34	1.48	1.42
31	b	611	CLA	CMB-C2B	-2.34	1.45	1.50
31	C	512	CLA	C4B-NB	2.34	1.40	1.37
31	b	606	CLA	C4B-NB	2.34	1.40	1.37
31	c	512	CLA	C4B-NB	2.34	1.40	1.37
31	P	610	CLA	C1B-C2B	2.34	1.48	1.43
37	11	301	LMG	C3-C2	2.34	1.58	1.52
43	16	301	A86	C13-C11	-2.34	1.45	1.49
31	1	321	CLA	C4B-NB	2.34	1.40	1.37
31	A	403	CLA	MG-ND	-2.34	2.01	2.05
31	6	311	CLA	C3B-C4B	2.34	1.48	1.42
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	407	PL9	C26-C24	-2.34	1.46	1.51
31	P	607	CLA	CMC-C2C	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	610	CLA	CMD-C2D	-2.34	1.45	1.50
31	d	406	CLA	CMD-C2D	-2.34	1.45	1.50
32	d	403	PHO	CAC-C3C	-2.34	1.47	1.51
31	C	505	CLA	CMB-C2B	-2.34	1.45	1.50
31	c	505	CLA	CMB-C2B	-2.34	1.45	1.50
31	13	313	CLA	CMC-C2C	-2.34	1.45	1.50
45	10	310	KC2	C1A-CHA	2.33	1.46	1.40
31	b	603	CLA	C1B-C2B	2.33	1.48	1.43
31	17	307	CLA	C1B-C2B	2.33	1.48	1.43
45	9	309	KC2	C4A-C3A	2.33	1.49	1.44
43	5	304	A86	O1-C20	-2.33	1.42	1.46
37	5	316	LMG	O8-C9	-2.33	1.39	1.45
31	p	601	CLA	MG-ND	-2.33	2.01	2.05
31	B	602	CLA	C1B-C2B	2.33	1.48	1.43
31	B	606	CLA	MG-NB	-2.33	2.01	2.05
38	c	519	DGD	O3D-C3D	-2.33	1.37	1.43
31	P	607	CLA	C1B-C2B	2.33	1.48	1.43
45	19	309	KC2	C1A-CHA	2.33	1.46	1.40
31	C	508	CLA	MG-ND	-2.33	2.01	2.05
45	13	311	KC2	C1D-C2D	2.33	1.48	1.43
37	D	404	LMG	C3-C2	2.33	1.58	1.52
31	b	608	CLA	CMC-C2C	-2.33	1.45	1.50
45	3	309	KC2	C4D-ND	2.33	1.40	1.37
45	12	311	KC2	C3C-C4C	2.33	1.49	1.44
35	a	409	PL9	C10-C9	-2.33	1.44	1.50
31	c	512	CLA	CMC-C2C	-2.33	1.45	1.50
31	c	513	CLA	CMC-C2C	-2.33	1.45	1.50
38	B	621	DGD	O4D-C4D	-2.33	1.37	1.43
31	2	307	CLA	CHC-C1C	2.33	1.43	1.38
42	10	315	KC1	C4B-NB	-2.33	1.34	1.37
31	P	602	CLA	CMC-C2C	-2.33	1.45	1.50
37	D	404	LMG	O1-C7	-2.33	1.39	1.43
31	b	616	CLA	C1B-NB	-2.33	1.34	1.37
31	b	614	CLA	C4B-NB	2.33	1.40	1.37
31	W	202	CLA	CMB-C2B	-2.33	1.45	1.50
37	K	101	LMG	O4-C4	-2.33	1.37	1.43
37	k	101	LMG	O4-C4	-2.33	1.37	1.43
31	1	312	CLA	CMB-C2B	-2.32	1.45	1.50
31	5	307	CLA	CMB-C2B	-2.32	1.45	1.50
31	B	614	CLA	CMB-C2B	-2.32	1.45	1.50
31	0	313	CLA	C3B-C4B	2.32	1.48	1.42
42	P	609	KC1	C4D-ND	2.32	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	313	CLA	CHC-C1C	2.32	1.43	1.38
31	p	607	CLA	C1B-C2B	2.32	1.48	1.43
31	15	311	CLA	CHC-C4B	-2.32	1.34	1.39
31	1	307	CLA	MG-ND	-2.32	2.01	2.05
31	13	310	CLA	C1B-C2B	2.32	1.48	1.43
31	C	514	CLA	CMD-C2D	-2.32	1.45	1.50
31	19	311	CLA	CHC-C1C	2.32	1.43	1.38
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	B	614	CLA	C4B-NB	2.32	1.40	1.37
31	7	313	CLA	CAA-C2A	-2.32	1.49	1.54
31	18	306	CLA	C1B-NB	-2.32	1.34	1.37
31	W	202	CLA	CMD-C2D	-2.32	1.45	1.50
37	W	201	LMG	O8-C9	-2.32	1.39	1.45
31	C	503	CLA	MG-NB	-2.32	2.01	2.05
45	1	309	KC2	C1A-CHA	2.32	1.46	1.40
31	10	313	CLA	CMB-C2B	-2.32	1.45	1.50
42	19	314	KC1	C4A-C3A	2.32	1.49	1.44
31	17	312	CLA	MG-NB	-2.32	2.01	2.05
31	2	312	CLA	C1D-ND	2.32	1.40	1.37
31	r	101	CLA	CMD-C2D	-2.32	1.45	1.50
31	B	613	CLA	C1B-C2B	2.31	1.48	1.43
31	b	615	CLA	CMB-C2B	-2.31	1.45	1.50
31	R	101	CLA	MG-NB	-2.31	2.01	2.05
37	1	317	LMG	C7-C8	2.31	1.57	1.50
31	Z	101	CLA	CMD-C2D	-2.31	1.45	1.50
45	6	312	KC2	C4A-C3A	2.31	1.49	1.44
42	2	313	KC1	C1B-NB	-2.31	1.34	1.37
31	B	613	CLA	C3B-C4B	2.31	1.48	1.42
37	11	317	LMG	C7-C8	2.31	1.57	1.50
38	C	519	DGD	O3D-C3D	-2.31	1.37	1.43
31	p	602	CLA	CMC-C2C	-2.31	1.45	1.50
31	11	312	CLA	C1B-NB	-2.31	1.34	1.37
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	407	PL9	C41-C39	-2.31	1.46	1.51
31	B	615	CLA	CMB-C2B	-2.31	1.45	1.50
31	0	308	CLA	CMD-C2D	-2.31	1.45	1.50
31	b	614	CLA	C1B-NB	-2.31	1.34	1.37
43	8	306	A86	C30-C29	-2.31	1.28	1.32
31	15	313	CLA	C1B-C2B	2.31	1.48	1.43
31	C	513	CLA	MG-ND	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
45	18	310	KC2	C4D-ND	2.30	1.40	1.37
37	W	201	LMG	O7-C8	-2.30	1.40	1.46
31	b	615	CLA	MG-ND	-2.30	2.01	2.05
45	12	311	KC2	C4D-ND	2.30	1.40	1.37
31	19	308	CLA	CHC-C1C	2.30	1.43	1.38
31	R	101	CLA	CMD-C2D	-2.30	1.45	1.50
31	w	203	CLA	CMB-C2B	-2.30	1.45	1.50
45	4	308	KC2	C4D-ND	2.30	1.40	1.37
31	0	314	CLA	MG-NB	-2.30	2.01	2.05
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	A	404	CLA	C4B-NB	2.30	1.40	1.37
31	a	404	CLA	C4B-NB	2.30	1.40	1.37
31	Z	101	CLA	C1B-C2B	2.30	1.48	1.43
31	B	602	CLA	MG-ND	-2.30	2.01	2.05
31	r	101	CLA	MG-NB	-2.30	2.01	2.05
43	0	303	A86	C5-C6	-2.30	1.32	1.35
45	5	308	KC2	C4D-ND	2.30	1.40	1.37
45	14	308	KC2	C4D-ND	2.30	1.40	1.37
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	b	615	CLA	C4B-NB	2.30	1.40	1.37
43	P	611	A86	C5-C6	-2.30	1.32	1.35
32	a	405	PHO	CBD-CGD	-2.30	1.49	1.52
31	1	308	CLA	CMB-C2B	-2.30	1.45	1.50
37	w	201	LMG	O7-C8	-2.30	1.40	1.46
31	c	508	CLA	MG-ND	-2.30	2.01	2.05
31	5	312	CLA	CHC-C1C	2.30	1.43	1.38
45	17	311	KC2	C3C-C4C	2.30	1.49	1.44
31	B	614	CLA	C1B-NB	-2.30	1.35	1.37
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
38	b	622	DGD	C4E-C3E	2.29	1.58	1.52
31	C	503	CLA	MG-ND	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	0	311	CLA	MG-ND	-2.29	2.01	2.05
42	6	315	KC1	C1D-ND	-2.29	1.35	1.37
31	1	310	CLA	MG-NB	-2.29	2.01	2.05
31	B	610	CLA	CMB-C2B	-2.29	1.45	1.50
31	3	312	CLA	MG-NB	-2.29	2.01	2.05
45	8	309	KC2	C4D-ND	2.29	1.40	1.37
31	C	510	CLA	C4B-NB	2.29	1.40	1.37
35	d	407	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	C	502	CLA	C4B-NB	2.29	1.40	1.37
31	c	502	CLA	C4B-NB	2.29	1.40	1.37
31	12	308	CLA	CHC-C1C	2.29	1.43	1.38
31	p	608	CLA	MG-NB	-2.29	2.01	2.05
31	z	101	CLA	C1B-C2B	2.29	1.48	1.43
42	11	314	KC1	C1D-ND	-2.29	1.35	1.37
37	d	409	LMG	O8-C9	-2.29	1.39	1.45
31	13	315	CLA	C1B-C2B	2.29	1.48	1.43
31	19	313	CLA	CHC-C1C	2.29	1.43	1.38
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	407	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	616	CLA	CMB-C2B	-2.28	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	p	605	CLA	MG-NB	-2.28	2.01	2.05
45	5	308	KC2	C4A-C3A	2.28	1.49	1.44
31	c	510	CLA	C1B-C2B	2.28	1.48	1.43
31	9	313	CLA	CHC-C1C	2.28	1.43	1.38
31	13	308	CLA	CMD-C2D	-2.28	1.46	1.50
45	6	310	KC2	C1D-C2D	2.28	1.48	1.43
37	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	9	315	CLA	CHC-C1C	2.28	1.43	1.38
45	5	310	KC2	C4D-ND	2.28	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
37	c	521	LMG	C3-C2	2.28	1.58	1.52
31	10	311	CLA	MG-ND	-2.28	2.01	2.05
42	9	314	KC1	C4C-C3C	2.28	1.49	1.45
31	c	503	CLA	MG-NB	-2.28	2.01	2.05
31	18	314	CLA	CMB-C2B	-2.28	1.46	1.50
43	12	306	A86	C26-C27	-2.28	1.32	1.35
45	9	309	KC2	C4D-ND	2.28	1.40	1.37
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
31	10	317	CLA	C1B-NB	-2.28	1.35	1.37
31	11	308	CLA	CMB-C2B	-2.28	1.46	1.50
31	p	607	CLA	CHC-C1C	2.27	1.43	1.38
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	B	616	CLA	MG-NB	-2.27	2.01	2.05
31	d	406	CLA	CMB-C2B	-2.27	1.46	1.50
43	p	611	A86	C26-C27	-2.27	1.32	1.35
31	p	601	CLA	CMD-C2D	-2.27	1.46	1.50
35	D	407	PL9	C26-C24	-2.27	1.46	1.51
31	0	314	CLA	C1B-C2B	2.27	1.48	1.43
31	C	511	CLA	C1B-NB	-2.27	1.35	1.37
45	11	311	KC2	C3C-C4C	2.27	1.49	1.44
31	C	504	CLA	C1B-NB	-2.27	1.35	1.37
31	B	614	CLA	MG-ND	-2.27	2.01	2.05
31	b	617	CLA	MG-NB	-2.27	2.01	2.05
31	b	602	CLA	CMD-C2D	-2.27	1.46	1.50
31	b	604	CLA	CHC-C4B	-2.27	1.34	1.39
45	16	309	KC2	C4D-ND	2.27	1.40	1.37
31	b	606	CLA	CMB-C2B	-2.27	1.46	1.50
31	C	506	CLA	C1B-C2B	2.27	1.48	1.43
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	6	308	CLA	MG-NB	-2.27	2.01	2.05
45	5	310	KC2	C1D-C2D	2.27	1.48	1.43
31	C	510	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	602	CLA	C3B-C4B	2.27	1.48	1.42
31	b	603	CLA	C3B-C4B	2.27	1.48	1.42
31	b	615	CLA	CMC-C2C	-2.27	1.46	1.50
31	b	614	CLA	CMD-C2D	-2.27	1.46	1.50
31	8	315	CLA	CMB-C2B	-2.27	1.46	1.50
45	8	311	KC2	C4D-ND	2.27	1.40	1.37
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	c	503	CLA	MG-ND	-2.27	2.01	2.05
31	C	511	CLA	CMC-C2C	-2.27	1.46	1.50
31	18	307	CLA	C1D-ND	2.27	1.40	1.37
33	b	619	BCR	C1-C6	-2.26	1.50	1.53
41	V	201	HEM	C2A-C3A	-2.26	1.32	1.38
31	D	402	CLA	MG-ND	-2.26	2.01	2.05
34	l	101	SQD	O2-C2	-2.26	1.37	1.43
31	19	315	CLA	CHC-C1C	2.26	1.43	1.38
34	i	101	SQD	O2-C2	-2.26	1.37	1.43
31	16	308	CLA	MG-NB	-2.26	2.01	2.05
31	c	511	CLA	CMC-C2C	-2.26	1.46	1.50
31	18	307	CLA	C4B-NB	2.26	1.40	1.37
45	3	309	KC2	C4B-NB	-2.26	1.35	1.37
31	c	510	CLA	CMB-C2B	-2.26	1.46	1.50
31	4	309	CLA	MG-NB	-2.26	2.01	2.05
31	c	506	CLA	C1B-C2B	2.26	1.48	1.43
31	11	310	CLA	MG-NB	-2.26	2.01	2.05
45	16	311	KC2	C1D-ND	-2.26	1.35	1.37
43	1	306	A86	C13-C11	-2.26	1.45	1.49
42	2	313	KC1	C1D-ND	-2.26	1.35	1.37
45	16	311	KC2	C4A-C3A	2.26	1.48	1.44
34	10	320	SQD	O4-C4	-2.26	1.37	1.43
31	C	504	CLA	CMD-C2D	-2.26	1.46	1.50
31	D	406	CLA	CMB-C2B	-2.26	1.46	1.50
31	c	504	CLA	CMD-C2D	-2.26	1.46	1.50
42	4	313	KC1	C4D-ND	2.26	1.40	1.37
38	c	518	DGD	O2E-C2E	-2.26	1.37	1.43
45	13	311	KC2	C3C-C4C	2.26	1.49	1.44
31	B	603	CLA	CHC-C4B	-2.26	1.34	1.39
43	16	302	A86	C26-C27	-2.26	1.32	1.35
31	1	315	CLA	MG-NB	-2.26	2.01	2.05
31	13	308	CLA	MG-ND	-2.26	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	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
31	19	313	CLA	C1B-C2B	2.26	1.48	1.43
42	14	313	KC1	C4B-NB	-2.26	1.35	1.37
43	4	305	A86	C26-C27	-2.26	1.32	1.35
38	c	520	DGD	O3D-C3D	-2.26	1.37	1.43
34	b	601	SQD	O2-C2	-2.26	1.37	1.43
37	C	522	LMG	C3-C2	2.26	1.58	1.52
37	w	201	LMG	O4-C4	-2.26	1.37	1.43
31	c	502	CLA	CMC-C2C	-2.25	1.46	1.50
38	C	520	DGD	O4D-C4D	-2.25	1.37	1.43
43	17	316	A86	C40-C32	-2.25	1.49	1.53
31	A	404	CLA	C1B-NB	-2.25	1.35	1.37
42	1	314	KC1	C4B-NB	-2.25	1.35	1.37
38	C	519	DGD	O2E-C2E	-2.25	1.37	1.43
31	0	313	CLA	CMD-C2D	-2.25	1.46	1.50
31	18	309	CLA	C1B-NB	-2.25	1.35	1.37
43	1	302	A86	O1-C20	-2.25	1.43	1.46
31	15	311	CLA	C1B-C2B	2.25	1.48	1.43
43	13	305	A86	C13-C11	-2.25	1.45	1.49
45	2	308	KC2	C4A-C3A	2.25	1.48	1.44
38	C	520	DGD	O3D-C3D	-2.25	1.37	1.43
31	P	605	CLA	MG-NB	-2.25	2.01	2.05
31	b	604	CLA	C4B-NB	2.25	1.40	1.37
31	b	616	CLA	CMD-C2D	-2.25	1.46	1.50
31	7	307	CLA	C1B-C2B	2.25	1.48	1.43
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
31	7	312	CLA	MG-NB	-2.25	2.01	2.05
31	A	406	CLA	C1B-NB	-2.25	1.35	1.37
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
31	p	607	CLA	MG-ND	-2.25	2.01	2.05
31	B	602	CLA	CHC-C4B	-2.25	1.34	1.39
31	1	316	CLA	C3B-C4B	2.25	1.48	1.42
31	6	309	CLA	MG-ND	-2.25	2.01	2.05
42	15	317	KC1	C1D-C2D	2.25	1.48	1.43
42	19	314	KC1	C1D-C2D	2.25	1.48	1.43
31	p	607	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	307	CLA	MG-ND	-2.25	2.01	2.05
31	14	309	CLA	MG-NB	-2.25	2.01	2.05
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
38	c	519	DGD	O2E-C2E	-2.25	1.37	1.43
31	B	613	CLA	C1B-NB	-2.25	1.35	1.37
31	P	601	CLA	CMD-C2D	-2.24	1.46	1.50
45	1	309	KC2	C1D-C2D	2.24	1.48	1.43
45	17	309	KC2	C4A-C3A	2.24	1.48	1.44
31	9	308	CLA	CHC-C1C	2.24	1.43	1.38
37	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	c	510	CLA	C4B-NB	2.24	1.40	1.37
31	11	312	CLA	MG-ND	-2.24	2.01	2.05
31	11	315	CLA	MG-NB	-2.24	2.01	2.05
35	D	407	PL9	C20-C19	-2.24	1.44	1.50
31	11	316	CLA	CHC-C1C	2.24	1.43	1.38
31	B	615	CLA	C1B-NB	-2.24	1.35	1.37
43	11	305	A86	O1-C20	-2.24	1.43	1.46
31	P	603	CLA	CMB-C2B	-2.24	1.46	1.50
31	15	311	CLA	C1A-CHA	-2.24	1.33	1.43
31	Z	101	CLA	CMB-C2B	-2.24	1.46	1.50
31	14	307	CLA	CMB-C2B	-2.24	1.46	1.50
38	C	518	DGD	O2E-C2E	-2.24	1.37	1.43
31	d	402	CLA	MG-ND	-2.24	2.01	2.05
42	16	314	KC1	C1A-CHA	2.24	1.46	1.40
31	12	307	CLA	C1B-NB	-2.24	1.35	1.37
31	0	316	CLA	C1B-C2B	2.24	1.48	1.43
43	4	303	A86	C19-C20	2.24	1.55	1.52
31	8	312	CLA	CMC-C2C	-2.24	1.46	1.50
31	4	307	CLA	MG-ND	-2.24	2.01	2.05
31	b	615	CLA	C1B-NB	-2.24	1.35	1.37
31	8	310	CLA	C1B-NB	-2.24	1.35	1.37
31	1	310	CLA	C3B-C4B	2.24	1.48	1.42
45	18	308	KC2	C4D-ND	2.24	1.40	1.37
31	c	504	CLA	C1B-C2B	2.24	1.48	1.43
34	A	411	SQD	O2-C2	-2.24	1.37	1.43
31	8	310	CLA	C1B-C2B	2.24	1.48	1.43
43	11	302	A86	O3-C36	2.24	1.47	1.43
43	10	318	A86	C33-C34	2.24	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
31	a	406	CLA	C1B-NB	-2.24	1.35	1.37
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
31	12	312	CLA	MG-NB	-2.24	2.01	2.05
43	2	301	A86	C13-C11	-2.24	1.45	1.49
41	v	201	HEM	C2A-C3A	-2.24	1.32	1.38
31	4	314	CLA	MG-NB	-2.24	2.01	2.05
38	11	318	DGD	C3G-C2G	2.24	1.57	1.50
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
37	b	621	LMG	O3-C3	-2.23	1.37	1.43
31	B	612	CLA	C3B-C4B	2.23	1.48	1.42
31	0	314	CLA	CMC-C2C	-2.23	1.46	1.50
31	16	313	CLA	CHC-C1C	2.23	1.43	1.38
31	P	607	CLA	CHC-C1C	2.23	1.43	1.38
31	c	511	CLA	C1B-NB	-2.23	1.35	1.37
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
31	P	610	CLA	MG-ND	-2.23	2.01	2.05
31	12	315	CLA	MG-NB	-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	6	309	CLA	C1B-C2B	2.23	1.48	1.43
31	1	315	CLA	CMD-C2D	-2.23	1.46	1.50
31	b	613	CLA	C3B-C4B	2.23	1.48	1.42
43	4	304	A86	C13-C11	-2.23	1.45	1.49
31	C	510	CLA	CMB-C2B	-2.23	1.46	1.50
31	8	315	CLA	CMD-C2D	-2.23	1.46	1.50
43	8	306	A86	C32-C31	-2.23	1.50	1.54
31	A	404	CLA	MG-ND	-2.23	2.01	2.05
45	15	310	KC2	C1D-C2D	2.23	1.48	1.43
31	14	311	CLA	MG-NB	-2.23	2.01	2.05
31	B	604	CLA	C4B-NB	2.23	1.40	1.37
31	4	314	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	8	304	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
45	6	312	KC2	C1D-ND	-2.22	1.35	1.37
31	A	406	CLA	CMC-C2C	-2.22	1.46	1.50
31	7	310	CLA	MG-NB	-2.22	2.01	2.05
34	8	301	SQD	O2-C2	-2.22	1.37	1.43
43	14	303	A86	C13-C11	-2.22	1.45	1.49
31	W	202	CLA	MG-NB	-2.22	2.01	2.05
42	4	313	KC1	C4B-NB	-2.22	1.35	1.37
45	7	311	KC2	C1D-ND	-2.22	1.35	1.37
45	6	310	KC2	C4D-ND	2.22	1.40	1.37
37	B	620	LMG	O3-C3	-2.22	1.37	1.43
31	A	406	CLA	MG-ND	-2.22	2.01	2.05
31	P	608	CLA	MG-NB	-2.22	2.01	2.05
31	D	405	CLA	CAA-C2A	-2.22	1.50	1.54
31	12	315	CLA	CMB-C2B	-2.22	1.46	1.50
31	B	607	CLA	CMD-C2D	-2.22	1.46	1.50
31	B	603	CLA	C4B-NB	2.22	1.40	1.37
31	10	308	CLA	CMC-C2C	-2.22	1.46	1.50
31	R	101	CLA	CMB-C2B	-2.22	1.46	1.50
42	12	314	KC1	C4C-C3C	2.22	1.48	1.45
34	L	102	SQD	O2-C2	-2.22	1.37	1.43
37	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
31	B	614	CLA	CMC-C2C	-2.22	1.46	1.50
31	P	606	CLA	CMB-C2B	-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	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	13	315	CLA	CHC-C1C	2.22	1.43	1.38
31	c	505	CLA	MG-NB	-2.22	2.01	2.05
31	12	310	CLA	MG-NB	-2.22	2.01	2.05
45	3	311	KC2	C1D-ND	-2.22	1.35	1.37
31	C	504	CLA	C1B-C2B	2.22	1.48	1.43
31	17	310	CLA	MG-NB	-2.22	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	9	314	KC1	C1D-C2D	2.22	1.48	1.43
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
31	c	505	CLA	C1B-C2B	2.21	1.48	1.43
31	B	605	CLA	CMB-C2B	-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	z	101	CLA	CMB-C2B	-2.21	1.46	1.50
31	a	403	CLA	C4B-NB	2.21	1.40	1.37
45	7	311	KC2	C3C-C4C	2.21	1.49	1.44
45	7	309	KC2	C4A-C3A	2.21	1.48	1.44
38	c	518	DGD	O3G-C1D	-2.21	1.36	1.40
31	C	502	CLA	C1B-NB	-2.21	1.35	1.37
31	18	311	CLA	CMC-C2C	-2.21	1.46	1.50
38	1	318	DGD	O1G-C1G	-2.21	1.40	1.45
31	b	603	CLA	CHC-C4B	-2.21	1.34	1.39
31	14	307	CLA	C1B-C2B	2.21	1.48	1.43
31	3	316	CLA	CMB-C2B	-2.21	1.46	1.50
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
31	w	203	CLA	MG-NB	-2.21	2.01	2.05
31	0	311	CLA	C1B-NB	-2.21	1.35	1.37
31	0	316	CLA	CMD-C2D	-2.21	1.46	1.50
45	13	309	KC2	C4D-ND	2.21	1.40	1.37
31	C	506	CLA	CMC-C2C	-2.21	1.46	1.50
31	P	607	CLA	CMB-C2B	-2.21	1.46	1.50
31	9	308	CLA	CMD-C2D	-2.21	1.46	1.50
31	11	315	CLA	CMB-C2B	-2.21	1.46	1.50
31	c	514	CLA	C1B-NB	-2.21	1.35	1.37
34	8	301	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	5	309	CLA	C1B-C2B	2.20	1.48	1.43
31	b	609	CLA	MG-ND	-2.20	2.01	2.05
31	d	405	CLA	CAA-C2A	-2.20	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	406	CLA	CMC-C2C	-2.20	1.46	1.50
31	b	603	CLA	CMD-C2D	-2.20	1.46	1.50
37	n	701	LMG	C7-C8	2.20	1.57	1.50
43	18	302	A86	C32-C31	-2.20	1.50	1.54
31	b	614	CLA	CMB-C2B	-2.20	1.46	1.50
31	P	608	CLA	CMB-C2B	-2.20	1.46	1.50
31	2	309	CLA	MG-NB	-2.20	2.01	2.05
43	1	304	A86	C5-C6	-2.20	1.32	1.35
37	J	101	LMG	O4-C4	-2.20	1.37	1.43
37	j	101	LMG	O4-C4	-2.20	1.37	1.43
31	6	309	CLA	CHC-C1C	2.20	1.43	1.38
31	16	312	CLA	MG-ND	-2.20	2.01	2.05
43	0	304	A86	C32-C31	-2.20	1.50	1.54
45	5	310	KC2	C1A-CHA	2.20	1.46	1.40
43	17	303	A86	C13-C11	-2.20	1.45	1.49
31	c	512	CLA	C3B-C4B	2.20	1.47	1.42
45	2	310	KC2	C1D-ND	-2.20	1.35	1.37
31	8	312	CLA	CMB-C2B	-2.20	1.46	1.50
31	18	311	CLA	CMB-C2B	-2.20	1.46	1.50
31	z	103	CLA	MG-ND	-2.20	2.01	2.05
31	6	311	CLA	MG-NB	-2.20	2.01	2.05
31	2	312	CLA	CMC-C2C	-2.20	1.46	1.50
31	b	612	CLA	CMD-C2D	-2.20	1.46	1.50
31	C	505	CLA	C1B-C2B	2.20	1.48	1.43
31	P	605	CLA	CMD-C2D	-2.20	1.46	1.50
31	11	313	CLA	C1D-ND	2.20	1.40	1.37
42	8	314	KC1	C1D-C2D	2.20	1.48	1.43
31	P	605	CLA	CMC-C2C	-2.20	1.46	1.50
31	c	502	CLA	CMB-C2B	-2.20	1.46	1.50
31	10	316	CLA	CMC-C2C	-2.20	1.46	1.50
31	C	505	CLA	MG-NB	-2.20	2.01	2.05
31	15	309	CLA	C1B-C2B	2.20	1.48	1.43
42	17	314	KC1	C4D-ND	2.20	1.40	1.37
43	5	302	A86	C40-C32	-2.19	1.49	1.53
31	8	308	CLA	C4B-NB	2.19	1.40	1.37
31	r	101	CLA	CMB-C2B	-2.19	1.46	1.50
31	D	405	CLA	CHD-C1D	-2.19	1.34	1.38
31	d	405	CLA	CHD-C1D	-2.19	1.34	1.38
31	7	313	CLA	C1B-NB	-2.19	1.35	1.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	16	310	CLA	MG-NB	-2.19	2.01	2.05
31	0	316	CLA	CMC-C2C	-2.19	1.46	1.50
31	c	508	CLA	C3B-C4B	2.19	1.47	1.42
31	b	603	CLA	MG-NB	-2.19	2.01	2.05
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	b	608	CLA	CMD-C2D	-2.19	1.46	1.50
31	p	606	CLA	CMB-C2B	-2.19	1.46	1.50
31	B	612	CLA	C1B-C2B	2.19	1.48	1.43
31	p	603	CLA	CMB-C2B	-2.19	1.46	1.50
31	r	101	CLA	MG-ND	-2.19	2.01	2.05
31	C	502	CLA	C1B-C2B	2.19	1.48	1.43
31	c	502	CLA	C1B-C2B	2.19	1.48	1.43
31	12	312	CLA	CMD-C2D	-2.19	1.46	1.50
43	19	305	A86	C14-C15	2.19	1.57	1.52
43	12	306	A86	C35-C34	2.19	1.55	1.51
38	C	520	DGD	O3E-C3E	-2.19	1.37	1.43
31	b	605	CLA	C4B-NB	2.19	1.40	1.37
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
45	13	309	KC2	C1D-C2D	2.18	1.48	1.43
44	p	612	DD6	C36-C31	-2.18	1.32	1.34
31	18	309	CLA	C1B-C2B	2.18	1.48	1.43
31	10	316	CLA	CMD-C2D	-2.18	1.46	1.50
31	B	606	CLA	C3B-C4B	2.18	1.47	1.42
31	B	602	CLA	CMD-C2D	-2.18	1.46	1.50
31	b	613	CLA	C1B-C2B	2.18	1.48	1.43
37	D	404	LMG	O6-C1	2.18	1.47	1.41
31	2	311	CLA	MG-ND	-2.18	2.01	2.05
31	16	308	CLA	C1B-C2B	2.18	1.48	1.43
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	10	308	CLA	C1B-NB	-2.18	1.35	1.37
42	9	314	KC1	C1D-ND	-2.18	1.35	1.37
31	z	101	CLA	C1B-NB	-2.18	1.35	1.37
31	p	608	CLA	CMB-C2B	-2.18	1.46	1.50
31	16	313	CLA	C1A-CHA	-2.18	1.34	1.43
31	p	605	CLA	CMD-C2D	-2.18	1.46	1.50
45	9	309	KC2	C1D-C2D	2.18	1.48	1.43
33	H	101	BCR	C33-C5	-2.18	1.47	1.50
31	13	308	CLA	CHC-C1C	2.18	1.42	1.38
31	10	309	CLA	CMC-C2C	-2.18	1.46	1.50
31	C	502	CLA	CMB-C2B	-2.18	1.46	1.50
45	12	309	KC2	C1D-C2D	2.18	1.48	1.43
43	19	303	A86	C35-C34	2.18	1.55	1.51
37	p	614	LMG	O7-C8	-2.18	1.41	1.46
31	0	308	CLA	MG-NB	-2.18	2.01	2.05
31	10	311	CLA	CMD-C2D	-2.18	1.46	1.50
43	16	304	A86	C5-C6	-2.18	1.32	1.35
31	13	312	CLA	CMD-C2D	-2.18	1.46	1.50
31	B	601	CLA	MG-ND	-2.18	2.01	2.05
45	19	309	KC2	C1D-C2D	2.18	1.48	1.43
31	4	314	CLA	CMB-C2B	-2.18	1.46	1.50
43	17	301	A86	C30-C29	-2.18	1.28	1.32
31	0	312	CLA	CMB-C2B	-2.18	1.46	1.50
43	1	320	A86	C35-C34	2.18	1.55	1.51
31	19	315	CLA	CMC-C2C	-2.17	1.46	1.50
38	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
45	15	310	KC2	C4D-ND	2.17	1.40	1.37
31	P	601	CLA	CMB-C2B	-2.17	1.46	1.50
31	Z	101	CLA	C1B-NB	-2.17	1.35	1.37
31	6	308	CLA	CMB-C2B	-2.17	1.46	1.50
31	P	602	CLA	CHC-C1C	2.17	1.42	1.38
31	19	312	CLA	MG-ND	-2.17	2.01	2.05
31	5	307	CLA	CMC-C2C	-2.17	1.46	1.50
31	6	309	CLA	CMB-C2B	-2.17	1.46	1.50
31	16	308	CLA	CMB-C2B	-2.17	1.46	1.50
31	A	403	CLA	C4B-NB	2.17	1.40	1.37
31	A	406	CLA	CMB-C2B	-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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	1	314	KC1	C4A-C3A	2.17	1.48	1.44
31	9	313	CLA	C4B-NB	2.17	1.40	1.37
31	0	311	CLA	CMD-C2D	-2.17	1.46	1.50
35	d	407	PL9	C35-C34	-2.17	1.45	1.50
31	C	512	CLA	C3B-C4B	2.17	1.47	1.42
31	B	602	CLA	MG-NB	-2.17	2.01	2.05
31	10	314	CLA	MG-ND	-2.17	2.01	2.05
31	16	308	CLA	CHC-C1C	2.17	1.42	1.38
31	p	601	CLA	CMB-C2B	-2.17	1.46	1.50
31	b	607	CLA	MG-ND	-2.17	2.01	2.05
42	17	314	KC1	C1D-C2D	2.17	1.48	1.43
43	8	302	A86	C5-C6	-2.17	1.32	1.35
31	10	316	CLA	C1B-C2B	2.17	1.48	1.43
31	P	604	CLA	CHC-C1C	2.17	1.42	1.38
43	3	304	A86	C13-C11	-2.17	1.45	1.49
31	B	613	CLA	CMB-C2B	-2.17	1.46	1.50
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	D	402	CLA	C3B-C4B	2.17	1.47	1.42
37	10	319	LMG	C3-C2	2.17	1.57	1.52
31	c	502	CLA	C1B-NB	-2.17	1.35	1.37
42	14	313	KC1	C1B-NB	-2.17	1.35	1.37
31	14	314	CLA	CMD-C2D	-2.17	1.46	1.50
45	17	311	KC2	C1D-ND	-2.16	1.35	1.37
37	d	404	LMG	O6-C1	2.16	1.47	1.41
31	b	607	CLA	C3B-C4B	2.16	1.47	1.42
43	14	305	A86	C17-C18	-2.16	1.49	1.52
31	p	603	CLA	C1B-NB	-2.16	1.35	1.37
31	C	508	CLA	C3B-C4B	2.16	1.47	1.42
31	4	315	CLA	MG-NB	-2.16	2.01	2.05
31	C	512	CLA	C1B-C2B	2.16	1.48	1.43
31	c	512	CLA	C1B-C2B	2.16	1.48	1.43
38	c	518	DGD	O4E-C4E	-2.16	1.37	1.43
33	h	101	BCR	C33-C5	-2.16	1.47	1.50
31	2	307	CLA	C1D-ND	2.16	1.40	1.37
38	C	518	DGD	O4E-C4E	-2.16	1.37	1.43
31	C	505	CLA	MG-ND	-2.16	2.01	2.05
31	c	505	CLA	MG-ND	-2.16	2.01	2.05
31	10	316	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	518	DGD	O6D-C5D	-2.16	1.39	1.44
31	C	507	CLA	CMD-C2D	-2.16	1.46	1.50
31	3	307	CLA	CMB-C2B	-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
31	19	308	CLA	MG-NB	-2.16	2.01	2.05
37	d	404	LMG	C7-C8	2.16	1.57	1.50
31	b	602	CLA	C1B-C2B	2.16	1.48	1.43
43	13	304	A86	O4-C34	-2.16	1.41	1.46
43	14	305	A86	C5-C6	-2.16	1.32	1.35
31	13	315	CLA	CMB-C2B	-2.16	1.46	1.50
31	13	315	CLA	CMD-C2D	-2.16	1.46	1.50
31	C	506	CLA	C1B-NB	-2.16	1.35	1.37
31	c	506	CLA	C1B-NB	-2.16	1.35	1.37
42	12	314	KC1	C1D-ND	-2.16	1.35	1.37
38	b	622	DGD	C6E-C5E	2.16	1.59	1.51
31	0	309	CLA	MG-ND	-2.15	2.01	2.05
38	C	518	DGD	O3G-C1D	-2.15	1.36	1.40
31	12	307	CLA	CMD-C2D	-2.15	1.46	1.50
31	14	314	CLA	CMB-C2B	-2.15	1.46	1.50
38	C	520	DGD	O2D-C2D	-2.15	1.37	1.43
31	B	606	CLA	MG-ND	-2.15	2.01	2.05
31	W	202	CLA	C1B-C2B	2.15	1.48	1.43
43	P	611	A86	C2-C1	-2.15	1.32	1.35
38	C	519	DGD	O3G-C3G	-2.15	1.39	1.43
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
38	C	519	DGD	O6E-C5E	-2.15	1.39	1.44
38	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	1	312	CLA	C1B-NB	-2.15	1.35	1.37
31	d	402	CLA	C3B-C4B	2.15	1.47	1.42
42	11	314	KC1	C1A-CHA	2.15	1.46	1.40
35	D	407	PL9	C35-C34	-2.15	1.45	1.50
45	4	310	KC2	C4B-NB	-2.15	1.35	1.37
37	B	620	LMG	C4-C5	2.15	1.57	1.53
31	z	101	CLA	MG-ND	-2.15	2.01	2.05
31	10	309	CLA	C1B-C2B	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	304	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	2	307	CLA	C1B-C2B	2.15	1.48	1.43
31	17	315	CLA	MG-NB	-2.15	2.01	2.05
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	14	312	CLA	CHC-C1C	2.15	1.42	1.38
31	a	406	CLA	CMB-C2B	-2.15	1.46	1.50
31	d	406	CLA	CMC-C2C	-2.15	1.46	1.50
31	3	310	CLA	MG-NB	-2.15	2.01	2.05
31	14	314	CLA	MG-NB	-2.15	2.01	2.05
31	d	402	CLA	C4B-NB	2.15	1.40	1.37
42	14	313	KC1	C4C-C3C	2.15	1.48	1.45
31	19	310	CLA	CHC-C1C	2.15	1.42	1.38
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
45	8	311	KC2	C3C-C4C	2.15	1.49	1.44
31	9	308	CLA	MG-NB	-2.15	2.01	2.05
31	15	312	CLA	MG-ND	-2.15	2.01	2.05
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	B	601	CLA	C1B-C2B	2.15	1.48	1.43
31	p	602	CLA	CHC-C1C	2.15	1.42	1.38
31	8	307	CLA	MG-ND	-2.14	2.01	2.05
31	P	603	CLA	C1B-NB	-2.14	1.35	1.37
31	C	510	CLA	MG-ND	-2.14	2.01	2.05
45	0	310	KC2	C4A-C3A	2.14	1.48	1.44
31	C	504	CLA	CMB-C2B	-2.14	1.46	1.50
31	c	504	CLA	CMB-C2B	-2.14	1.46	1.50
42	17	314	KC1	C1D-ND	-2.14	1.35	1.37
43	14	302	A86	C32-C31	-2.14	1.51	1.54
31	a	404	CLA	C1B-NB	-2.14	1.35	1.37
31	10	311	CLA	C1B-NB	-2.14	1.35	1.37
37	5	315	LMG	C1-C2	2.14	1.58	1.52
31	18	309	CLA	CMD-C2D	-2.14	1.46	1.50
31	0	314	CLA	CHC-C1C	2.14	1.42	1.38
31	1	321	CLA	CMB-C2B	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	318	DGD	C4E-C5E	2.14	1.57	1.53
31	0	311	CLA	CMC-C2C	-2.14	1.46	1.50
31	p	604	CLA	CHC-C1C	2.14	1.42	1.38
31	11	315	CLA	C4C-C3C	2.14	1.48	1.45
31	5	307	CLA	C1B-NB	-2.14	1.35	1.37
31	14	307	CLA	MG-ND	-2.14	2.01	2.05
31	8	313	CLA	CMC-C2C	-2.14	1.46	1.50
31	10	314	CLA	MG-NB	-2.14	2.01	2.05
31	4	307	CLA	C1B-C2B	2.14	1.48	1.43
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
31	4	311	CLA	MG-NB	-2.14	2.01	2.05
37	P	614	LMG	O7-C8	-2.14	1.41	1.46
31	17	313	CLA	C1D-ND	2.14	1.40	1.37
31	12	307	CLA	CHC-C1C	2.14	1.42	1.38
38	c	520	DGD	O2D-C2D	-2.13	1.37	1.43
31	B	612	CLA	CMB-C2B	-2.13	1.46	1.50
31	b	613	CLA	CMB-C2B	-2.13	1.46	1.50
31	1	310	CLA	CMC-C2C	-2.13	1.46	1.50
31	2	307	CLA	CMB-C2B	-2.13	1.46	1.50
31	w	203	CLA	C1B-C2B	2.13	1.48	1.43
31	11	308	CLA	MG-ND	-2.13	2.01	2.05
45	19	309	KC2	C4D-ND	2.13	1.40	1.37
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	310	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	10	317	CLA	C1B-C2B	2.13	1.48	1.43
45	9	309	KC2	C1D-ND	-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
45	8	311	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
31	9	310	CLA	CHC-C1C	2.13	1.42	1.38
31	c	508	CLA	C1B-C2B	2.13	1.48	1.43
31	D	406	CLA	CMC-C2C	-2.13	1.46	1.50
31	D	402	CLA	C4B-NB	2.13	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	7	302	A86	C13-C11	-2.13	1.45	1.49
38	c	518	DGD	O6D-C5D	-2.13	1.39	1.44
31	c	507	CLA	CMD-C2D	-2.13	1.46	1.50
31	0	312	CLA	MG-NB	-2.13	2.01	2.05
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
42	0	315	KC1	C1D-C2D	2.13	1.48	1.43
31	15	306	CLA	CMD-C2D	-2.13	1.46	1.50
31	19	313	CLA	CMC-C2C	-2.13	1.46	1.50
31	7	315	CLA	MG-NB	-2.13	2.01	2.05
34	A	411	SQD	O4-C4	-2.13	1.38	1.43
38	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	9	313	CLA	C1B-C2B	2.13	1.48	1.43
31	9	310	CLA	MG-NB	-2.13	2.01	2.05
34	a	408	SQD	O4-C4	-2.13	1.38	1.43
31	b	615	CLA	C1B-C2B	2.13	1.48	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
37	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	317	LHG	P-O6	2.13	1.67	1.59
45	3	311	KC2	C3C-C4C	2.13	1.49	1.44
31	19	312	CLA	CHC-C1C	2.13	1.42	1.38
31	9	312	CLA	MG-ND	-2.13	2.01	2.05
38	C	519	DGD	O6D-C5D	-2.13	1.39	1.44
43	17	301	A86	C26-C27	-2.12	1.33	1.35
31	P	603	CLA	C1B-C2B	2.12	1.48	1.43
43	17	305	A86	C14-C13	2.12	1.53	1.51
31	C	508	CLA	C1B-C2B	2.12	1.48	1.43
42	5	313	KC1	C1D-C2D	2.12	1.48	1.43
31	8	308	CLA	C1B-NB	-2.12	1.35	1.37
38	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	313	CLA	CMC-C2C	-2.12	1.46	1.50
43	5	303	A86	C17-C18	-2.12	1.49	1.52
31	14	315	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	307	CLA	C4B-NB	2.12	1.40	1.37
31	12	308	CLA	C1B-NB	-2.12	1.35	1.37
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
31	14	315	CLA	CMB-C2B	-2.12	1.46	1.50
31	16	315	CLA	CMD-C2D	-2.12	1.46	1.50
31	C	513	CLA	C1B-C2B	2.12	1.48	1.43
31	9	312	CLA	CHC-C1C	2.12	1.42	1.38
31	15	309	CLA	CMB-C2B	-2.12	1.46	1.50
31	12	316	CLA	CHC-C1C	2.12	1.42	1.38
43	8	306	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
45	15	310	KC2	C1A-CHA	2.12	1.46	1.40
31	C	511	CLA	MG-ND	-2.12	2.01	2.05
31	17	308	CLA	C1B-C2B	2.12	1.48	1.43
31	Z	101	CLA	CMC-C2C	-2.12	1.46	1.50
31	14	314	CLA	C1B-C2B	2.12	1.48	1.43
31	C	513	CLA	CMB-C2B	-2.12	1.46	1.50
42	19	314	KC1	C1D-ND	-2.12	1.35	1.37
37	w	201	LMG	C7-C8	2.12	1.57	1.50
42	14	313	KC1	C1D-ND	-2.12	1.35	1.37
31	B	609	CLA	CMC-C2C	-2.12	1.46	1.50
38	W	203	DGD	C4D-C3D	2.12	1.57	1.52
31	17	315	CLA	CMD-C2D	-2.11	1.46	1.50
31	10	311	CLA	C1B-C2B	2.11	1.48	1.43
31	14	306	CLA	CMB-C2B	-2.11	1.46	1.50
31	7	308	CLA	C1B-C2B	2.11	1.48	1.43
43	5	305	A86	C5-C6	-2.11	1.33	1.35
31	16	307	CLA	CMB-C2B	-2.11	1.46	1.50
31	3	313	CLA	C1B-NB	-2.11	1.35	1.37
34	A	411	SQD	O3-C3	-2.11	1.38	1.43
31	13	307	CLA	CMB-C2B	-2.11	1.46	1.50
31	17	313	CLA	CMC-C2C	-2.11	1.46	1.50
31	19	308	CLA	CMD-C2D	-2.11	1.46	1.50
31	15	307	CLA	C1B-NB	-2.11	1.35	1.37
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	11	316	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	18	306	CLA	CMD-C2D	-2.11	1.46	1.50
37	f	102	LMG	O4-C4	-2.11	1.38	1.43
31	3	315	CLA	MG-NB	-2.11	2.01	2.05
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	D	402	CLA	CAC-C3C	-2.11	1.45	1.51
31	8	307	CLA	CMC-C2C	-2.11	1.46	1.50
42	9	314	KC1	C3B-C4B	2.11	1.49	1.46
31	7	310	CLA	CHC-C1C	2.11	1.42	1.38
31	0	311	CLA	C1B-C2B	2.11	1.48	1.43
37	B	620	LMG	O4-C4	-2.11	1.38	1.43
31	C	514	CLA	C1B-NB	-2.11	1.35	1.37
31	b	607	CLA	C4B-NB	2.11	1.40	1.37
37	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	311	KC2	C3C-C4C	2.11	1.49	1.44
31	C	509	CLA	CHC-C1C	2.11	1.42	1.38
31	c	509	CLA	CHC-C1C	2.11	1.42	1.38
31	3	310	CLA	CHC-C1C	2.11	1.42	1.38
31	c	510	CLA	MG-ND	-2.11	2.01	2.05
38	H	102	DGD	O4D-C4D	-2.11	1.38	1.43
31	14	311	CLA	CHC-C1C	2.11	1.42	1.38
31	15	309	CLA	MG-ND	-2.11	2.01	2.05
31	b	613	CLA	CMA-C3A	-2.10	1.48	1.53
37	W	201	LMG	C7-C8	2.10	1.57	1.50
43	7	304	A86	C14-C13	2.10	1.53	1.51
31	p	604	CLA	CMB-C2B	-2.10	1.46	1.50
31	b	612	CLA	CAC-C3C	-2.10	1.45	1.51
31	B	602	CLA	C4B-NB	2.10	1.40	1.37
31	P	604	CLA	CMB-C2B	-2.10	1.46	1.50
34	L	102	SQD	O3-C3	-2.10	1.38	1.43
31	8	307	CLA	CMD-C2D	-2.10	1.46	1.50
31	11	310	CLA	CMC-C2C	-2.10	1.46	1.50
31	B	606	CLA	CAC-C3C	-2.10	1.45	1.51
43	0	303	A86	C37-C36	-2.10	1.49	1.52
45	13	311	KC2	C4D-ND	2.10	1.40	1.37
31	z	103	CLA	C1B-C2B	2.10	1.48	1.43
31	0	309	CLA	C1B-C2B	2.10	1.48	1.43
36	C	521	LHG	O7-C5	-2.10	1.41	1.46
36	w	202	LHG	O7-C5	-2.10	1.41	1.46
31	b	602	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	L	102	SQD	O4-C4	-2.10	1.38	1.43
31	17	312	CLA	CHC-C1C	2.10	1.42	1.38
31	b	611	CLA	MG-ND	-2.10	2.01	2.05
45	12	311	KC2	C1D-ND	-2.10	1.35	1.37
31	10	309	CLA	CMD-C2D	-2.10	1.46	1.50
38	c	519	DGD	O3G-C3G	-2.10	1.39	1.43
31	10	311	CLA	CMB-C2B	-2.10	1.46	1.50
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	6	313	CLA	CHC-C1C	2.10	1.42	1.38
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	306	CLA	MG-NB	-2.10	2.01	2.05
31	19	310	CLA	MG-NB	-2.10	2.01	2.05
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	3	307	CLA	MG-NB	-2.10	2.01	2.05
42	0	315	KC1	C4D-ND	2.09	1.40	1.37
31	P	610	CLA	CMB-C2B	-2.09	1.46	1.50
45	11	309	KC2	C1D-C2D	2.09	1.48	1.43
31	15	313	CLA	MG-NB	-2.09	2.01	2.05
31	c	503	CLA	CMC-C2C	-2.09	1.46	1.50
31	0	308	CLA	C1B-NB	-2.09	1.35	1.37
31	p	604	CLA	MG-ND	-2.09	2.01	2.05
31	0	311	CLA	CMB-C2B	-2.09	1.46	1.50
43	15	303	A86	C17-C18	-2.09	1.49	1.52
45	11	309	KC2	C1A-CHA	2.09	1.46	1.40
31	16	312	CLA	CHC-C1C	2.09	1.42	1.38
42	19	314	KC1	C4C-C3C	2.09	1.48	1.45
43	8	304	A86	C5-C6	-2.09	1.33	1.35
38	c	519	DGD	O6D-C5D	-2.09	1.39	1.44
31	8	310	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
31	17	308	CLA	CMB-C2B	-2.09	1.46	1.50
45	8	309	KC2	O2A-CGA	-2.09	1.24	1.30
31	P	610	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	16	309	KC2	C4B-NB	-2.09	1.35	1.37
31	7	308	CLA	CMB-C2B	-2.09	1.46	1.50
42	4	313	KC1	C4C-C3C	2.09	1.48	1.45
31	B	614	CLA	C1B-C2B	2.09	1.48	1.43
31	10	312	CLA	CMB-C2B	-2.09	1.46	1.50
43	14	304	A86	C32-C31	-2.09	1.51	1.54
37	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	p	610	CLA	CHC-C1C	2.09	1.42	1.38
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
37	F	102	LMG	O3-C3	-2.09	1.38	1.43
31	p	603	CLA	C1B-C2B	2.09	1.48	1.43
31	4	314	CLA	C1B-C2B	2.09	1.48	1.43
45	12	311	KC2	C1D-C2D	2.09	1.48	1.43
31	d	402	CLA	CAC-C3C	-2.09	1.45	1.51
37	5	315	LMG	O7-C8	-2.09	1.41	1.46
38	w	204	DGD	C4D-C3D	2.09	1.57	1.52
31	0	307	CLA	CMC-C2C	-2.09	1.46	1.50
31	B	606	CLA	C4B-NB	2.09	1.40	1.37
31	9	315	CLA	MG-NB	-2.09	2.01	2.05
45	5	310	KC2	O2A-CGA	-2.09	1.24	1.30
31	B	601	CLA	CMB-C2B	-2.09	1.46	1.50
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	5	309	CLA	CMB-C2B	-2.09	1.46	1.50
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	18	314	CLA	C1B-NB	-2.08	1.35	1.37
31	b	609	CLA	CMC-C2C	-2.08	1.46	1.50
36	18	316	LHG	P-O6	2.08	1.67	1.59
31	19	315	CLA	MG-NB	-2.08	2.01	2.05
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
45	2	310	KC2	C1D-C2D	2.08	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	604	CLA	CMA-C3A	-2.08	1.48	1.53
31	2	309	CLA	CMC-C2C	-2.08	1.46	1.50
38	B	621	DGD	C4E-C3E	2.08	1.57	1.52
45	19	309	KC2	C1D-ND	-2.08	1.35	1.37
31	0	314	CLA	CMB-C2B	-2.08	1.46	1.50
43	6	305	A86	C40-C32	-2.08	1.49	1.53
31	10	312	CLA	MG-NB	-2.08	2.01	2.05
34	B	623	SQD	O3-C3	-2.08	1.38	1.43
37	N	101	LMG	O4-C4	-2.08	1.38	1.43
37	15	314	LMG	C9-C8	2.08	1.57	1.50
31	0	312	CLA	CHC-C1C	2.08	1.42	1.38
31	C	511	CLA	CMB-C2B	-2.08	1.46	1.50
31	c	511	CLA	CMB-C2B	-2.08	1.46	1.50
31	4	314	CLA	CMC-C2C	-2.08	1.46	1.50
31	c	513	CLA	C1B-C2B	2.08	1.48	1.43
45	18	308	KC2	C1D-C2D	2.08	1.48	1.43
31	14	312	CLA	CMC-C2C	-2.08	1.46	1.50
31	18	307	CLA	CHC-C1C	2.08	1.42	1.38
31	p	610	CLA	CMB-C2B	-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
31	18	312	CLA	C1B-NB	-2.08	1.35	1.37
45	14	308	KC2	C1D-C2D	2.08	1.48	1.43
34	b	601	SQD	O3-C3	-2.08	1.38	1.43
38	11	318	DGD	O2G-C2G	-2.08	1.41	1.46
45	6	312	KC2	C1D-C2D	2.08	1.48	1.43
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	2	314	CLA	CMB-C2B	-2.08	1.46	1.50
31	c	513	CLA	C4B-NB	2.08	1.40	1.37
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	C	505	CLA	C1B-NB	-2.07	1.35	1.37
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	306	A86	C33-C34	2.07	1.55	1.51
31	3	308	CLA	MG-ND	-2.07	2.01	2.05
31	3	308	CLA	CMB-C2B	-2.07	1.46	1.50
35	A	409	PL9	C53-C6	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	16	311	KC2	C1D-C2D	2.07	1.48	1.43
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
37	n	701	LMG	O4-C4	-2.07	1.38	1.43
31	c	506	CLA	MG-ND	-2.07	2.01	2.05
31	13	313	CLA	CMA-C3A	-2.07	1.48	1.53
38	B	621	DGD	O2D-C2D	-2.07	1.38	1.43
43	0	303	A86	C32-C31	-2.07	1.51	1.54
31	12	316	CLA	CMB-C2B	-2.07	1.46	1.50
31	P	602	CLA	C1B-NB	-2.07	1.35	1.37
43	p	611	A86	C2-C1	-2.07	1.33	1.35
43	14	305	A86	C33-C34	2.07	1.55	1.51
31	7	315	CLA	CMB-C2B	-2.07	1.46	1.50
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	p	602	CLA	C1B-NB	-2.07	1.35	1.37
42	19	314	KC1	C1B-NB	-2.07	1.35	1.37
31	3	315	CLA	CMB-C2B	-2.07	1.46	1.50
31	16	308	CLA	CMC-C2C	-2.07	1.46	1.50
31	18	306	CLA	C1B-C2B	2.07	1.48	1.43
31	13	312	CLA	MG-NB	-2.07	2.01	2.05
38	W	203	DGD	O1G-C1G	-2.07	1.40	1.45
31	c	513	CLA	CMB-C2B	-2.07	1.46	1.50
37	Z	102	LMG	O1-C1	2.07	1.43	1.40
31	16	307	CLA	MG-NB	-2.07	2.01	2.05
31	B	608	CLA	CMC-C2C	-2.07	1.46	1.50
43	P	613	A86	C13-C11	-2.07	1.45	1.49
37	w	201	LMG	O2-C2	-2.07	1.38	1.43
31	b	603	CLA	C4B-NB	2.07	1.40	1.37
31	10	308	CLA	MG-NB	-2.07	2.01	2.05
43	10	303	A86	C37-C36	-2.07	1.49	1.52
42	8	314	KC1	O2A-CGA	-2.07	1.24	1.30
31	C	514	CLA	CMB-C2B	-2.07	1.46	1.50
31	6	316	CLA	CMB-C2B	-2.07	1.46	1.50
37	n	701	LMG	C4-C5	2.07	1.57	1.53
31	5	311	CLA	CHC-C4B	-2.07	1.34	1.39
31	14	311	CLA	MG-ND	-2.07	2.01	2.05
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
37	N	101	LMG	C4-C5	2.06	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	18	311	CLA	C1B-C2B	2.06	1.48	1.43
31	7	312	CLA	CHC-C1C	2.06	1.42	1.38
31	0	307	CLA	CHC-C1C	2.06	1.42	1.38
31	7	307	CLA	MG-NB	-2.06	2.01	2.05
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	13	313	CLA	CMB-C2B	-2.06	1.46	1.50
31	13	316	CLA	CMD-C2D	-2.06	1.46	1.50
31	4	315	CLA	CMA-C3A	-2.06	1.48	1.53
42	18	313	KC1	C1A-CHA	2.06	1.46	1.40
38	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	14	307	CLA	CHC-C1C	2.06	1.42	1.38
31	17	310	CLA	CHC-C1C	2.06	1.42	1.38
31	10	317	CLA	CMC-C2C	-2.06	1.46	1.50
31	10	309	CLA	C1B-NB	-2.06	1.35	1.37
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	2	314	CLA	MG-NB	-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
37	c	522	LMG	C1-C2	2.06	1.58	1.52
37	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
31	14	315	CLA	MG-NB	-2.06	2.01	2.05
31	15	313	CLA	CHC-C1C	2.06	1.42	1.38
45	6	310	KC2	C4B-NB	-2.06	1.35	1.37
31	7	307	CLA	CMB-C2B	-2.06	1.46	1.50
45	4	308	KC2	C1D-C2D	2.06	1.48	1.43
31	0	316	CLA	CHC-C1C	2.06	1.42	1.38
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
31	b	607	CLA	C1B-NB	-2.06	1.35	1.37
42	0	315	KC1	C1A-CHA	2.06	1.46	1.40
36	4	317	LHG	P-O6	2.05	1.67	1.59
34	8	301	SQD	O3-C3	-2.05	1.38	1.43
31	13	313	CLA	C1A-CHA	-2.05	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
37	F	102	LMG	O4-C4	-2.05	1.38	1.43
45	15	310	KC2	C4A-C3A	2.05	1.48	1.44
37	W	201	LMG	O2-C2	-2.05	1.38	1.43
31	13	310	CLA	CHC-C1C	2.05	1.42	1.38
38	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	5	306	CLA	CMD-C2D	-2.05	1.46	1.50
31	c	514	CLA	CHC-C1C	2.05	1.42	1.38
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	P	604	CLA	C1B-C2B	2.05	1.48	1.43
31	16	308	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
31	p	608	CLA	C1B-NB	-2.05	1.35	1.37
31	10	314	CLA	CHC-C1C	2.05	1.42	1.38
37	5	315	LMG	O4-C4	-2.05	1.38	1.43
45	17	311	KC2	C1D-C2D	2.05	1.48	1.43
31	b	607	CLA	CAC-C3C	-2.05	1.45	1.51
45	7	311	KC2	C1D-C2D	2.05	1.48	1.43
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	A	406	CLA	CHC-C1C	2.04	1.42	1.38
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	313	CLA	C1A-CHA	-2.04	1.34	1.43
31	4	307	CLA	CHC-C1C	2.04	1.42	1.38
31	10	312	CLA	CHC-C1C	2.04	1.42	1.38
33	a	407	BCR	C38-C26	-2.04	1.47	1.50
31	d	406	CLA	MG-ND	-2.04	2.01	2.05
31	C	506	CLA	CHC-C1C	2.04	1.42	1.38
38	h	102	DGD	O2G-C2G	-2.04	1.41	1.46
31	11	310	CLA	CMB-C2B	-2.04	1.46	1.50
43	1	303	A86	O4-C34	-2.04	1.41	1.46
31	17	312	CLA	CMB-C2B	-2.04	1.46	1.50
43	6	304	A86	C5-C6	-2.04	1.33	1.35
31	18	309	CLA	MG-ND	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	621	LMG	C4-C5	2.04	1.57	1.53
31	10	314	CLA	CMB-C2B	-2.04	1.46	1.50
31	C	514	CLA	CHC-C1C	2.04	1.42	1.38
31	8	308	CLA	CHC-C1C	2.04	1.42	1.38
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	15	317	KC1	C4C-C3C	2.04	1.48	1.45
43	6	305	A86	C13-C11	-2.04	1.45	1.49
42	5	313	KC1	C4D-ND	2.04	1.40	1.37
31	C	506	CLA	CMB-C2B	-2.04	1.46	1.50
31	7	312	CLA	CMB-C2B	-2.04	1.46	1.50
31	17	312	CLA	MG-ND	-2.04	2.01	2.05
43	10	303	A86	C32-C31	-2.04	1.51	1.54
38	H	102	DGD	O2G-C2G	-2.04	1.41	1.46
42	14	313	KC1	C1D-C2D	2.04	1.48	1.43
31	18	314	CLA	MG-ND	-2.04	2.01	2.05
37	F	102	LMG	O2-C2	-2.04	1.38	1.43
31	c	506	CLA	CHC-C1C	2.04	1.42	1.38
38	C	520	DGD	O4E-C4E	-2.04	1.38	1.43
38	c	520	DGD	O4E-C4E	-2.04	1.38	1.43
42	3	314	KC1	C1C-C2C	2.04	1.48	1.44
31	b	605	CLA	C1C-NC	-2.03	1.34	1.37
31	b	606	CLA	C3B-C4B	2.03	1.47	1.42
31	16	310	CLA	CMD-C2D	-2.03	1.46	1.50
43	3	305	A86	C35-C34	2.03	1.55	1.51
31	B	612	CLA	C4B-NB	2.03	1.40	1.37
31	P	605	CLA	CMB-C2B	-2.03	1.46	1.50
31	1	307	CLA	CMB-C2B	-2.03	1.46	1.50
43	17	301	A86	C37-C36	-2.03	1.49	1.52
45	10	310	KC2	C1D-C2D	2.03	1.48	1.43
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	605	CLA	C3B-C4B	2.03	1.47	1.42
31	b	606	CLA	MG-ND	-2.03	2.01	2.05
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	p	605	CLA	CMB-C2B	-2.03	1.46	1.50
37	Z	102	LMG	C1-C2	2.03	1.58	1.52
38	b	622	DGD	O2D-C2D	-2.03	1.38	1.43
43	16	306	A86	O3-C36	2.03	1.46	1.43
31	C	506	CLA	MG-ND	-2.03	2.01	2.05
42	1	314	KC1	C4C-C3C	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	306	CLA	CMB-C2B	-2.03	1.46	1.50
31	17	315	CLA	CMB-C2B	-2.03	1.46	1.50
31	8	308	CLA	CMA-C3A	-2.03	1.48	1.53
31	19	307	CLA	CMD-C2D	-2.03	1.46	1.50
31	5	314	CLA	CMB-C2B	-2.03	1.46	1.50
31	6	309	CLA	CMC-C2C	-2.03	1.46	1.50
31	12	310	CLA	CHC-C1C	2.03	1.42	1.38
33	A	407	BCR	C38-C26	-2.03	1.47	1.50
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	B	605	CLA	MG-ND	-2.03	2.01	2.05
31	0	308	CLA	CMB-C2B	-2.03	1.46	1.50
31	1	310	CLA	CMB-C2B	-2.03	1.46	1.50
31	18	306	CLA	CMC-C2C	-2.03	1.46	1.50
31	b	606	CLA	CAC-C3C	-2.03	1.45	1.51
31	2	315	CLA	CHD-C1D	-2.03	1.34	1.38
37	d	409	LMG	O1-C7	-2.03	1.40	1.43
31	13	307	CLA	MG-NB	-2.03	2.01	2.05
31	18	306	CLA	CMB-C2B	-2.03	1.46	1.50
31	C	513	CLA	C4B-NB	2.03	1.40	1.37
31	c	514	CLA	CMB-C2B	-2.02	1.46	1.50
43	12	306	A86	C5-C6	-2.02	1.33	1.35
31	19	311	CLA	CMD-C2D	-2.02	1.46	1.50
31	2	311	CLA	CHC-C1C	2.02	1.42	1.38
31	4	311	CLA	CHC-C1C	2.02	1.42	1.38
31	15	313	CLA	CMB-C2B	-2.02	1.46	1.50
31	0	313	CLA	CHC-C1C	2.02	1.42	1.38
31	17	307	CLA	CMB-C2B	-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
45	5	308	KC2	C1D-C2D	2.02	1.48	1.43
43	4	303	A86	C19-C18	2.02	1.55	1.52
45	16	309	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
31	p	604	CLA	C1B-C2B	2.02	1.48	1.43
31	c	506	CLA	CMB-C2B	-2.02	1.46	1.50
31	B	601	CLA	C1B-NB	-2.02	1.35	1.37
36	14	317	LHG	P-O6	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	307	CLA	CMD-C2D	-2.02	1.46	1.50
45	15	308	KC2	C1D-C2D	2.02	1.48	1.43
31	8	315	CLA	CMC-C2C	-2.02	1.46	1.50
31	a	406	CLA	C4B-NB	2.02	1.40	1.37
31	B	610	CLA	MG-ND	-2.02	2.01	2.05
31	3	315	CLA	CMD-C2D	-2.02	1.46	1.50
42	9	314	KC1	C1C-C2C	2.02	1.48	1.44
31	c	505	CLA	C1B-NB	-2.02	1.35	1.37
37	B	620	LMG	O8-C9	-2.02	1.40	1.45
37	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
42	6	315	KC1	C1A-CHA	2.02	1.45	1.40
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
37	b	621	LMG	O8-C9	-2.02	1.40	1.45
37	f	102	LMG	O2-C2	-2.02	1.38	1.43
31	8	315	CLA	MG-ND	-2.02	2.01	2.05
45	4	310	KC2	C4D-ND	2.02	1.40	1.37
45	4	310	KC2	C1D-C2D	2.02	1.48	1.43
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
31	P	608	CLA	C1B-NB	-2.02	1.35	1.37
38	W	203	DGD	C1D-C2D	2.02	1.58	1.52
34	a	408	SQD	O47-C45	-2.02	1.41	1.46
31	b	611	CLA	C1B-C2B	2.02	1.48	1.43
31	19	311	CLA	CMC-C2C	-2.02	1.46	1.50
38	W	203	DGD	C6D-C5D	2.02	1.57	1.51
31	B	605	CLA	CAC-C3C	-2.02	1.45	1.51
31	3	312	CLA	CMB-C2B	-2.01	1.46	1.50
38	C	519	DGD	O4D-C4D	-2.01	1.38	1.43
38	c	519	DGD	O4D-C4D	-2.01	1.38	1.43
31	3	312	CLA	CHC-C1C	2.01	1.42	1.38
31	8	315	CLA	C1B-NB	-2.01	1.35	1.37
43	3	304	A86	C5-C6	-2.01	1.33	1.35
43	6	303	A86	C13-C11	-2.01	1.45	1.49
31	D	406	CLA	CHC-C1C	2.01	1.42	1.38
31	D	402	CLA	CHC-C4B	-2.01	1.34	1.39
43	6	304	A86	C26-C27	-2.01	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	8	316	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
43	11	302	A86	C13-C11	-2.01	1.45	1.49
31	4	315	CLA	CHC-C1C	2.01	1.42	1.38
31	19	307	CLA	MG-NB	-2.01	2.01	2.05
43	8	306	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	15	306	CLA	CMB-C2B	-2.01	1.46	1.50
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	P	604	CLA	C1B-NB	-2.01	1.35	1.37
31	12	313	CLA	C1D-ND	2.01	1.40	1.37
31	9	307	CLA	MG-NB	-2.01	2.01	2.05
45	14	310	KC2	C1D-C2D	2.01	1.48	1.43
31	b	616	CLA	CAC-C3C	-2.01	1.46	1.51
42	18	313	KC1	O2A-CGA	-2.01	1.25	1.30
37	c	522	LMG	O1-C1	2.01	1.43	1.40
31	19	313	CLA	C4B-NB	2.01	1.40	1.37
31	a	406	CLA	CHC-C1C	2.01	1.42	1.38
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	13	310	CLA	CMB-C2B	-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
31	b	613	CLA	C4B-NB	2.01	1.40	1.37
38	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
37	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	310	CLA	MG-ND	-2.00	2.01	2.05
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	p	609	KC1	O2A-CGA	-2.00	1.25	1.30
38	w	204	DGD	C1D-C2D	2.00	1.58	1.52
31	6	314	CLA	CMC-C2C	-2.00	1.46	1.50
31	13	316	CLA	MG-NB	-2.00	2.01	2.05
31	10	308	CLA	CMB-C2B	-2.00	1.46	1.50
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	15	317	KC1	C4B-NB	-2.00	1.35	1.37

All (8544) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	303	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	314	KC1	CMD-C2D-C1D	-23.89	88.98	125.37
42	6	315	KC1	C4D-C3D-CAD	22.82	122.80	107.42
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
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	305	A86	O1-C20-C19	-22.19	96.71	113.38
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
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	6	315	KC1	CMD-C2D-C1D	-20.77	93.73	125.37
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
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
43	12	304	A86	O1-C20-C19	20.62	128.87	113.38
43	8	305	A86	O1-C20-C19	20.36	128.67	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	3	314	KC1	CMD-C2D-C1D	-19.05	96.35	125.37
43	1	306	A86	O1-C20-C19	18.86	127.55	113.38
42	17	314	KC1	CMD-C2D-C1D	-18.81	96.72	125.37
42	5	313	KC1	CMD-C2D-C1D	18.60	153.69	125.37
43	19	302	A86	C28-C27-C26	-18.44	97.10	122.92
42	18	313	KC1	C4D-C3D-CAD	18.27	119.73	107.42
42	16	314	KC1	C4D-C3D-CAD	18.06	119.59	107.42
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
42	16	314	KC1	CMD-C2D-C1D	-16.90	99.63	125.37
43	P	611	A86	O1-C20-C21	-16.89	94.82	115.06
43	p	611	A86	O1-C20-C21	-16.85	94.86	115.06
42	18	313	KC1	CMD-C2D-C1D	-16.81	99.77	125.37
43	17	301	A86	C33-C32-C31	-16.67	93.01	109.21
45	14	308	KC2	CMD-C2D-C1D	-16.67	99.98	125.37
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
43	8	302	A86	C33-C32-C31	-16.11	93.55	109.21
45	4	308	KC2	CMD-C2D-C1D	-16.07	100.89	125.37
42	0	315	KC1	CMD-C2D-C1D	-16.05	100.93	125.37
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
43	6	301	A86	C33-C32-C31	-15.42	94.23	109.21
43	16	305	A86	O1-C20-C21	-15.31	96.72	115.06
43	15	305	A86	C40-C32-C31	15.29	124.16	110.47
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	8	311	KC2	CMD-C2D-C1D	-14.97	102.57	125.37
42	14	313	KC1	CMD-C2D-C1D	-14.95	102.61	125.37
43	14	305	A86	C33-C32-C31	-14.94	94.69	109.21
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})
43	1	319	A86	C33-C32-C31	-14.86	94.77	109.21
42	8	314	KC1	CMD-C2D-C3D	14.85	166.05	125.93
45	18	310	KC2	CMD-C2D-C1D	-14.83	102.78	125.37
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	3	309	KC2	CHD-C1D-ND	-14.72	108.68	124.26
45	2	308	KC2	CHD-C1D-ND	-14.64	108.76	124.26
43	1	303	A86	C33-C32-C31	-14.63	94.99	109.21
45	16	311	KC2	CMD-C2D-C1D	-14.61	103.12	125.37
43	10	303	A86	O1-C15-C14	-14.56	84.00	113.21
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	304	A86	O1-C15-C14	-14.45	84.21	113.21
43	16	304	A86	O1-C15-C14	-14.43	84.25	113.21
45	6	312	KC2	CMD-C2D-C1D	-14.42	103.40	125.37
43	10	306	A86	O1-C15-C14	-14.41	84.30	113.21
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
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	10	315	KC1	CMD-C2D-C1D	-14.15	103.82	125.37
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
45	3	311	KC2	CMD-C2D-C1D	-14.11	103.87	125.37
45	2	310	KC2	CMD-C2D-C1D	-14.11	103.88	125.37
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	6	310	KC2	CHD-C1D-ND	-13.99	109.45	124.26
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
43	1	302	A86	C33-C32-C31	-13.91	95.69	109.21
43	16	301	A86	O1-C15-C14	-13.91	85.30	113.21
43	19	303	A86	O1-C15-C14	-13.90	85.31	113.21
45	16	309	KC2	CHD-C1D-ND	-13.87	109.57	124.26
45	7	309	KC2	CHD-C1D-ND	-13.87	109.58	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	314	KC1	C4D-C3D-CAD	13.85	116.75	107.42
43	11	320	A86	O1-C15-C14	-13.84	85.43	113.21
43	19	302	A86	C33-C32-C31	-13.72	95.88	109.21
43	1	302	A86	C40-C32-C31	13.71	122.74	110.47
45	17	309	KC2	CHD-C1D-ND	-13.70	109.75	124.26
43	11	303	A86	C33-C32-C31	-13.69	95.90	109.21
42	4	313	KC1	CMD-C2D-C1D	-13.56	104.72	125.37
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
43	1	306	A86	O1-C15-C14	-13.31	86.50	113.21
45	13	311	KC2	CHD-C1D-ND	-13.30	110.17	124.26
45	7	311	KC2	CMD-C2D-C1D	-13.21	105.24	125.37
43	5	301	A86	C41-C32-C31	-13.18	98.68	110.47
45	9	309	KC2	CMD-C2D-C1D	-13.17	105.32	125.37
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
45	19	309	KC2	CMD-C2D-C1D	-13.10	105.42	125.37
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
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	314	KC1	C1A-C2A-C3A	-12.98	96.81	107.11
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
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
45	18	308	KC2	CHD-C1D-ND	-12.89	110.61	124.26
43	4	301	A86	O1-C20-C19	-12.88	103.71	113.38
43	16	301	A86	C33-C32-C31	-12.84	96.73	109.21
43	18	301	A86	O1-C15-C14	-12.81	87.51	113.21
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	10	310	KC2	CHC-C4B-NB	12.60	136.03	124.45
42	1	314	KC1	CMD-C2D-C1D	12.60	144.56	125.37
42	5	313	KC1	C1A-NA-C4A	-12.59	101.05	106.71
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
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
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	3	314	KC1	CMD-C2D-C3D	12.48	159.64	125.93
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
42	5	313	KC1	C1A-C2A-C3A	-12.43	97.24	107.11
42	17	314	KC1	CMD-C2D-C3D	12.43	159.49	125.93
43	7	302	A86	C23-C16-C22	-12.41	89.06	107.37
43	12	302	A86	C40-C32-C31	12.38	121.55	110.47
42	7	314	KC1	C4D-C3D-CAD	12.37	115.76	107.42
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	15	317	KC1	CHD-C1D-ND	-12.29	111.24	124.26
43	1	303	A86	C40-C32-C31	12.25	121.44	110.47
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
43	16	305	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
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
43	13	301	A86	O1-C15-C14	-12.08	88.96	113.21
43	11	303	A86	C40-C32-C31	12.05	121.26	110.47
43	19	305	A86	C23-C16-C22	-12.04	89.62	107.37
43	15	302	A86	O1-C15-C14	-12.02	89.09	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	8	309	KC2	CHD-C1D-ND	-12.01	111.54	124.26
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
42	13	314	KC1	CMD-C2D-C1D	11.99	143.63	125.37
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
42	6	315	KC1	CMD-C2D-C3D	11.97	158.25	125.93
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	14	308	KC2	CHD-C1D-ND	-11.84	111.72	124.26
45	4	308	KC2	CHD-C1D-ND	-11.84	111.72	124.26
42	16	314	KC1	C1A-NA-C4A	-11.83	101.39	106.71
43	8	302	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	311	KC2	CHC-C4B-NB	11.75	135.25	124.45
43	16	306	A86	C40-C32-C31	11.73	120.97	110.47
42	8	314	KC1	CHC-C4B-NB	11.72	135.23	124.45
43	7	304	A86	C21-C20-C19	-11.72	101.09	114.28
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
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
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
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
43	14	305	A86	O1-C15-C14	-11.57	89.99	113.21
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	5	308	KC2	CHD-C1D-ND	-11.46	112.12	124.26
43	11	304	A86	O1-C15-C14	-11.46	90.20	113.21
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	302	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
45	3	309	KC2	C4C-C3C-C2C	-11.30	98.14	107.11
45	8	309	KC2	C4C-C3C-C2C	-11.30	98.14	107.11
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	314	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
45	13	309	KC2	CHD-C1D-ND	-11.17	112.43	124.26
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
43	16	305	A86	O1-C15-C14	11.11	135.50	113.21
45	14	308	KC2	CMD-C2D-C3D	11.10	155.90	125.93
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
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
45	1	309	KC2	CHD-C1D-ND	-11.00	112.61	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	15	308	KC2	CHD-C1D-ND	-10.93	112.68	124.26
45	13	309	KC2	CHC-C4B-NB	10.93	134.50	124.45
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
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	306	A86	O1-C15-C14	-10.80	91.54	113.21
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
45	4	308	KC2	CMD-C2D-C3D	10.74	154.95	125.93
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	311	KC2	CHC-C4B-NB	10.71	134.29	124.45
43	8	306	A86	O1-C15-C14	-10.71	91.72	113.21
42	13	314	KC1	C1A-C2A-C3A	-10.71	98.61	107.11
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	309	KC2	CHC-C4B-NB	10.61	134.20	124.45
42	0	315	KC1	CMD-C2D-C3D	10.60	154.56	125.93
45	9	309	KC2	CHC-C4B-NB	10.60	134.19	124.45
42	15	317	KC1	C1A-C2A-C3A	-10.60	98.70	107.11
45	15	308	KC2	C1A-C2A-C3A	-10.59	98.70	107.11
42	8	314	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	CMD-C2D-C3D	10.55	154.43	125.93
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	309	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	5	310	KC2	CAB-C3B-C4B	10.47	150.18	124.90
42	6	315	KC1	C1D-ND-C4D	10.46	113.77	106.33
45	15	310	KC2	CHC-C4B-NB	10.46	134.06	124.45
42	17	314	KC1	CHD-C4C-C3C	-10.45	105.70	125.33
43	3	306	A86	O1-C15-C14	-10.45	92.23	113.21
42	14	313	KC1	CMD-C2D-C3D	10.45	154.15	125.93
45	15	310	KC2	CAB-C3B-C4B	10.44	150.11	124.90
45	18	310	KC2	CMD-C2D-C3D	10.43	154.11	125.93
45	8	311	KC2	CMD-C2D-C3D	10.43	154.10	125.93
42	5	313	KC1	CHC-C4B-NB	10.43	134.03	124.45
42	16	314	KC1	CMD-C2D-C3D	10.42	154.08	125.93
42	15	317	KC1	CHC-C4B-NB	10.41	134.02	124.45
42	8	314	KC1	CAB-C3B-C4B	10.39	149.99	124.90
43	8	303	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	311	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	16	311	KC2	CMD-C2D-C3D	10.20	153.49	125.93
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	10	315	KC1	CMD-C2D-C3D	10.14	153.31	125.93
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
45	6	312	KC2	CMD-C2D-C3D	10.07	153.14	125.93
42	11	314	KC1	CHD-C4C-C3C	-10.07	106.42	125.33
45	3	311	KC2	CMD-C2D-C3D	10.06	153.11	125.93
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
43	16	305	A86	C21-C20-C19	-10.05	102.97	114.28
42	4	313	KC1	CHD-C4C-C3C	-10.05	106.46	125.33
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
42	18	313	KC1	OBD-CAD-C3D	-10.05	104.34	128.52
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
45	4	310	KC2	CMD-C2D-C1D	-10.02	110.11	125.37
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
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	8	314	KC1	CHD-C1D-ND	-9.93	113.74	124.26
42	5	313	KC1	CMD-C2D-C3D	-9.93	99.09	125.93
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	2	310	KC2	CMD-C2D-C3D	9.88	152.62	125.93
45	17	311	KC2	C1A-C2A-C3A	-9.87	99.28	107.11
43	15	305	A86	O1-C20-C19	9.86	120.79	113.38
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
42	4	313	KC1	CMD-C2D-C3D	9.83	152.49	125.93
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	314	KC1	CAB-C3B-C4B	9.74	148.42	124.90
42	4	313	KC1	CAB-C3B-C4B	9.73	148.41	124.90
42	10	315	KC1	CHD-C1D-ND	-9.67	114.02	124.26
45	2	310	KC2	OBD-CAD-C3D	-9.67	105.26	128.52
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	18	313	KC1	CHD-C4C-C3C	-9.62	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
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	303	A86	O1-C20-C21	-9.59	103.57	115.06
45	14	310	KC2	CMD-C2D-C1D	-9.57	110.79	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	6	315	KC1	OBD-CAD-C3D	-9.57	105.48	128.52
45	16	309	KC2	CHB-C1B-NB	9.56	133.24	124.45
43	4	302	A86	O4-C34-C33	9.56	131.40	107.59
42	5	313	KC1	CHD-C4C-C3C	-9.56	107.39	125.33
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	7	311	KC2	CMD-C2D-C3D	9.52	151.66	125.93
45	1	311	KC2	C1A-C2A-C3A	-9.52	99.56	107.11
42	5	313	KC1	CHD-C1D-ND	-9.52	114.18	124.26
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
42	16	314	KC1	OBD-CAD-C3D	-9.47	105.73	128.52
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
45	0	310	KC2	CHB-C1B-NB	9.42	133.11	124.45
45	5	310	KC2	CHD-C1D-ND	-9.41	114.30	124.26
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	309	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	15	317	KC1	CAB-C3B-C4B	9.35	147.47	124.90
45	10	310	KC2	CHB-C1B-NB	9.35	133.04	124.45
45	14	310	KC2	OBD-CAD-C3D	-9.32	106.09	128.52
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
45	10	310	KC2	OBD-CAD-C3D	-9.31	106.11	128.52
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
45	10	310	KC2	CHD-C1D-ND	-9.27	114.45	124.26
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	4	310	KC2	OBD-CAD-C3D	-9.23	106.31	128.52
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
45	9	309	KC2	CMD-C2D-C3D	9.21	150.81	125.93
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
44	P	612	DD6	O1-C20-C19	9.18	120.28	113.38
43	8	302	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	309	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
45	2	308	KC2	C4C-C3C-C2C	-9.14	99.86	107.11
45	13	311	KC2	CHD-C4C-NC	-9.13	110.35	124.20
42	2	313	KC1	C4D-C3D-CAD	9.13	113.57	107.42
42	16	314	KC1	CHD-C4C-C3C	-9.13	108.19	125.33
42	13	314	KC1	CAB-C3B-C4B	9.13	146.94	124.90
45	3	309	KC2	C1D-ND-C4D	9.13	112.82	106.33
45	19	309	KC2	CMD-C2D-C3D	9.12	150.58	125.93
42	11	314	KC1	C1A-C2A-C3A	-9.12	99.87	107.11
42	15	317	KC1	CHD-C4C-C3C	-9.11	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
45	8	311	KC2	OBD-CAD-C3D	-9.10	106.63	128.52
43	16	304	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	7	311	KC2	OBD-CAD-C3D	-9.06	106.72	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	7	314	KC1	CHD-C4C-NC	9.02	137.89	124.20
45	6	312	KC2	C1A-C2A-C3A	-9.01	99.96	107.11
45	3	311	KC2	OBD-CAD-C3D	-9.00	106.86	128.52
43	0	302	A86	O1-C20-C19	8.99	120.14	113.38
45	8	311	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
42	2	313	KC1	OBD-CAD-C3D	-8.95	106.99	128.52
31	b	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
43	8	306	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
42	12	314	KC1	C4D-C3D-CAD	8.93	113.44	107.42
45	7	311	KC2	CHB-C1B-NB	8.92	132.66	124.45
42	2	313	KC1	CMD-C2D-C1D	-8.92	111.78	125.37
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	18	310	KC2	OBD-CAD-C3D	-8.91	107.08	128.52
42	3	314	KC1	OBD-CAD-C3D	-8.91	107.08	128.52
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
45	17	311	KC2	OBD-CAD-C3D	-8.87	107.18	128.52
42	18	313	KC1	C1D-ND-C4D	8.86	112.63	106.33
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	11	314	KC1	OBD-CAD-C3D	-8.82	107.28	128.52
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
42	8	314	KC1	OBD-CAD-C3D	-8.78	107.39	128.52
45	16	311	KC2	C1A-C2A-C3A	-8.77	100.15	107.11
45	2	308	KC2	C1D-ND-C4D	8.77	112.57	106.33
45	15	310	KC2	CHD-C1D-ND	-8.76	114.98	124.26
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	16	314	KC1	C1D-ND-C4D	8.75	112.55	106.33
42	P	609	KC1	OBD-CAD-C3D	-8.75	107.47	128.52
45	11	309	KC2	OBD-CAD-C3D	-8.74	107.48	128.52
45	7	309	KC2	C1D-ND-C4D	8.73	112.54	106.33
42	p	609	KC1	OBD-CAD-C3D	-8.73	107.52	128.52
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	305	A86	C17-C16-C15	8.72	118.06	109.16
42	8	314	KC1	CHB-C1B-NB	8.72	132.47	124.45
42	9	314	KC1	CHB-C1B-NB	8.72	132.46	124.45
42	0	315	KC1	CHD-C1D-ND	-8.71	115.03	124.26
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
42	8	314	KC1	C4D-C3D-CAD	8.70	113.28	107.42
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
45	6	312	KC2	OBD-CAD-C3D	-8.68	107.64	128.52
45	5	308	KC2	C1D-ND-C4D	8.67	112.50	106.33
43	6	305	A86	C17-C16-C15	8.66	118.00	109.16
45	6	310	KC2	C1D-ND-C4D	8.66	112.49	106.33
31	c	505	CLA	C4A-NA-C1A	8.66	110.60	106.71
43	11	306	A86	C17-C16-C15	8.66	118.00	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	306	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	17	309	KC2	C1D-ND-C4D	8.64	112.47	106.33
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	12	309	KC2	OBD-CAD-C3D	-8.64	107.73	128.52
45	15	308	KC2	OBD-CAD-C3D	-8.63	107.75	128.52
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
45	16	311	KC2	OBD-CAD-C3D	-8.60	107.83	128.52
42	15	317	KC1	C1D-ND-C4D	8.60	112.44	106.33
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
45	12	309	KC2	CHD-C1D-ND	-8.58	115.18	124.26
31	b	616	CLA	C4A-NA-C1A	8.57	110.56	106.71
45	3	309	KC2	OBD-CAD-C3D	-8.57	107.90	128.52
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
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
45	5	308	KC2	OBD-CAD-C3D	-8.55	107.94	128.52
42	14	313	KC1	C1A-NA-C4A	-8.55	102.86	106.71
42	p	609	KC1	CHD-C1D-ND	-8.55	115.21	124.26
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	10	315	KC1	CHB-C4A-C3A	-8.54	111.64	124.98
42	6	315	KC1	CHD-C4C-C3C	-8.54	109.30	125.33
45	11	311	KC2	OBD-CAD-C3D	-8.54	107.97	128.52
45	16	309	KC2	C1D-ND-C4D	8.54	112.40	106.33
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
45	1	311	KC2	OBD-CAD-C3D	-8.52	108.01	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	303	A86	C17-C16-C15	8.52	117.85	109.16
45	0	310	KC2	OBD-CAD-C3D	-8.52	108.03	128.52
44	p	612	DD6	C8-C6-C5	8.52	132.01	118.94
45	0	310	KC2	CHD-C1D-ND	-8.52	115.24	124.26
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	301	A86	C41-C32-C31	8.49	118.07	110.47
42	P	609	KC1	CHD-C1D-ND	-8.49	115.27	124.26
45	12	311	KC2	OBD-CAD-C3D	-8.49	108.09	128.52
31	c	508	CLA	C4A-NA-C1A	8.47	110.51	106.71
45	19	309	KC2	CHD-C1D-ND	-8.46	115.30	124.26
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
45	15	308	KC2	C1D-ND-C4D	8.45	112.33	106.33
45	18	308	KC2	C1D-ND-C4D	8.45	112.33	106.33
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
45	4	310	KC2	CHD-C1D-ND	-8.44	115.33	124.26
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
43	12	302	A86	C17-C16-C15	8.41	117.75	109.16
43	8	305	A86	C40-C32-C31	8.40	117.99	110.47
45	8	309	KC2	OBD-CAD-C3D	-8.39	108.32	128.52
42	p	609	KC1	CHB-C1B-NB	8.38	132.15	124.45
45	8	311	KC2	CHB-C1B-NB	8.37	132.15	124.45
43	16	306	A86	C17-C16-C15	8.36	117.69	109.16
43	8	303	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	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
45	9	309	KC2	CHD-C1D-ND	-8.33	115.44	124.26
43	17	305	A86	O1-C15-C14	8.33	129.93	113.21
43	8	305	A86	C41-C32-C31	8.33	117.93	110.47
42	4	313	KC1	OBD-CAD-C3D	-8.33	108.48	128.52
43	8	306	A86	C17-C16-C15	8.33	117.66	109.16
45	6	310	KC2	C4C-C3C-C2C	-8.32	100.51	107.11
43	13	302	A86	C17-C16-C15	8.31	117.64	109.16
42	12	314	KC1	OBD-CAD-C3D	-8.31	108.52	128.52
42	4	313	KC1	CHD-C4C-NC	8.30	136.79	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	4	308	KC2	OBD-CAD-C3D	-8.29	108.56	128.52
45	17	311	KC2	C4D-C3D-CAD	8.29	113.01	107.42
45	7	311	KC2	C4D-C3D-CAD	8.29	113.01	107.42
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
45	13	309	KC2	OBD-CAD-C3D	-8.27	108.61	128.52
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
42	19	314	KC1	OBD-CAD-C3D	-8.26	108.64	128.52
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	14	310	KC2	CHD-C1D-ND	-8.24	115.53	124.26
45	17	309	KC2	OBD-CAD-C3D	-8.24	108.69	128.52
42	15	317	KC1	OBD-CAD-C3D	-8.24	108.69	128.52
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
45	18	308	KC2	OBD-CAD-C3D	-8.23	108.71	128.52
45	1	309	KC2	OBD-CAD-C3D	-8.22	108.73	128.52
45	7	309	KC2	OBD-CAD-C3D	-8.22	108.73	128.52
43	8	304	A86	C41-C32-C31	8.22	117.83	110.47
42	9	314	KC1	OBD-CAD-C3D	-8.22	108.74	128.52
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
45	3	311	KC2	C4D-C3D-CAD	8.19	112.94	107.42
45	14	308	KC2	OBD-CAD-C3D	-8.19	108.82	128.52
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
45	2	308	KC2	OBD-CAD-C3D	-8.13	108.96	128.52
43	P	611	A86	C21-C20-C19	-8.12	105.14	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	6	315	KC1	C2D-C1D-ND	-8.12	104.79	110.23
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	314	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	306	A86	O4-C38-C39	8.09	125.98	111.09
45	8	309	KC2	C1D-ND-C4D	8.08	112.07	106.33
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
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
42	17	314	KC1	CHD-C1D-ND	-8.05	115.74	124.26
31	C	510	CLA	C4A-NA-C1A	8.05	110.32	106.71
42	0	315	KC1	OBD-CAD-C3D	-8.05	109.16	128.52
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
45	1	311	KC2	CHD-C1D-ND	-8.02	115.77	124.26
43	3	303	A86	C34-O4-C38	-8.01	102.97	117.90
45	19	309	KC2	OBD-CAD-C3D	-8.01	109.25	128.52
45	9	309	KC2	OBD-CAD-C3D	-8.01	109.25	128.52
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	311	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
45	13	311	KC2	CHC-C4B-NB	7.97	131.78	124.45
42	16	314	KC1	CHD-C4C-NC	7.96	136.29	124.20
45	13	311	KC2	C1D-ND-C4D	7.96	111.99	106.33
43	5	303	A86	C21-C20-C19	-7.96	105.32	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	2	310	KC2	C2C-C1C-NC	7.96	119.26	110.57
42	14	313	KC1	CHD-C1D-ND	-7.95	115.84	124.26
45	15	310	KC2	C4C-C3C-C2C	-7.94	100.81	107.11
42	14	313	KC1	OBD-CAD-C3D	-7.93	109.45	128.52
31	10	312	CLA	C4A-NA-C1A	7.92	110.27	106.71
45	12	309	KC2	CMD-C2D-C1D	-7.92	113.31	125.37
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
31	14	306	CLA	CMB-C2B-C1B	-7.87	113.39	125.37
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
45	11	311	KC2	CHD-C1D-ND	-7.85	115.95	124.26
42	8	314	KC1	C3C-C4C-NC	7.84	117.26	109.88
45	15	310	KC2	OBD-CAD-C3D	-7.84	109.66	128.52
45	11	309	KC2	CHD-C1D-ND	-7.83	115.97	124.26
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
42	9	314	KC1	CHD-C1D-ND	-7.82	115.97	124.26
45	14	310	KC2	CHD-C4C-NC	7.82	136.06	124.20
45	2	310	KC2	C4D-C3D-CAD	7.82	112.69	107.42
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
45	3	311	KC2	C1A-C2A-C3A	-7.79	100.93	107.11
43	8	306	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
42	19	314	KC1	CHD-C1D-ND	-7.78	116.02	124.26
43	p	611	A86	C17-C16-C15	7.77	117.09	109.16
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
45	6	312	KC2	C4D-C3D-CAD	7.74	112.64	107.42
45	6	310	KC2	OBD-CAD-C3D	-7.74	109.90	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	4	310	KC2	CMD-C2D-C3D	7.74	146.83	125.93
43	10	305	A86	C17-C16-C15	7.73	117.05	109.16
45	16	311	KC2	C4D-C3D-CAD	7.73	112.63	107.42
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	402	CLA	C4A-NA-C1A	7.70	110.17	106.71
45	4	308	KC2	C1D-ND-C4D	7.70	111.81	106.33
42	15	317	KC1	CHB-C1B-NB	7.70	131.53	124.45
43	2	302	A86	O4-C38-C39	7.70	125.25	111.09
45	12	309	KC2	C4D-C3D-CAD	7.70	112.61	107.42
42	11	314	KC1	CAB-C3B-C4B	7.70	143.48	124.90
42	10	315	KC1	C4D-C3D-CAD	7.68	112.60	107.42
31	2	315	CLA	CAC-C3C-C4C	-7.68	114.84	124.81
43	8	302	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	311	KC2	C2C-C1C-NC	7.68	118.95	110.57
43	3	301	A86	C3-C2-C1	-7.67	116.36	127.31
45	5	310	KC2	OBD-CAD-C3D	-7.67	110.05	128.52
43	17	302	A86	O4-C38-C39	7.67	125.20	111.09
45	18	310	KC2	C4D-C3D-CAD	7.67	112.59	107.42
42	17	314	KC1	C1A-NA-C4A	-7.66	103.26	106.71
45	14	308	KC2	C1D-ND-C4D	7.66	111.78	106.33
42	15	317	KC1	C1A-NA-C4A	-7.66	103.26	106.71
45	16	309	KC2	CHD-C4C-NC	-7.66	112.58	124.20
31	16	313	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
31	6	311	CLA	C4A-NA-C1A	7.65	110.14	106.71
42	10	315	KC1	OBD-CAD-C3D	-7.64	110.13	128.52
43	11	320	A86	O4-C38-C39	7.64	125.14	111.09
43	8	305	A86	O1-C15-C14	-7.64	97.88	113.21
31	13	316	CLA	C4A-NA-C1A	7.64	110.14	106.71
31	d	402	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	314	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	302	A86	C17-C16-C15	7.60	116.92	109.16
42	3	314	KC1	CHD-C1D-ND	-7.60	116.21	124.26
31	8	310	CLA	C4A-NA-C1A	7.60	110.12	106.71
31	16	310	CLA	C4A-NA-C1A	7.59	110.12	106.71
42	8	314	KC1	CBD-CHA-C1A	7.59	143.03	128.88
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
45	14	310	KC2	CMD-C2D-C3D	7.57	146.39	125.93
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	304	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
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
42	4	313	KC1	CHD-C1D-ND	-7.53	116.28	124.26
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	16	309	KC2	OBD-CAD-C3D	-7.53	110.41	128.52
45	8	309	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	302	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
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
31	1	321	CLA	CMB-C2B-C1B	-7.49	113.95	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	14	310	KC2	C4D-C3D-CAD	7.48	112.46	107.42
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
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	314	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	314	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
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
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
32	A	405	PHO	C4D-CHA-CBD	-7.35	105.19	108.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	302	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
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
42	2	313	KC1	CMD-C2D-C3D	7.28	145.58	125.93
31	12	312	CLA	C4A-NA-C1A	7.28	109.98	106.71
42	15	317	KC1	C4D-C3D-CAD	7.27	112.32	107.42
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
32	a	405	PHO	C4D-CHA-CBD	-7.26	105.23	108.52
31	B	601	CLA	C4A-NA-C1A	7.26	109.97	106.71
45	13	311	KC2	OBD-CAD-C3D	-7.26	111.06	128.52
45	16	311	KC2	C2C-C1C-NC	7.26	118.49	110.57
42	12	314	KC1	CHD-C1D-ND	-7.25	116.58	124.26
43	16	306	A86	O4-C34-C35	7.24	125.63	107.59
43	8	306	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	308	CLA	C4A-NA-C1A	7.23	109.96	106.71
43	8	302	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	307	CLA	C4A-NA-C1A	7.22	109.95	106.71
45	0	310	KC2	C2C-C1C-NC	7.22	118.46	110.57
31	8	308	CLA	C4A-NA-C1A	7.22	109.95	106.71
31	8	315	CLA	C4A-NA-C1A	7.22	109.95	106.71
45	12	309	KC2	C1A-C2A-C3A	-7.21	101.39	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	4	310	KC2	C1D-ND-C4D	7.21	111.46	106.33
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
42	11	314	KC1	CMD-C2D-C1D	-7.20	114.41	125.37
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	8	311	KC2	C4D-C3D-CAD	7.18	112.26	107.42
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	305	A86	C35-C34-C33	-7.16	97.39	109.88
43	5	302	A86	C17-C16-C15	7.15	116.46	109.16
42	6	315	KC1	CHD-C1D-ND	-7.15	116.69	124.26
42	9	314	KC1	CAB-C3B-C2B	-7.15	105.05	128.60
45	2	310	KC2	C1D-ND-C4D	7.15	111.41	106.33
31	5	309	CLA	C4A-NA-C1A	7.14	109.92	106.71
31	16	315	CLA	C4A-NA-C1A	7.14	109.92	106.71
42	19	314	KC1	C4D-C3D-CAD	7.14	112.23	107.42
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
45	1	309	KC2	C1D-ND-C4D	7.13	111.40	106.33
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
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
45	4	310	KC2	C4D-C3D-CAD	7.12	112.22	107.42
42	2	313	KC1	CHB-C4A-C3A	-7.11	113.86	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	314	KC1	C2C-C1C-NC	7.11	118.34	110.57
31	6	309	CLA	C4A-NA-C1A	7.11	109.90	106.71
42	16	314	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
45	12	311	KC2	CHD-C1D-ND	-7.07	116.77	124.26
42	17	314	KC1	OBD-CAD-C3D	-7.07	111.50	128.52
43	5	301	A86	C4-C5-C6	-7.07	117.22	127.31
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
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
42	6	315	KC1	CAD-C3D-C2D	-7.03	129.27	144.44
31	c	502	CLA	C4A-NA-C1A	7.02	109.86	106.71
42	11	314	KC1	CHD-C1D-ND	-7.01	116.83	124.26
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
45	11	311	KC2	C4D-C3D-CAD	7.00	112.14	107.42
42	2	313	KC1	CHD-C1D-ND	-7.00	116.85	124.26
45	8	311	KC2	CHD-C1D-ND	-7.00	116.85	124.26
42	18	313	KC1	C2C-C1C-NC	7.00	118.21	110.57
45	6	312	KC2	CHD-C1D-ND	-6.99	116.85	124.26
45	12	311	KC2	C2C-C1C-NC	6.99	118.21	110.57
42	16	314	KC1	CAC-C3C-C4C	6.99	133.88	124.81
45	14	310	KC2	C1D-ND-C4D	6.99	111.30	106.33
45	12	311	KC2	C4C-C3C-C2C	-6.98	101.57	107.11
45	17	311	KC2	CHD-C1D-ND	-6.98	116.86	124.26
31	b	611	CLA	C4A-NA-C1A	6.98	109.84	106.71
31	8	312	CLA	C4A-NA-C1A	6.98	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	12	311	KC2	C4D-C3D-CAD	6.97	112.12	107.42
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	311	KC2	CHB-C1B-NB	6.96	130.85	124.45
45	13	309	KC2	CMD-C2D-C1D	-6.96	114.77	125.37
31	B	610	CLA	C4A-NA-C1A	6.96	109.83	106.71
42	p	609	KC1	C4D-C3D-CAD	6.95	112.11	107.42
42	6	315	KC1	C3C-C4C-NC	6.95	116.42	109.88
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
45	16	311	KC2	CHD-C1D-ND	-6.94	116.91	124.26
43	12	306	A86	C3-C2-C1	-6.93	117.42	127.31
42	8	314	KC1	C1D-ND-C4D	6.93	111.26	106.33
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	311	KC2	C4C-C3C-C2C	-6.92	101.62	107.11
42	P	609	KC1	C4D-C3D-CAD	6.92	112.09	107.42
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
42	7	314	KC1	C1D-ND-C4D	6.92	111.25	106.33
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	311	KC2	CHC-C4B-C3B	-6.92	113.43	125.26
42	9	314	KC1	C4D-C3D-CAD	6.92	112.08	107.42
45	2	310	KC2	CHD-C1D-ND	-6.91	116.94	124.26
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	314	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	0	315	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
45	3	311	KC2	CHD-C1D-ND	-6.89	116.96	124.26
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	314	KC1	CHB-C1B-NB	6.88	130.78	124.45
42	3	314	KC1	C1D-ND-C4D	6.88	111.22	106.33
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
45	18	310	KC2	CHD-C1D-ND	-6.87	116.98	124.26
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	303	A86	O1-C15-C14	6.86	126.98	113.21
43	P	611	A86	O1-C15-C14	6.86	126.98	113.21
42	1	314	KC1	CHD-C1D-ND	-6.86	117.00	124.26
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	406	CLA	C4A-NA-C1A	6.85	109.78	106.71
42	8	314	KC1	CHC-C1C-NC	-6.85	113.42	124.20
31	9	307	CLA	C4A-NA-C1A	6.84	109.78	106.71
45	17	311	KC2	C1D-ND-C4D	6.84	111.20	106.33
43	8	302	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	11	314	KC1	C4D-C3D-CAD	6.79	112.00	107.42
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	303	A86	C41-C32-C31	6.77	116.53	110.47
31	D	406	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
45	15	310	KC2	CAB-C3B-C2B	-6.75	106.36	128.60
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	1	311	KC2	C4D-C3D-CAD	6.73	111.95	107.42
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	314	KC1	CHC-C4B-C3B	-6.72	113.77	125.26
45	5	308	KC2	CBD-CHA-C1A	6.72	141.40	128.88
31	11	307	CLA	CMB-C2B-C1B	-6.72	115.14	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	302	A86	C17-C16-C15	6.68	115.98	109.16
45	15	308	KC2	CMD-C2D-C1D	-6.67	115.20	125.37
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	309	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
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	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
31	2	312	CLA	CHB-C1B-NB	6.63	131.27	124.26
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
45	7	311	KC2	CHD-C1D-ND	-6.62	117.25	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	302	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
43	0	302	A86	O1-C20-C21	-6.56	107.20	115.06
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
45	1	309	KC2	C4D-C3D-CAD	6.55	111.84	107.42
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
42	18	313	KC1	CHD-C1D-ND	-6.54	117.33	124.26
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
45	13	309	KC2	C1D-ND-C4D	6.53	110.97	106.33
45	10	310	KC2	C4D-C3D-CAD	6.52	111.82	107.42
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	311	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	302	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	405	CLA	C4A-NA-C1A	6.51	109.63	106.71
31	19	308	CLA	C4A-NA-C1A	6.51	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	405	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
45	5	310	KC2	C1D-ND-C4D	6.47	110.93	106.33
45	18	310	KC2	C1D-ND-C4D	6.47	110.93	106.33
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	15	317	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
45	8	311	KC2	C1D-ND-C4D	6.45	110.92	106.33
43	17	302	A86	C23-C16-C17	-6.45	97.78	108.98
31	4	312	CLA	CHB-C1B-NB	6.44	131.08	124.26
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	312	CLA	C4A-NA-C1A	6.44	109.60	106.71
42	3	314	KC1	CHC-C1C-NC	-6.44	114.06	124.20
42	3	314	KC1	CHC-C4B-C3B	-6.44	114.24	125.26
45	12	311	KC2	CMD-C2D-C1D	-6.43	115.57	125.37
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
42	13	314	KC1	CMD-C2D-C3D	-6.42	108.58	125.93
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	318	A86	C4-C5-C6	-6.40	118.18	127.31
43	8	305	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
43	11	302	A86	C4-C5-C6	-6.37	118.22	127.31
42	16	314	KC1	CHC-C4B-C3B	-6.37	114.36	125.26
42	11	314	KC1	CHC-C4B-C3B	-6.37	114.37	125.26
45	12	309	KC2	CMD-C2D-C3D	6.36	143.12	125.93
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	301	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	314	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
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
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
42	7	314	KC1	OBD-CAD-C3D	-6.33	113.30	128.52
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	p	603	CLA	C4A-NA-C1A	6.30	109.54	106.71
43	8	303	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
42	16	314	KC1	CHD-C1D-ND	-6.29	117.60	124.26
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	12	309	KC2	C1D-ND-C4D	6.28	110.80	106.33
45	8	311	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
45	8	309	KC2	C4D-C3D-CAD	6.28	111.65	107.42
31	14	312	CLA	CHB-C1B-NB	6.28	130.90	124.26
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
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
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
42	1	314	KC1	CMD-C2D-C3D	-6.25	109.05	125.93
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	15	317	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
45	11	309	KC2	C4D-C3D-CAD	6.15	111.56	107.42
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	303	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
31	11	316	CLA	C4A-NA-C1A	6.13	109.46	106.71
43	8	305	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
42	18	313	KC1	CHB-C4A-C3A	-6.12	115.42	124.98
45	15	308	KC2	C4D-C3D-CAD	6.12	111.55	107.42
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	10	305	A86	C3-C2-C1	-6.11	118.60	127.31
43	16	304	A86	C3-C2-C1	-6.11	118.60	127.31
42	14	313	KC1	C1D-ND-C4D	6.11	110.67	106.33
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
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
42	P	609	KC1	C1D-ND-C4D	6.08	110.66	106.33
45	5	308	KC2	C4D-C3D-CAD	6.08	111.52	107.42
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	15	317	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	15	317	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	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
31	16	307	CLA	CED-O2D-CGD	6.05	129.61	115.94
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
42	p	609	KC1	C1D-ND-C4D	6.04	110.62	106.33
31	8	307	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	7	311	KC2	C1D-ND-C4D	6.04	110.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	6	312	KC2	CHD-C4C-NC	6.03	133.36	124.20
42	18	313	KC1	CAD-C3D-C2D	-6.03	131.42	144.44
42	4	313	KC1	C1D-ND-C4D	6.03	110.62	106.33
43	7	302	A86	C25-C26-C27	-6.03	118.71	127.31
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
31	4	312	CLA	CMB-C2B-C1B	-6.01	116.22	125.37
43	4	301	A86	C17-C16-C15	6.01	115.29	109.16
42	16	314	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	314	KC1	CHC-C1C-NC	-6.00	114.76	124.20
42	16	314	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	305	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
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	309	KC2	C2C-C1C-NC	5.98	117.10	110.57
45	16	309	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	309	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
42	11	314	KC1	CMD-C2D-C3D	5.96	142.02	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	10	306	A86	C41-C32-C31	5.96	115.80	110.47
43	8	306	A86	C41-C32-C40	-5.96	90.25	108.53
45	15	308	KC2	CBD-CHA-C1A	5.95	139.98	128.88
45	15	310	KC2	C1D-ND-C4D	5.95	110.56	106.33
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	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
45	10	310	KC2	C1D-ND-C4D	5.94	110.55	106.33
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
42	P	609	KC1	CHB-C4A-C3A	-5.92	115.72	124.98
42	17	314	KC1	C1D-ND-C4D	5.92	110.54	106.33
45	8	309	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
43	16	304	A86	O1-C20-C19	5.91	117.82	113.38
45	12	309	KC2	CHB-C4A-C3A	-5.90	115.76	124.98
45	2	308	KC2	CHD-C1D-C2D	5.90	143.89	127.24
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
45	3	309	KC2	CHD-C1D-C2D	5.88	143.85	127.24
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	3	311	KC2	C1D-ND-C4D	5.87	110.51	106.33
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	11	302	A86	C25-C26-C27	-5.87	118.94	127.31
45	16	311	KC2	C1D-ND-C4D	5.86	110.50	106.33
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	302	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
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	6	312	KC2	C1D-ND-C4D	5.84	110.48	106.33
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	302	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	309	KC2	CHC-C4B-C3B	-5.83	115.28	125.26
43	6	301	A86	C4-C5-C6	-5.83	118.99	127.31
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
31	P	606	CLA	C2B-C1B-NB	5.82	114.14	110.23
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
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
31	12	313	CLA	C3B-C4B-NB	-5.80	105.14	110.52
42	8	314	KC1	CAC-C3C-C4C	5.80	132.33	124.81
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
45	13	309	KC2	CMD-C2D-C3D	5.78	141.55	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	p	606	CLA	C2B-C1B-NB	5.78	114.11	110.23
45	12	309	KC2	CHC-C4B-C3B	-5.78	115.38	125.26
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
45	18	308	KC2	C4D-C3D-CAD	5.78	111.31	107.42
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	311	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	311	KC2	CHC-C1C-NC	-5.76	115.13	124.20
31	14	312	CLA	CMB-C2B-C1B	-5.76	116.60	125.37
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
31	16	313	CLA	CHB-C1B-NB	5.74	130.34	124.26
42	8	314	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
42	2	313	KC1	CHC-C1C-NC	-5.73	115.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	14	306	CLA	CHB-C1B-NB	5.71	130.30	124.26
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	311	KC2	CHD-C4C-NC	5.70	132.86	124.20
43	16	305	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	305	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
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	301	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
45	8	309	KC2	CHC-C1C-NC	-5.66	115.30	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	307	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
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	12	311	KC2	C1D-ND-C4D	5.64	110.34	106.33
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	5	308	KC2	CMD-C2D-C1D	-5.63	116.80	125.37
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
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	314	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
42	4	313	KC1	CHB-C4A-C3A	-5.61	116.22	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	0	315	KC1	C1D-ND-C4D	5.61	110.32	106.33
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
45	7	309	KC2	CHD-C1D-C2D	5.60	143.04	127.24
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	303	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	303	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
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
42	11	314	KC1	C1D-ND-C4D	5.57	110.29	106.33
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
45	6	310	KC2	CHD-C1D-C2D	5.56	142.94	127.24
42	5	313	KC1	CAA-C2A-C1A	5.56	150.30	124.75
45	11	309	KC2	C1D-ND-C4D	5.56	110.28	106.33
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
42	16	314	KC1	CAD-C3D-C2D	-5.55	132.45	144.44
45	16	309	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	16	314	KC1	C2D-C1D-ND	-5.55	106.51	110.23
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
31	0	314	CLA	C4A-NA-C1A	5.54	109.20	106.71
45	16	311	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
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	311	KC2	C4C-C3C-C2C	-5.54	102.72	107.11
45	15	308	KC2	CMD-C2D-C3D	5.54	140.88	125.93
31	8	313	CLA	C2D-C1D-ND	-5.53	106.03	110.10
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
45	17	309	KC2	CHD-C1D-C2D	5.52	142.84	127.24
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	306	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	311	KC2	CHD-C4C-C3C	-5.52	106.12	126.11
45	16	309	KC2	CHD-C1D-C2D	5.51	142.81	127.24
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	311	KC2	CBD-CHA-C1A	5.49	139.12	128.88
43	8	305	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	305	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
42	15	317	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	15	317	KC1	CAA-C2A-C1A	5.48	149.92	124.75
45	6	310	KC2	CHC-C4B-C3B	-5.48	115.89	125.26
45	19	309	KC2	C1D-ND-C4D	5.47	110.22	106.33
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
38	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
31	1	307	CLA	CMB-C2B-C1B	-5.46	117.05	125.37
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
38	c	520	DGD	O3G-C3G-C2G	-5.46	97.72	110.90
43	5	305	A86	C3-C2-C1	-5.46	119.52	127.31
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	309	KC2	C1A-C2A-C3A	-5.44	102.79	107.11
45	3	309	KC2	C2C-C1C-NC	5.44	116.51	110.57
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	9	314	KC1	CHB-C4A-C3A	-5.43	116.50	124.98
45	8	311	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	309	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
31	2	312	CLA	C3B-C4B-NB	-5.42	105.49	110.52
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
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	303	A86	O4-C38-O5	-5.41	112.22	122.96
42	0	315	KC1	CHB-C4A-NA	5.41	132.72	124.20
45	13	311	KC2	CHD-C1D-C2D	5.41	142.50	127.24
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	d	405	CLA	C3B-C4B-NB	-5.40	105.51	110.52
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	311	KC2	C4B-CHC-C1C	-5.39	114.43	126.06
43	1	306	A86	C25-C26-C27	-5.39	119.62	127.31
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	309	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	6	315	KC1	CHB-C4A-C3A	-5.38	116.58	124.98
45	12	311	KC2	CMD-C2D-C3D	5.37	140.43	125.93
45	9	309	KC2	C1D-ND-C4D	5.37	110.15	106.33
43	15	301	A86	C3-C2-C1	-5.37	119.65	127.31
45	8	309	KC2	O2D-CGD-CBD	5.37	120.81	111.27
45	12	311	KC2	O2D-CGD-CBD	5.37	120.81	111.27
31	D	405	CLA	C3B-C4B-NB	-5.37	105.53	110.52
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	309	KC2	CHB-C4A-C3A	-5.36	116.60	124.98
45	0	310	KC2	C1D-ND-C4D	5.36	110.14	106.33
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
45	4	308	KC2	C4D-C3D-CAD	5.35	111.03	107.42
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
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
38	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	302	A86	C4-C5-C6	-5.34	119.70	127.31
43	16	306	A86	O4-C38-O5	-5.33	112.37	122.96
45	4	308	KC2	CHC-C1C-NC	-5.33	115.81	124.20
38	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
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	15	317	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
42	7	314	KC1	CHD-C1D-ND	-5.31	118.63	124.26
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
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
45	16	311	KC2	CHB-C4A-C3A	-5.31	116.69	124.98
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
42	9	314	KC1	CAC-C3C-C4C	5.30	131.69	124.81
43	18	302	A86	O1-C20-C21	-5.30	108.71	115.06
31	3	313	CLA	CHB-C1B-NB	5.30	129.87	124.26
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
31	16	313	CLA	CMB-C2B-C1B	-5.28	117.32	125.37
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	311	KC2	O2D-CGD-CBD	5.27	120.64	111.27
43	8	305	A86	C19-C18-C17	-5.27	100.60	110.77
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	311	KC2	O2D-CGD-CBD	5.25	120.60	111.27
42	18	313	KC1	C2D-C1D-ND	-5.25	106.71	110.23
43	8	303	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	314	KC1	C4B-CHC-C1C	-5.25	114.73	126.06
31	5	314	CLA	C4A-NA-C1A	5.25	109.07	106.71
31	2	312	CLA	CMB-C2B-C1B	-5.25	117.38	125.37
40	D	401	BCT	O2-C-O1	5.25	133.16	119.55
40	d	401	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
42	15	317	KC1	CMD-C2D-C3D	5.24	140.08	125.93
43	8	304	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
45	13	309	KC2	C4D-C3D-CAD	5.22	110.94	107.42
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	301	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
31	6	314	CLA	CHB-C1B-NB	5.20	129.76	124.26
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
42	13	314	KC1	C1D-ND-C4D	5.19	110.03	106.33
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	11	314	KC1	C1A-NA-C4A	-5.19	104.37	106.71
43	16	304	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
42	15	317	KC1	CMD-C2D-C1D	-5.18	117.48	125.37
45	14	310	KC2	C2C-C1C-NC	5.18	116.22	110.57
31	14	306	CLA	CMB-C2B-C3B	5.17	139.12	126.59
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
45	11	311	KC2	C1D-ND-C4D	5.16	110.00	106.33
42	6	315	KC1	C4B-CHC-C1C	-5.16	114.93	126.06
43	5	304	A86	C17-C16-C15	5.16	114.42	109.16
42	10	315	KC1	C1D-ND-C4D	5.16	110.00	106.33
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	13	309	KC2	C4B-CHC-C1C	-5.16	114.94	126.06
31	6	314	CLA	CMB-C2B-C1B	-5.16	117.52	125.37
43	8	303	A86	C25-C26-C27	-5.15	119.95	127.31
45	18	308	KC2	CHD-C1D-C2D	5.15	141.79	127.24
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	311	KC2	C4B-CHC-C1C	-5.15	114.96	126.06
42	0	315	KC1	C2A-C3A-C4A	5.15	110.30	106.49
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
31	15	311	CLA	C2B-C1B-NB	-5.14	106.79	110.23
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
31	4	312	CLA	C3B-C4B-NB	-5.14	105.75	110.52
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
31	13	313	CLA	C3B-C4B-NB	-5.13	105.75	110.52
45	8	309	KC2	C4B-CHC-C1C	-5.13	115.00	126.06
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	301	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
42	17	314	KC1	C3C-C4C-NC	5.11	114.69	109.88
43	5	304	A86	C21-C20-C19	-5.11	108.53	114.28
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
43	8	302	A86	C23-C16-C17	-5.10	100.12	108.98
31	10	307	CLA	CMB-C2B-C1B	-5.10	117.60	125.37
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	314	KC1	C2A-C3A-C4A	5.10	110.27	106.49
43	16	303	A86	C3-C2-C1	-5.10	120.03	127.31
45	5	310	KC2	O2D-CGD-CBD	5.10	120.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	314	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	314	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
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
45	13	311	KC2	CMD-C2D-C1D	5.09	133.12	125.37
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
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
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	4	310	KC2	CAA-C2A-C1A	5.07	148.04	124.75
43	16	302	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	302	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
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
31	7	313	CLA	CHB-C1B-NB	5.04	129.59	124.26
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	15	317	KC1	C2A-C3A-C4A	5.04	110.22	106.49
43	6	303	A86	O4-C34-C33	5.04	120.14	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	1	321	CLA	CMB-C2B-C3B	5.03	138.78	126.59
43	7	306	A86	O3-C36-C37	-5.03	100.44	109.39
42	2	313	KC1	C1D-ND-C4D	5.03	109.91	106.33
43	14	301	A86	C4-C3-C2	5.03	133.78	123.47
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
45	11	311	KC2	O2D-CGD-CBD	5.02	120.19	111.27
43	16	303	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
42	13	314	KC1	C4D-C3D-CAD	5.00	110.79	107.42
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
43	6	305	A86	C41-C32-C31	5.00	114.94	110.47
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
31	15	311	CLA	CHC-C4B-NB	4.99	129.54	124.26
45	11	311	KC2	C4B-CHC-C1C	-4.99	115.29	126.06
31	12	313	CLA	CHB-C1B-NB	4.99	129.54	124.26
31	B	616	CLA	CAA-C2A-C3A	-4.99	99.12	112.78
31	0	307	CLA	CMB-C2B-C1B	-4.99	117.77	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	5	313	KC1	CHB-C4A-NA	4.99	132.06	124.20
43	16	301	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
45	14	308	KC2	C4D-C3D-CAD	4.98	110.78	107.42
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
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	1	311	KC2	C1D-ND-C4D	4.96	109.86	106.33
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
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	309	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
31	17	313	CLA	C3B-C4B-NB	-4.94	105.94	110.52
31	12	307	CLA	C4A-NA-C1A	4.94	108.92	106.71
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	17	313	CLA	CHB-C1B-NB	4.93	129.48	124.26
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
31	3	313	CLA	CMB-C2B-C1B	-4.93	117.86	125.37
43	5	318	A86	C3-C2-C1	-4.93	120.28	127.31
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
45	5	310	KC2	CHD-C4C-C3C	-4.92	108.29	126.11
45	5	308	KC2	CMD-C2D-C3D	4.92	139.21	125.93
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	301	A86	O4-C38-C39	4.91	120.12	111.09
42	15	317	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
42	12	314	KC1	C1D-ND-C4D	4.90	109.82	106.33
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
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
43	11	305	A86	O4-C38-C39	4.89	120.08	111.09
43	8	304	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	8	305	A86	C33-C32-C31	-4.88	104.47	109.21
43	4	304	A86	C3-C2-C1	-4.88	120.35	127.31
31	12	307	CLA	CMB-C2B-C1B	-4.88	117.94	125.37
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	8	301	SQD	O7-S-C6	4.86	112.72	106.94
43	16	306	A86	C4-C5-C6	-4.86	120.37	127.31
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	309	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
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
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
45	8	309	KC2	CHD-C1D-C2D	4.83	140.89	127.24
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	15	317	KC1	O2D-CGD-CBD	4.81	119.82	111.27
43	10	303	A86	C25-C26-C27	-4.81	120.44	127.31
43	11	306	A86	O-C13-C11	-4.81	110.53	121.15
31	11	313	CLA	C3B-C4B-NB	-4.81	106.06	110.52
42	5	313	KC1	C1D-ND-C4D	4.80	109.75	106.33
42	10	315	KC1	C3C-C4C-NC	4.80	114.40	109.88
37	15	315	LMG	O6-C5-C4	4.80	118.41	109.69
31	1	313	CLA	C3B-C4B-NB	-4.80	106.06	110.52
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
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
31	7	313	CLA	C3B-C4B-NB	-4.79	106.07	110.52
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
31	10	307	CLA	CHB-C1B-NB	4.78	129.32	124.26
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
42	3	314	KC1	CAD-C3D-C2D	-4.78	134.13	144.44
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	306	A86	C4-C5-C6	-4.77	120.51	127.31
45	3	309	KC2	C4D-C3D-CAD	4.77	110.63	107.42
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	306	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
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
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
43	16	301	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	302	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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	304	A86	C25-C26-C27	-4.73	120.56	127.31
43	8	302	A86	C3-C2-C1	-4.73	120.56	127.31
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	15	310	KC2	C4D-C3D-CAD	4.73	110.61	107.42
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
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	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	309	KC2	C1B-CHB-C4A	-4.71	115.90	126.06
43	16	304	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
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
37	D	404	LMG	O1-C1-C2	-4.69	100.97	108.30
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
45	15	310	KC2	O2D-CGD-CBD	4.69	119.60	111.27
43	8	303	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
45	8	311	KC2	CAA-C2A-C1A	4.68	146.27	124.75
43	6	304	A86	O4-C38-C39	4.68	119.70	111.09
45	5	310	KC2	C4D-C3D-CAD	4.68	110.57	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	303	A86	C35-C34-C33	-4.68	101.71	109.88
43	16	306	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	314	KC1	C1B-CHB-C4A	-4.67	115.98	126.06
43	12	302	A86	O4-C34-C35	4.67	119.22	107.59
31	1	308	CLA	CMB-C2B-C1B	-4.67	118.26	125.37
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
45	0	310	KC2	C4D-C3D-CAD	4.66	110.56	107.42
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
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
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	307	CLA	CAC-C3C-C4C	4.65	130.84	124.81
43	12	302	A86	O4-C38-O5	-4.65	113.72	122.96
31	11	307	CLA	CMB-C2B-C3B	4.65	137.85	126.59
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	314	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	309	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	316	A86	O4-C38-O5	-4.64	113.75	122.96
45	17	311	KC2	CMD-C2D-C3D	4.63	138.45	125.93
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	302	A86	C25-C26-C27	-4.63	120.71	127.31
42	15	317	KC1	CHD-C1D-C2D	4.63	140.31	127.24
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
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
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
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	309	KC2	CHB-C1B-C2B	-4.61	115.80	125.48
42	1	314	KC1	C1D-ND-C4D	4.61	109.61	106.33
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	311	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
37	5	316	LMG	O1-C7-C8	-4.61	99.78	110.90
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
43	1	319	A86	C20-C19-C18	4.60	121.84	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	314	KC1	O2D-CGD-CBD	4.59	119.43	111.27
43	17	316	A86	O1-C15-C20	-4.59	54.91	59.40
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	14	312	CLA	C3B-C4B-NB	-4.59	106.26	110.52
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
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
45	17	311	KC2	CMD-C2D-C1D	-4.58	118.39	125.37
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
42	19	314	KC1	C1D-ND-C4D	4.58	109.59	106.33
43	4	306	A86	C3-C2-C1	-4.58	120.78	127.31
45	14	308	KC2	CHD-C1D-C2D	4.58	140.16	127.24
42	9	314	KC1	C1D-ND-C4D	4.58	109.59	106.33
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
45	4	308	KC2	CHD-C1D-C2D	4.57	140.16	127.24
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
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	311	KC2	CHB-C4A-NA	4.57	131.40	124.20
45	5	308	KC2	C1B-CHB-C4A	-4.57	116.21	126.06
43	8	302	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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
43	6	302	A86	O4-C34-C33	4.54	118.90	107.59
45	16	311	KC2	CAA-C2A-C1A	4.54	145.62	124.75
37	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
43	6	303	A86	C35-C34-C33	-4.53	101.97	109.88
43	16	303	A86	C35-C34-C33	-4.53	101.97	109.88
43	18	305	A86	O4-C38-C39	4.53	119.43	111.09
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	302	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
45	5	308	KC2	CHD-C1D-C2D	4.51	139.98	127.24
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	303	A86	O4-C34-C35	-4.50	96.38	107.59
43	8	306	A86	O1-C20-C19	4.50	116.76	113.38
45	16	311	KC2	C1B-CHB-C4A	-4.50	116.35	126.06
43	19	304	A86	O1-C20-C21	-4.50	109.67	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
32	A	405	PHO	C2B-C1B-NB	-4.50	106.42	109.53
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
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
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
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
43	1	306	A86	C3-C2-C1	-4.48	120.92	127.31
32	a	405	PHO	C2B-C1B-NB	-4.48	106.43	109.53
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
42	13	314	KC1	CHD-C1D-ND	-4.48	119.52	124.26
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
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
45	9	309	KC2	C4D-C3D-CAD	4.46	110.43	107.42
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	403	PHO	CMB-C2B-C3B	4.45	133.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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
41	V	201	HEM	CAA-C2A-C1A	4.44	133.63	124.89
31	18	312	CLA	CHB-C1B-NB	4.44	128.96	124.26
45	8	309	KC2	CHB-C4A-NA	4.44	131.20	124.20
32	d	403	PHO	CBC-CAC-C3C	4.44	119.38	112.88
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	403	PHO	CMB-C2B-C3B	4.44	132.98	124.68
37	5	316	LMG	O6-C1-O1	-4.44	99.47	109.97
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
34	A	411	SQD	C4-C3-C2	4.43	118.56	110.82
37	d	404	LMG	O1-C1-C2	-4.43	101.39	108.30
45	8	311	KC2	CHB-C1B-C2B	-4.43	116.19	125.48
43	11	320	A86	O3-C36-C37	-4.43	101.51	109.39
32	D	403	PHO	CBC-CAC-C3C	4.42	119.36	112.88
41	v	201	HEM	CAA-C2A-C1A	4.42	133.60	124.89
31	16	313	CLA	CHA-C4D-ND	4.42	141.75	132.50
45	8	309	KC2	CHD-C4C-NC	-4.42	117.49	124.20
43	17	305	A86	O1-C15-C20	-4.42	55.08	59.40
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	301	A86	O1-C20-C21	-4.42	109.76	115.06
43	13	304	A86	O-C13-C14	4.42	130.63	121.66
45	11	311	KC2	C4B-C3B-C2B	-4.41	103.13	106.75
43	16	301	A86	O2-C18-C17	4.41	118.57	109.80
31	8	313	CLA	C3B-C4B-NB	-4.41	106.42	110.52
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
43	11	320	A86	O1-C20-C19	4.41	116.69	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	101	SQD	C4-C3-C2	4.41	118.52	110.82
34	8	301	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
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
31	11	308	CLA	CMB-C2B-C1B	-4.40	118.67	125.37
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
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
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
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
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
42	2	313	KC1	C3C-C4C-NC	4.38	114.00	109.88
43	0	301	A86	C25-C26-C27	-4.38	121.07	127.31
43	16	301	A86	C17-C16-C15	4.37	113.63	109.16
43	16	302	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	8	313	CLA	CHB-C1B-NB	4.37	128.88	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	C	509	CLA	CMB-C2B-C1B	-4.36	118.72	125.37
45	12	311	KC2	C1B-CHB-C4A	-4.36	116.65	126.06
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	14	306	CLA	C3B-C4B-NB	-4.36	106.47	110.52
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
42	p	609	KC1	CMD-C2D-C3D	4.35	137.68	125.93
31	11	307	CLA	O2D-CGD-O1D	-4.35	115.33	123.84
45	6	310	KC2	C4D-C3D-CAD	4.35	110.35	107.42
42	1	314	KC1	CAA-C2A-C1A	4.35	144.74	124.75
45	16	309	KC2	CHD-C4C-C3C	-4.35	110.35	126.11
37	15	315	LMG	O6-C1-O1	-4.35	99.68	109.97
42	P	609	KC1	CMD-C2D-C3D	4.35	137.67	125.93
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
31	c	509	CLA	CMB-C2B-C1B	-4.35	118.75	125.37
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
45	13	311	KC2	C2D-C1D-ND	-4.34	107.32	110.23
43	14	304	A86	C28-C27-C26	-4.34	116.84	122.92
43	11	303	A86	C3-C2-C1	-4.34	121.12	127.31
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	303	A86	O1-C15-C20	-4.32	55.17	59.40
31	7	313	CLA	CMB-C2B-C1B	-4.32	118.78	125.37
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
45	17	309	KC2	C4D-C3D-CAD	4.32	110.33	107.42
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
45	7	309	KC2	C4D-C3D-CAD	4.31	110.33	107.42
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
43	9	306	A86	C28-C27-C29	4.31	128.91	118.93
37	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
45	2	308	KC2	C2D-C1D-ND	-4.30	107.35	110.23
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
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	304	A86	C35-C34-C33	-4.29	102.39	109.88
38	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
45	2	308	KC2	C4D-C3D-CAD	4.29	110.31	107.42
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
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	317	LHG	O4-P-O5	4.28	133.41	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	313	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
43	0	301	A86	C3-C2-C1	-4.28	121.20	127.31
45	16	309	KC2	C4D-C3D-CAD	4.28	110.30	107.42
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
37	10	319	LMG	O6-C5-C4	4.27	117.45	109.69
45	15	308	KC2	CHD-C1D-C2D	4.27	139.29	127.24
34	i	101	SQD	O9-S-C6	4.27	112.01	106.94
45	8	311	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
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	7	309	KC2	C2D-C1D-ND	-4.26	107.38	110.23
45	5	308	KC2	CAA-C2A-C1A	4.26	144.31	124.75
43	11	306	A86	C35-C34-C33	-4.26	102.45	109.88
37	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
45	12	311	KC2	C4B-C3B-C2B	-4.25	103.26	106.75
43	8	306	A86	C36-C31-C32	-4.25	115.48	119.70
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
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	303	A86	C35-C34-C33	-4.24	102.48	109.88
32	d	403	PHO	C4D-CHA-CBD	-4.24	106.60	108.52
42	1	314	KC1	OBD-CAD-C3D	-4.24	118.32	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	312	CLA	CMD-C2D-C1D	-4.24	117.24	124.71
43	14	304	A86	C35-C34-C33	4.24	117.27	109.88
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
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
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
45	17	309	KC2	C2D-C1D-ND	-4.22	107.40	110.23
34	L	102	SQD	O9-S-C6	4.22	111.95	106.94
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
42	12	314	KC1	CMD-C2D-C3D	4.21	137.31	125.93
31	0	307	CLA	CHB-C1B-NB	4.21	128.72	124.26
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
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	309	KC2	CHD-C4C-C3C	-4.20	110.88	126.11
38	1	318	DGD	O3G-C3G-C2G	-4.20	100.76	110.90
34	A	411	SQD	O5-C5-C4	4.20	117.32	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	b	622	DGD	C1E-O6E-C5E	4.20	121.93	113.69
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
43	15	303	A86	O1-C15-C20	-4.20	55.30	59.40
31	1	313	CLA	CHB-C1B-NB	4.19	128.70	124.26
43	13	303	A86	C41-C32-C31	4.19	114.23	110.47
43	8	303	A86	O1-C15-C20	-4.19	55.30	59.40
36	d	408	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	316	LHG	O4-P-O5	4.19	132.94	112.24
31	18	312	CLA	C4D-C3D-CAD	-4.19	103.16	108.10
36	18	315	LHG	O4-P-O5	4.18	132.93	112.24
36	D	408	LHG	O4-P-O5	4.18	132.93	112.24
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
38	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
45	10	310	KC2	CMD-C2D-C3D	4.18	137.22	125.93
36	p	615	LHG	O4-P-O5	4.18	132.90	112.24
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
42	13	314	KC1	C4C-C3C-C2C	-4.18	100.81	106.90
31	1	321	CLA	CHB-C1B-NB	4.18	128.68	124.26
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
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
42	0	315	KC1	C4D-C3D-CAD	4.17	110.23	107.42
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
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
32	D	403	PHO	C4D-CHA-CBD	-4.16	106.64	108.52
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	b	612	CLA	CMB-C2B-C1B	-4.15	119.04	125.37
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	C	503	CLA	CMB-C2B-C1B	4.15	131.69	125.37
31	7	313	CLA	CAA-C2A-C3A	-4.15	101.42	112.78
31	c	503	CLA	CMB-C2B-C1B	4.15	131.69	125.37
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
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	16	313	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
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	306	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	306	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	303	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	302	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
43	5	302	A86	C34-O4-C38	4.12	125.58	117.90
43	16	306	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
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	B	611	CLA	CMB-C2B-C1B	-4.12	119.10	125.37
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
38	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	3	309	KC2	C2D-C1D-ND	-4.11	107.47	110.23
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
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
43	8	302	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
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	311	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
36	Z	103	LHG	O4-P-O5	4.10	132.49	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	309	KC2	CHB-C4A-NA	4.09	130.65	124.20
43	19	306	A86	C25-C26-C27	-4.09	121.47	127.31
37	15	315	LMG	O1-C7-C8	-4.09	101.03	110.90
45	1	309	KC2	CHD-C1D-C2D	4.09	138.79	127.24
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	302	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
32	D	403	PHO	C2B-C1B-NB	-4.08	106.71	109.53
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
31	a	403	CLA	CMB-C2B-C1B	-4.07	119.16	125.37
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	303	A86	C4-C5-C6	-4.07	121.50	127.31
43	13	304	A86	C40-C32-C31	-4.07	106.83	110.47
45	19	309	KC2	C4B-C3B-C2B	-4.07	103.41	106.75
43	9	305	A86	C4-C5-C6	-4.07	121.50	127.31
31	A	403	CLA	CMB-C2B-C1B	-4.07	119.18	125.37
43	10	305	A86	O1-C15-C20	-4.07	55.42	59.40
32	d	403	PHO	C2B-C1B-NB	-4.07	106.72	109.53
42	13	314	KC1	CHB-C1B-C2B	-4.06	116.96	125.48
43	8	306	A86	C23-C16-C22	4.06	113.36	107.37
45	6	312	KC2	CHB-C4A-NA	4.06	130.60	124.20
31	3	313	CLA	C3B-C4B-NB	-4.06	106.75	110.52
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	304	A86	C28-C27-C26	-4.06	117.24	122.92
37	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
43	5	305	A86	C25-C26-C27	-4.05	121.53	127.31
31	1	307	CLA	CMB-C2B-C3B	4.05	136.40	126.59
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
38	b	622	DGD	O6E-C5E-C4E	4.05	117.04	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	0	305	A86	O1-C15-C20	-4.04	55.45	59.40
31	17	313	CLA	CMB-C2B-C1B	-4.04	119.21	125.37
42	P	609	KC1	CMD-C2D-C1D	-4.04	119.21	125.37
45	13	309	KC2	CHD-C1D-C2D	4.04	138.65	127.24
31	3	308	CLA	C3B-C4B-NB	-4.04	106.77	110.52
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
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	15	317	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
37	11	301	LMG	O6-C5-C4	4.02	116.99	109.69
43	8	304	A86	C25-C26-C27	-4.02	121.58	127.31
43	12	306	A86	O4-C38-C39	4.02	118.48	111.09
37	p	614	LMG	O6-C5-C4	4.01	116.98	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	317	KC1	CHB-C1B-C2B	-4.01	117.06	125.48
31	16	307	CLA	CAC-C3C-C4C	4.01	130.01	124.81
43	1	305	A86	C8-C6-C5	4.01	125.09	118.94
42	p	609	KC1	CMD-C2D-C1D	-4.01	119.26	125.37
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
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
37	1	301	LMG	O6-C5-C4	4.00	116.96	109.69
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
31	C	503	CLA	C2B-C1B-NB	-4.00	107.55	110.23
43	0	301	A86	C12-C11-C13	4.00	122.74	116.02
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
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	6	315	KC1	CHD-C1D-C2D	3.99	138.51	127.24
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	314	KC1	O2D-CGD-CBD	3.99	118.36	111.27
43	11	306	A86	C4-C5-C6	-3.99	121.62	127.31
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
43	1	320	A86	O3-C36-C37	-3.98	102.31	109.39
45	8	309	KC2	C2D-C1D-ND	-3.98	107.56	110.23
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	311	KC2	CBD-CHA-C1A	3.98	136.29	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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
38	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
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
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
31	c	503	CLA	C2B-C1B-NB	-3.96	107.58	110.23
43	16	303	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	314	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
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
31	12	308	CLA	CMB-C2B-C1B	-3.95	119.36	125.37
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
31	4	312	CLA	CMB-C2B-C3B	3.94	136.13	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
38	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
38	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	302	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
45	18	308	KC2	C2D-C1D-ND	-3.93	107.60	110.23
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
45	19	309	KC2	C2A-C1A-NA	3.93	115.70	109.40
31	16	313	CLA	C3B-C4B-NB	-3.92	106.87	110.52
43	4	303	A86	C3-C2-C1	-3.92	121.71	127.31
38	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
42	8	314	KC1	CHD-C1D-C2D	3.92	138.30	127.24
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
37	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
45	6	310	KC2	C2D-C1D-ND	-3.91	107.61	110.23
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	302	A86	C9-C8-C6	-3.91	115.44	126.42
43	9	301	A86	C4-C5-C6	-3.91	121.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	B	620	LMG	C1-C2-C3	-3.90	101.87	110.00
31	17	308	CLA	C3B-C4B-NB	-3.90	106.90	110.52
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
43	17	305	A86	C33-C32-C31	-3.90	105.42	109.21
43	16	302	A86	O4-C38-O5	-3.90	115.22	122.96
45	16	309	KC2	C2D-C1D-ND	-3.90	107.62	110.23
42	16	314	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
43	8	302	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	302	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
32	a	405	PHO	C2D-C1D-ND	-3.88	106.85	109.53
43	3	305	A86	C14-C15-C16	-3.88	103.91	118.75
45	16	311	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	6	315	KC1	CHB-C1B-C2B	-3.87	117.36	125.48
32	A	405	PHO	C2D-C1D-ND	-3.87	106.85	109.53
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	306	A86	C3-C2-C1	-3.87	121.79	127.31
31	16	313	CLA	C3D-C2D-C1D	3.87	111.11	105.83
45	11	311	KC2	CMD-C2D-C3D	3.87	136.38	125.93
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
45	10	310	KC2	CMD-C2D-C1D	-3.86	119.48	125.37
31	2	307	CLA	CAA-C2A-C3A	-3.86	102.20	112.78
43	9	303	A86	C4-C5-C6	-3.86	121.80	127.31
43	5	304	A86	C14-C15-C16	3.86	133.54	118.75
31	7	308	CLA	C3B-C4B-NB	-3.86	106.93	110.52
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
31	15	312	CLA	CHB-C1B-NB	3.86	128.34	124.26
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
45	12	311	KC2	C2A-C3A-C4A	3.85	109.34	106.49
45	5	308	KC2	CHD-C4C-C3C	-3.85	112.14	126.11
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
43	10	318	A86	O4-C38-O5	-3.85	115.32	122.96
31	2	315	CLA	C3B-C4B-NB	-3.84	106.95	110.52
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	15	317	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	301	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	305	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	302	A86	C4-C3-C2	-3.83	115.63	123.47
45	1	309	KC2	C4B-C3B-C2B	-3.83	103.61	106.75
31	12	307	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
31	5	311	CLA	CHC-C4B-NB	3.83	128.31	124.26
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
42	5	313	KC1	CHD-C1D-C2D	3.83	138.04	127.24
38	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	303	A86	C3-C2-C1	-3.82	121.86	127.31
43	1	305	A86	C14-C15-C16	3.82	133.38	118.75
38	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	302	A86	C35-C34-C33	-3.81	103.22	109.88
45	13	311	KC2	C4D-C3D-CAD	3.81	109.99	107.42
31	11	307	CLA	C4A-NA-C1A	3.81	108.42	106.71
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
43	12	304	A86	C9-C10-C11	-3.80	115.43	126.61
42	6	315	KC1	CHB-C4A-NA	3.80	130.19	124.20
31	18	309	CLA	CMB-C2B-C1B	-3.80	119.59	125.37
45	19	309	KC2	CHB-C4A-NA	3.80	130.19	124.20
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
31	11	307	CLA	CHB-C1B-NB	3.79	128.27	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	305	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
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
31	12	307	CLA	CMB-C2B-C3B	3.77	135.73	126.59
43	8	306	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	313	CLA	C4A-NA-C1A	3.77	108.40	106.71
38	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
43	14	305	A86	C41-C32-C33	3.77	125.97	109.05
45	19	309	KC2	C4D-C3D-CAD	3.77	109.96	107.42
45	8	309	KC2	CAC-C3C-C4C	3.77	142.02	124.47
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
37	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	301	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
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	4	314	CLA	C3B-C4B-NB	-3.75	107.03	110.52
31	p	607	CLA	CAC-C3C-C4C	3.75	129.68	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	306	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
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
31	13	313	CLA	CHB-C1B-NB	3.74	128.22	124.26
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	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
37	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
43	7	305	A86	C41-C32-C31	3.73	113.81	110.47
31	18	312	CLA	C3B-C4B-NB	-3.73	107.05	110.52
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
31	b	605	CLA	C2B-C1B-NB	-3.73	107.73	110.23
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
43	9	306	A86	C4-C5-C6	-3.72	122.00	127.31
43	16	305	A86	C14-C15-C16	-3.72	104.50	118.75
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
43	19	302	A86	C41-C32-C31	3.71	113.80	110.47
45	11	309	KC2	CMD-C2D-C3D	3.71	135.96	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	303	A86	O1-C15-C20	-3.71	55.77	59.40
31	3	313	CLA	C2D-C1D-ND	-3.71	107.37	110.10
43	0	303	A86	O1-C20-C19	3.71	116.17	113.38
43	3	304	A86	C4-C3-C2	-3.71	115.88	123.47
45	8	311	KC2	C2A-C1A-NA	3.71	115.35	109.40
31	13	308	CLA	CMB-C2B-C1B	-3.71	119.72	125.37
31	8	313	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	6	308	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
32	D	403	PHO	C2D-C1D-ND	-3.70	106.97	109.53
31	2	312	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
42	13	314	KC1	C2D-C1D-ND	-3.70	107.75	110.23
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
43	16	306	A86	C19-C18-C17	-3.70	103.63	110.77
45	9	309	KC2	CAB-C3B-C2B	3.70	140.78	128.60
31	B	604	CLA	C2B-C1B-NB	-3.69	107.75	110.23
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
31	2	307	CLA	C3B-C4B-NB	-3.69	107.09	110.52
43	8	302	A86	C25-C24-C1	-3.69	116.04	126.42
43	8	306	A86	O1-C15-C20	-3.69	55.79	59.40
31	14	314	CLA	C3B-C4B-NB	-3.69	107.09	110.52
37	D	404	LMG	O6-C1-C2	3.69	118.16	110.35
32	d	403	PHO	C2D-C1D-ND	-3.69	106.98	109.53
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	305	A86	O-C13-C14	3.69	129.15	121.66
31	B	601	CLA	C3B-C4B-NB	-3.69	107.09	110.52
43	17	316	A86	C41-C32-C40	-3.68	97.22	108.53
31	b	602	CLA	C3B-C4B-NB	-3.68	107.10	110.52
45	7	311	KC2	C3B-C2B-C1B	-3.68	103.56	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	11	313	CLA	CHB-C1B-NB	3.68	128.15	124.26
31	B	606	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
38	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
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
43	12	301	A86	C28-C27-C26	-3.68	117.77	122.92
43	16	305	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	P	602	CLA	C3B-C4B-NB	-3.67	107.11	110.52
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
42	5	313	KC1	C2D-C1D-ND	-3.67	107.77	110.23
43	14	305	A86	C8-C6-C5	-3.67	113.31	118.94
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
31	B	608	CLA	CMB-C2B-C1B	-3.66	119.79	125.37
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	405	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
43	16	306	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
45	1	311	KC2	CMD-C2D-C3D	3.65	135.80	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	304	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
31	14	306	CLA	C2A-C1A-CHA	3.65	130.25	123.86
43	16	305	A86	C19-C18-C17	3.65	117.83	110.77
43	0	305	A86	C40-C32-C31	3.65	113.74	110.47
37	d	404	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	305	A86	C25-C26-C27	-3.65	122.11	127.31
31	c	512	CLA	C3B-C4B-NB	-3.65	107.13	110.52
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	307	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
31	b	609	CLA	CMB-C2B-C1B	-3.64	119.83	125.37
43	3	305	A86	C19-C18-C17	3.64	117.80	110.77
37	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	314	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	D	409	LMG	O1-C1-C2	-3.63	102.64	108.30
43	14	303	A86	C17-C16-C15	3.62	112.86	109.16
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
43	6	305	A86	C14-C15-C16	-3.62	104.88	118.75
45	16	309	KC2	CAA-C2A-C1A	3.62	141.40	124.75
31	C	512	CLA	C3B-C4B-NB	-3.62	107.15	110.52
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	405	CLA	CAC-C3C-C4C	3.62	129.50	124.81
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
37	d	409	LMG	O1-C1-C2	-3.61	102.66	108.30
42	1	314	KC1	C3B-C2B-C1B	-3.61	103.62	107.08
34	8	301	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
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	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
43	16	305	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	301	A86	C21-C20-C19	-3.61	110.22	114.28
31	p	602	CLA	C3B-C4B-NB	-3.61	107.17	110.52
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	16	310	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	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
31	8	310	CLA	CMB-C2B-C1B	-3.59	119.89	125.37
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	311	KC2	C4B-C3B-C2B	-3.59	103.80	106.75
31	19	313	CLA	C2B-C1B-NB	3.59	112.64	110.23
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
31	10	311	CLA	CMB-C2B-C1B	-3.59	119.91	125.37
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
42	8	314	KC1	C2B-C1B-NB	3.58	112.74	110.10
43	6	305	A86	C19-C18-C17	3.58	117.69	110.77
45	18	308	KC2	CAC-C3C-C4C	3.58	141.14	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	311	CLA	CMB-C2B-C1B	-3.58	119.92	125.37
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
43	1	304	A86	C28-C27-C26	-3.57	117.92	122.92
31	16	307	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
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	303	A86	C22-C16-C17	-3.57	102.78	108.98
34	i	101	SQD	O47-C7-C8	3.57	119.19	111.50
31	15	312	CLA	C3B-C4B-NB	-3.56	107.21	110.52
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
31	8	307	CLA	CMB-C2B-C1B	-3.56	119.95	125.37
44	P	612	DD6	C12-C11-C10	-3.56	117.94	122.92
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
31	6	309	CLA	C3B-C4B-NB	-3.55	107.22	110.52
45	5	310	KC2	CHD-C1D-C2D	3.55	137.27	127.24
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	9	313	CLA	C2B-C1B-NB	3.55	112.61	110.23
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
42	7	314	KC1	CAD-C3D-C2D	-3.55	136.78	144.44
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	301	A86	C21-C20-C19	3.54	118.26	114.28
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
44	P	612	DD6	C37-C36-C35	3.54	120.91	114.36
38	W	203	DGD	O6D-C1D-O3G	-3.54	101.60	109.97
31	p	603	CLA	C3B-C4B-NB	-3.53	107.24	110.52
43	2	301	A86	C33-C32-C31	-3.53	105.78	109.21
42	15	317	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	302	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
38	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	303	A86	C4-C3-C2	-3.52	116.26	123.47
43	17	316	A86	C19-C18-C17	-3.52	103.97	110.77
31	11	308	CLA	CHB-C1B-NB	3.52	127.98	124.26
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
42	11	314	KC1	CHB-C1B-C2B	-3.52	118.10	125.48
31	19	315	CLA	CAA-C2A-C3A	-3.52	107.89	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	308	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
45	5	308	KC2	C2D-C1D-ND	-3.50	107.88	110.23
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
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	5	311	CLA	C2B-C1B-NB	-3.49	107.89	110.23
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	303	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
43	8	302	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
43	4	304	A86	C28-C27-C26	-3.49	118.04	122.92
45	12	309	KC2	C4B-C3B-C2B	-3.49	103.89	106.75
43	2	301	A86	C10-C9-C8	-3.49	112.34	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	16	313	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
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	7	310	CLA	CMB-C2B-C1B	-3.48	120.07	125.37
31	P	603	CLA	C3B-C4B-NB	-3.48	107.29	110.52
31	5	312	CLA	C3B-C4B-NB	-3.48	107.29	110.52
37	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
38	c	518	DGD	O6D-C5D-C6D	-3.48	99.65	106.67
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	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
37	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
43	16	301	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
38	C	518	DGD	O6D-C5D-C6D	-3.47	99.67	106.67
42	16	314	KC1	C4B-C3B-C2B	-3.47	103.91	106.75
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
31	p	606	CLA	CHB-C1B-NB	3.47	127.93	124.26
31	16	308	CLA	C3B-C4B-NB	-3.47	107.30	110.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	605	CLA	CHC-C4B-NB	3.46	127.92	124.26
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	13	310	CLA	CAA-C2A-C3A	-3.45	108.04	116.10
31	0	309	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
43	14	302	A86	C3-C2-C1	-3.45	122.39	127.31
31	c	506	CLA	CMB-C2B-C1B	-3.45	120.12	125.37
43	12	305	A86	O1-C15-C20	-3.45	56.03	59.40
42	16	314	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
37	5	315	LMG	O6-C1-O1	-3.44	101.82	109.97
31	P	606	CLA	CHB-C1B-NB	3.44	127.90	124.26
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
45	16	311	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
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	15	317	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	C	506	CLA	CMB-C2B-C1B	-3.43	120.15	125.37
31	14	312	CLA	CMB-C2B-C3B	3.43	134.89	126.59
31	b	612	CLA	CHC-C1C-NC	3.43	129.40	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	12	303	A86	O1-C20-C19	3.43	115.95	113.38
31	8	310	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	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
43	15	302	A86	C41-C32-C33	3.42	124.41	109.05
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
38	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
38	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	8	314	KC1	C2D-C1D-ND	-3.41	107.95	110.23
42	15	317	KC1	CAC-C3C-C4C	3.41	129.23	124.81
43	9	303	A86	O1-C15-C20	-3.41	56.07	59.40
38	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
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
45	8	309	KC2	CMD-C2D-C1D	-3.40	120.19	125.37
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	302	A86	O-C13-C14	-3.40	114.75	121.66
42	7	314	KC1	C3B-C2B-C1B	-3.40	103.83	107.08
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
31	P	607	CLA	C3B-C4B-NB	-3.39	107.37	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	18	311	CLA	CHB-C1B-NB	3.39	127.85	124.26
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
38	B	621	DGD	O2D-C2D-C1D	-3.39	101.81	110.05
42	7	314	KC1	C2D-C1D-ND	-3.39	107.96	110.23
43	1	302	A86	C36-C31-C32	3.39	123.06	119.70
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	1	308	CLA	CMB-C2B-C3B	3.38	134.77	126.59
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	C	513	CLA	CMB-C2B-C1B	-3.38	120.23	125.37
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
31	b	606	CLA	CHC-C4B-NB	3.38	127.83	124.26
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
38	c	518	DGD	O6D-C1D-O3G	-3.37	101.99	109.97
31	8	313	CLA	CHA-C4D-ND	3.37	139.55	132.50
43	5	304	A86	C36-C31-C32	-3.37	116.35	119.70
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	306	A86	C23-C16-C22	3.37	112.34	107.37
45	2	310	KC2	CAB-C3B-C2B	3.37	139.70	128.60
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
37	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
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	C	507	CLA	CMB-C2B-C1B	-3.36	120.25	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	312	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
31	14	306	CLA	CHA-C1A-NA	-3.36	118.70	126.40
38	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
31	c	513	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
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
37	p	614	LMG	O6-C1-C2	3.36	117.46	110.35
38	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
31	8	312	CLA	CHB-C1B-NB	3.36	127.81	124.26
31	c	507	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
37	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
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	d	406	CLA	C3B-C4B-NB	-3.36	107.40	110.52
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
42	2	313	KC1	CAD-C3D-C2D	-3.35	137.21	144.44
34	A	411	SQD	C3-C4-C5	3.35	116.22	110.24
43	14	302	A86	O1-C20-C19	-3.35	110.86	113.38
31	p	607	CLA	C3B-C4B-NB	-3.35	107.41	110.52
33	c	515	BCR	C3-C4-C5	-3.35	108.09	114.08
43	16	305	A86	C25-C26-C27	-3.35	122.53	127.31
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
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
43	15	301	A86	C25-C24-C1	-3.34	117.03	126.42
31	P	606	CLA	CHB-C1B-C2B	-3.34	117.81	127.24
42	12	314	KC1	CAD-C3D-C2D	-3.34	137.23	144.44
31	p	606	CLA	CHB-C1B-C2B	-3.34	117.81	127.24
45	8	311	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	12	308	CLA	CHB-C1B-NB	3.33	127.78	124.26
31	13	313	CLA	C2D-C1D-ND	-3.33	107.65	110.10
31	d	402	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
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	301	A86	C9-C8-C6	-3.33	117.06	126.42
43	16	305	A86	C-C1-C2	-3.33	118.26	122.92
43	7	302	A86	C9-C8-C6	-3.33	117.07	126.42
31	D	406	CLA	C3B-C4B-NB	-3.33	107.43	110.52
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
31	D	402	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
31	10	307	CLA	CMB-C2B-C3B	3.33	134.64	126.59
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	17	310	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
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
41	V	201	HEM	CAA-C2A-C3A	-3.32	119.46	127.07
31	c	509	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
45	15	308	KC2	C2D-C1D-ND	-3.32	108.00	110.23
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
31	10	309	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
45	11	311	KC2	CMD-C2D-C1D	-3.32	120.31	125.37
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	311	KC2	CBC-CAC-C3C	-3.32	111.12	127.62
31	0	313	CLA	CHB-C1B-NB	3.32	127.77	124.26
31	3	316	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
31	12	307	CLA	CHB-C1B-NB	3.31	127.77	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	303	A86	C34-O4-C38	-3.31	111.72	117.90
41	v	201	HEM	CAA-C2A-C3A	-3.31	119.48	127.07
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
45	8	309	KC2	CMD-C2D-C3D	3.31	134.86	125.93
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	304	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	A	406	CLA	C3B-C4B-NB	-3.30	107.45	110.52
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
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	306	A86	O4-C38-C39	3.29	117.14	111.09
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
31	8	307	CLA	CHB-C1B-NB	3.29	127.74	124.26
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
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
37	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	309	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	304	A86	O1-C15-C20	-3.27	56.20	59.40
43	16	305	A86	C3-C4-C5	-3.27	116.77	123.47
31	18	307	CLA	CHB-C1B-NB	3.27	127.72	124.26
31	0	307	CLA	CMB-C2B-C3B	3.27	134.51	126.59
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
45	10	310	KC2	CHD-C1D-C2D	3.27	136.47	127.24
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	303	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
43	14	302	A86	C34-O4-C38	-3.27	111.81	117.90
31	a	406	CLA	C3B-C4B-NB	-3.27	107.49	110.52
43	17	301	A86	C25-C24-C1	-3.26	117.25	126.42
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	3	309	KC2	CAC-C3C-C4C	3.26	139.67	124.47
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	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	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	D	406	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
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	313	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
42	17	314	KC1	C4D-C3D-CAD	3.25	109.61	107.42
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
42	5	313	KC1	C4D-C3D-C2D	-3.25	103.07	107.30
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
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
43	7	303	A86	O1-C15-C20	-3.24	56.23	59.40
31	c	505	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	d	406	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	4	312	CLA	CHB-C1B-C2B	-3.24	118.10	127.24
42	15	317	KC1	C1D-CHD-C4C	-3.24	118.66	126.34
42	6	315	KC1	C3D-C4D-ND	-3.24	105.53	110.17
34	A	411	SQD	C44-O6-C1	3.24	120.06	113.74
43	16	304	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
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	309	KC2	C4B-C3B-C2B	-3.23	104.10	106.75
43	3	302	A86	O1-C20-C21	3.23	118.92	115.06
37	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	308	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
37	4	316	LMG	C9-C8-C7	-3.22	104.17	111.79
43	17	304	A86	O1-C15-C20	-3.22	56.25	59.40
43	6	301	A86	O1-C15-C20	-3.22	56.25	59.40
37	1	301	LMG	O6-C1-O1	-3.22	102.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	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	14	306	CLA	CHB-C1B-C2B	-3.21	118.16	127.24
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
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
45	3	311	KC2	CBC-CAC-C3C	-3.21	111.65	127.62
42	0	315	KC1	CHD-C1D-C2D	3.21	136.30	127.24
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	307	CLA	O2D-CGD-CBD	3.21	116.97	111.27
45	15	310	KC2	CHD-C1D-C2D	3.21	136.29	127.24
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	302	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
37	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
38	C	519	DGD	O3G-C3G-C2G	-3.20	103.17	110.90
38	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
43	17	301	A86	C22-C16-C17	-3.20	103.42	108.98
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
43	3	306	A86	C34-O4-C38	3.20	123.85	117.90
35	d	407	PL9	C36-C34-C33	-3.20	114.65	121.12
43	3	305	A86	O-C13-C14	3.20	128.15	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	311	CLA	C2D-C1D-ND	-3.20	107.75	110.10
38	b	622	DGD	O5D-C6D-C5D	-3.20	103.13	109.05
43	2	305	A86	C3-C2-C1	-3.19	122.75	127.31
42	13	314	KC1	OBD-CAD-C3D	-3.19	120.84	128.52
31	p	606	CLA	CMB-C2B-C3B	3.19	134.32	126.59
31	9	313	CLA	C3C-C4C-NC	-3.19	106.99	110.57
43	8	304	A86	C28-C27-C26	-3.19	118.45	122.92
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
31	P	606	CLA	CMB-C2B-C3B	3.19	134.31	126.59
43	15	302	A86	O1-C20-C21	3.19	118.87	115.06
31	6	314	CLA	C3B-C4B-NB	-3.19	107.56	110.52
45	2	310	KC2	C4B-C3B-C2B	-3.19	104.14	106.75
31	c	503	CLA	CHB-C1B-NB	-3.19	120.89	124.26
31	10	316	CLA	C3B-C4B-NB	-3.18	107.56	110.52
45	18	308	KC2	CAA-C2A-C1A	3.18	139.38	124.75
35	D	407	PL9	C36-C34-C33	-3.18	114.67	121.12
31	b	605	CLA	C1-C2-C3	-3.18	120.54	126.04
38	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	315	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	305	A86	C4-C3-C2	-3.18	116.97	123.47
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
37	D	404	LMG	O3-C3-C2	-3.18	103.00	110.35
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
31	a	404	CLA	CMB-C2B-C1B	-3.17	120.53	125.37
31	c	508	CLA	CHB-C4A-NA	3.17	128.90	124.51
45	1	309	KC2	O2D-CGD-O1D	-3.17	117.63	123.84
43	16	304	A86	C3-C4-C5	-3.17	116.97	123.47
42	12	314	KC1	CMD-C2D-C1D	-3.17	120.54	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	14	308	KC2	C2D-C1D-ND	-3.17	108.11	110.23
37	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	a	404	CLA	CHB-C1B-NB	3.17	127.61	124.26
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
38	C	518	DGD	O2D-C2D-C1D	-3.16	102.36	110.05
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
45	4	308	KC2	C2D-C1D-ND	-3.16	108.11	110.23
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	314	KC1	C4B-C3B-C2B	-3.16	104.16	106.75
31	18	309	CLA	CMB-C2B-C3B	3.16	134.24	126.59
33	Y	101	BCR	C3-C4-C5	-3.16	108.44	114.08
38	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
31	11	308	CLA	CMB-C2B-C3B	3.16	134.24	126.59
31	C	510	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
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	309	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
38	c	518	DGD	O2D-C2D-C1D	-3.15	102.39	110.05
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	503	CLA	CHC-C1C-NC	3.15	128.99	124.20
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	b	617	CLA	CHB-C1B-NB	3.15	127.59	124.26
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
31	A	404	CLA	CMB-C2B-C1B	-3.14	120.58	125.37
31	c	510	CLA	CMB-C2B-C1B	-3.14	120.58	125.37
43	1	305	A86	O1-C15-C20	-3.14	56.33	59.40
31	B	604	CLA	CHB-C4A-NA	3.14	128.86	124.51
43	16	301	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
31	c	507	CLA	CHB-C1B-NB	3.14	127.58	124.26
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
37	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	B	611	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
31	C	507	CLA	CHB-C1B-NB	3.13	127.58	124.26
31	B	607	CLA	CHB-C1B-NB	3.13	127.57	124.26
37	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
42	10	315	KC1	CHD-C1D-C2D	3.13	136.08	127.24
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
31	C	503	CLA	CHB-C1B-NB	-3.13	120.94	124.26
37	K	101	LMG	O1-C7-C8	-3.13	103.34	110.90
31	8	313	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
38	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
31	b	603	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
37	P	614	LMG	O6-C1-O1	-3.13	102.57	109.97
31	b	608	CLA	CHB-C1B-NB	3.13	127.57	124.26
37	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	313	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
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	315	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
31	P	610	CLA	CMB-C2B-C1B	-3.12	120.61	125.37
31	4	309	CLA	CMB-C2B-C1B	-3.12	120.62	125.37
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
31	B	616	CLA	CHB-C1B-NB	3.12	127.56	124.26
31	19	310	CLA	CMB-C2B-C1B	-3.12	120.62	125.37
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
38	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
31	B	602	CLA	CMB-C2B-C1B	-3.11	120.63	125.37
43	3	302	A86	C36-C31-C32	3.11	122.78	119.70
35	d	407	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
31	A	404	CLA	CHB-C1B-NB	3.11	127.55	124.26
35	D	407	PL9	C22-C23-C24	-3.11	120.17	127.66
43	12	304	A86	C28-C27-C26	-3.11	118.57	122.92
37	d	404	LMG	O3-C3-C2	-3.11	103.16	110.35
43	2	302	A86	C41-C32-C31	-3.11	107.69	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	305	A86	C3-C4-C5	-3.11	117.11	123.47
31	p	610	CLA	CMB-C2B-C1B	-3.11	120.64	125.37
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
37	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
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
38	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
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
45	11	309	KC2	CMD-C2D-C1D	-3.10	120.65	125.37
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
31	13	308	CLA	CHB-C1B-NB	3.10	127.54	124.26
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	314	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
37	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
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	4	307	CLA	CMB-C2B-C1B	-3.09	120.66	125.37
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	406	CLA	CHB-C4A-NA	3.09	128.78	124.51
43	10	305	A86	C22-C16-C17	-3.09	103.62	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	18	313	KC1	CHD-C1D-C2D	3.09	135.96	127.24
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
38	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
43	4	302	A86	C9-C8-C6	-3.08	117.75	126.42
31	C	509	CLA	CHB-C1B-NB	3.08	127.52	124.26
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
37	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	403	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	310	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	18	306	CLA	C3B-C4B-NB	-3.08	107.66	110.52
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	403	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	306	A86	C41-C32-C31	3.07	113.22	110.47
37	p	614	LMG	O1-C1-C2	-3.07	103.51	108.30
31	d	405	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
45	15	308	KC2	C3C-C2C-C1C	3.07	108.76	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	306	A86	C22-C16-C17	-3.07	103.65	108.98
31	A	404	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
42	16	314	KC1	C1B-CHB-C4A	-3.07	119.44	126.06
31	17	315	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
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	12	308	CLA	C3B-C4B-NB	-3.07	107.67	110.52
31	D	406	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
45	4	310	KC2	CHB-C1B-C2B	-3.06	119.06	125.48
42	16	314	KC1	CHD-C1D-C2D	3.06	135.89	127.24
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
38	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
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	306	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	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
31	9	310	CLA	CMB-C2B-C1B	-3.05	120.72	125.37
31	c	503	CLA	C3B-C4B-NB	3.05	113.35	110.52
43	12	302	A86	C40-C32-C33	3.05	122.76	109.05
45	8	311	KC2	C3B-C2B-C1B	-3.05	104.16	107.08
38	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

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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
42	15	317	KC1	CAD-C3D-C2D	-3.05	137.86	144.44
31	3	313	CLA	CMB-C2B-C3B	3.05	133.97	126.59
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
31	c	509	CLA	CHB-C1B-NB	3.05	127.48	124.26
45	18	308	KC2	CMD-C2D-C3D	3.05	134.16	125.93
31	d	405	CLA	CHB-C1B-NB	3.05	127.48	124.26
31	2	312	CLA	CHB-C1B-C2B	-3.05	118.63	127.24
43	6	307	A86	O1-C15-C20	-3.05	56.42	59.40
31	13	315	CLA	C3B-C4B-NB	-3.05	107.69	110.52
31	18	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	8	310	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
31	C	503	CLA	C3B-C4B-NB	3.05	113.34	110.52
31	B	606	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
31	B	612	CLA	CMB-C2B-C1B	-3.04	120.73	125.37
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
38	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
38	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	405	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
38	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
43	6	303	A86	C21-C20-C19	-3.04	110.86	114.28
31	p	604	CLA	C3B-C4B-NB	-3.04	107.70	110.52
38	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	0	309	CLA	C3B-C4B-NB	-3.04	107.70	110.52
31	0	316	CLA	C3B-C4B-NB	-3.04	107.70	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	13	310	CLA	C3B-C4B-NB	-3.04	107.70	110.52
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
31	b	613	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
45	3	311	KC2	CAB-C3B-C4B	-3.03	117.58	124.90
31	5	312	CLA	CHC-C4B-NB	3.03	127.47	124.26
43	9	305	A86	O-C13-C11	-3.03	114.45	121.15
43	8	304	A86	C26-C25-C24	-3.03	113.77	123.22
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
31	z	103	CLA	CHB-C1B-NB	3.02	127.46	124.26
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
43	16	301	A86	C22-C16-C17	-3.02	103.74	108.98
31	4	307	CLA	C3B-C4B-NB	-3.02	107.72	110.52
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
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	14	312	CLA	CHB-C1B-C2B	-3.01	118.72	127.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	313	CLA	CHD-C1D-C2D	3.01	131.80	125.48
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
45	12	309	KC2	CHD-C1D-C2D	3.01	135.74	127.24
43	16	302	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
31	19	308	CLA	CMB-C2B-C1B	-3.01	120.78	125.37
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	14	312	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
31	D	405	CLA	CHB-C1B-NB	3.01	127.44	124.26
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	P	604	CLA	C3B-C4B-NB	-3.01	107.72	110.52
31	14	307	CLA	C3B-C4B-NB	-3.01	107.72	110.52
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	311	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	B	610	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
31	1	307	CLA	CHB-C1B-NB	3.00	127.43	124.26
37	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	5	309	CLA	O2D-CGD-O1D	-2.99	117.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	15	313	CLA	C3B-C4B-NB	-2.99	107.74	110.52
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	303	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	308	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
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
31	C	502	CLA	C3B-C4B-NB	-2.99	107.74	110.52
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	b	612	CLA	CHB-C1B-NB	2.99	127.42	124.26
45	19	309	KC2	CHD-C1D-C2D	2.99	135.68	127.24
31	8	310	CLA	CMB-C2B-C3B	2.99	133.82	126.59
31	2	315	CLA	C2D-C1D-ND	2.99	112.30	110.10
45	4	310	KC2	CHD-C1D-C2D	2.98	135.67	127.24
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
43	0	306	A86	C36-C31-C32	-2.98	116.74	119.70
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	B	611	CLA	CHB-C1B-NB	2.98	127.41	124.26
43	13	302	A86	C3-C4-C5	-2.98	117.38	123.47
43	16	305	A86	C28-C27-C26	-2.98	118.75	122.92
31	16	308	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	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
31	c	502	CLA	C3B-C4B-NB	-2.97	107.76	110.52
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
31	8	315	CLA	C3B-C4B-NB	-2.97	107.76	110.52
31	19	313	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
45	17	311	KC2	CAD-C3D-C2D	-2.97	138.03	144.44
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	314	KC1	CAA-CBA-CGA	-2.97	112.01	127.26
43	16	303	A86	C9-C8-C6	-2.97	118.08	126.42
31	15	309	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
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
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
31	11	310	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
43	16	301	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	p	604	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
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
43	12	304	A86	C34-O4-C38	-2.96	112.39	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	10	307	CLA	C3B-C4B-NB	-2.96	107.77	110.52
43	17	301	A86	O1-C15-C20	-2.96	56.51	59.40
31	b	605	CLA	CHC-C4B-NB	2.96	127.39	124.26
41	V	201	HEM	CAA-CBA-CGA	-2.96	107.24	113.60
31	19	315	CLA	CHB-C4A-NA	2.96	128.60	124.51
31	8	308	CLA	OBD-CAD-C3D	2.96	135.63	128.52
45	8	309	KC2	C3B-C2B-C1B	-2.96	104.25	107.08
31	C	503	CLA	CMB-C2B-C3B	-2.96	119.43	126.59
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
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
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	313	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
31	3	310	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
45	16	311	KC2	C3C-C2C-C1C	-2.95	104.30	106.49
43	8	305	A86	C9-C10-C11	-2.95	117.94	126.61
31	R	101	CLA	CHB-C4A-NA	2.95	128.59	124.51
31	P	604	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
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	306	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	8	308	CLA	C3B-C4B-NB	-2.95	107.78	110.52
31	C	509	CLA	CHB-C4A-NA	2.95	128.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	503	CLA	CMB-C2B-C3B	-2.95	119.45	126.59
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	402	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
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	15	317	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	314	KC1	CMA-C3A-C4A	-2.94	120.56	125.04
31	c	504	CLA	C3B-C4B-NB	-2.94	107.79	110.52
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	402	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	8	307	CLA	C2A-C1A-CHA	2.94	129.00	123.86
45	16	311	KC2	CAB-C3B-C2B	2.94	138.29	128.60
43	8	303	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
31	1	313	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
43	5	302	A86	C4-C3-C2	-2.94	117.45	123.47
31	B	604	CLA	CHC-C4B-NB	2.94	127.37	124.26
31	P	603	CLA	CMD-C2D-C1D	-2.94	119.53	124.71
37	J	101	LMG	O1-C7-C8	-2.94	103.81	110.90
45	1	311	KC2	CMD-C2D-C1D	-2.94	120.89	125.37
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
41	v	201	HEM	CAA-CBA-CGA	-2.94	107.28	113.60
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	305	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
45	3	311	KC2	CAD-C3D-C2D	-2.93	138.11	144.44
38	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	0	309	CLA	CMB-C2B-C3B	2.93	133.68	126.59
31	17	307	CLA	CHB-C4A-NA	2.93	128.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	610	CLA	C3B-C4B-NB	-2.93	107.80	110.52
42	15	317	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
37	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
38	c	519	DGD	C3G-C2G-C1G	-2.92	104.87	111.79
43	16	301	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	311	KC2	CBC-CAC-C3C	-2.92	113.09	127.62
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
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
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
38	b	622	DGD	C2G-O2G-C1B	2.92	124.98	117.79
43	8	304	A86	O4-C34-C33	2.92	114.86	107.59
31	P	607	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
34	8	301	SQD	C44-O6-C1	2.92	119.44	113.74
38	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	303	A86	C10-C9-C8	-2.92	114.12	123.22
45	16	309	KC2	CMD-C2D-C1D	2.92	129.81	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	305	A86	O1-C15-C20	-2.91	56.55	59.40
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
31	2	314	CLA	C3B-C4B-NB	-2.91	107.81	110.52
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	307	CLA	C2A-C1A-CHA	2.91	128.95	123.86
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	402	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
45	7	311	KC2	CAD-C3D-C2D	-2.91	138.17	144.44
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	C	504	CLA	C3B-C4B-NB	-2.91	107.82	110.52
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
37	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
31	14	309	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
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
31	3	315	CLA	C3B-C4B-NB	-2.90	107.83	110.52
45	16	311	KC2	C2A-C1A-NA	2.90	114.05	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	307	CLA	CHB-C4A-NA	2.90	128.52	124.51
43	0	306	A86	O1-C15-C20	-2.90	56.57	59.40
31	15	311	CLA	C3B-C2B-C1B	2.90	110.66	107.16
31	2	309	CLA	CMB-C2B-C1B	-2.90	120.96	125.37
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	311	KC2	CAB-C3B-C4B	-2.90	117.90	124.90
31	p	601	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
31	1	312	CLA	C3B-C4B-NB	-2.90	107.83	110.52
42	18	313	KC1	C3D-C4D-ND	-2.90	106.01	110.17
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	303	A86	C4-C3-C2	-2.89	117.55	123.47
35	D	407	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	304	A86	C10-C9-C8	-2.89	114.19	123.22
43	1	306	A86	C36-C31-C32	-2.89	116.83	119.70
43	0	305	A86	C9-C8-C6	-2.89	118.29	126.42
31	16	307	CLA	CAC-C3C-C2C	-2.89	122.58	127.53
31	10	312	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
43	19	303	A86	O4-C38-O5	-2.89	117.22	122.96
31	14	307	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
31	d	402	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	C	509	CLA	CMB-C2B-C3B	2.89	133.58	126.59
31	18	307	CLA	CHB-C4A-NA	2.89	128.50	124.51
42	13	314	KC1	C1D-CHD-C4C	-2.88	119.50	126.34
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	b	611	CLA	C3B-C4B-NB	-2.88	107.84	110.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	603	CLA	CHB-C4A-NA	2.88	128.50	124.51
31	8	315	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
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
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
31	c	509	CLA	CMB-C2B-C3B	2.88	133.56	126.59
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
43	4	306	A86	C20-C19-C18	2.88	118.44	112.75
31	19	307	CLA	CHB-C4A-NA	2.88	128.49	124.51
31	10	309	CLA	C3B-C4B-NB	-2.88	107.85	110.52
37	w	201	LMG	O6-C5-C4	2.88	114.92	109.69
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
37	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
31	8	312	CLA	CHC-C4B-NB	2.87	127.30	124.26
43	6	301	A86	C34-O4-C38	-2.87	112.54	117.90
45	9	309	KC2	CHD-C1D-C2D	2.87	135.35	127.24
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	301	A86	C34-O4-C38	-2.87	112.54	117.90
43	15	305	A86	O4-C38-C39	2.87	116.37	111.09
31	C	504	CLA	CMB-C2B-C1B	-2.87	121.00	125.37
31	10	311	CLA	CMB-C2B-C3B	2.87	133.54	126.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	314	KC1	C3B-C2B-C1B	-2.87	104.34	107.08
31	9	313	CLA	CAA-C2A-C1A	-2.87	102.58	111.97
31	r	101	CLA	C3B-C4B-NB	-2.87	107.86	110.52
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
31	7	310	CLA	CMB-C2B-C3B	2.86	133.53	126.59
31	a	403	CLA	C3B-C4B-NB	-2.86	107.86	110.52
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	407	PL9	O1-C4-C3	-2.86	117.57	120.72
31	c	504	CLA	CMB-C2B-C1B	-2.86	121.01	125.37
45	10	310	KC2	C1D-CHD-C4C	-2.86	119.55	126.34
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
37	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
38	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
38	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	R	101	CLA	C3B-C4B-NB	-2.86	107.86	110.52
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
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	14	310	KC2	CAD-C3D-C2D	-2.86	138.27	144.44
43	8	302	A86	C9-C8-C6	-2.86	118.39	126.42
31	C	509	CLA	C3B-C4B-NB	-2.86	107.86	110.52
43	5	304	A86	O1-C15-C20	-2.86	56.61	59.40
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	a	403	CLA	CMB-C2B-C3B	2.85	133.50	126.59
31	C	511	CLA	CMB-C2B-C1B	-2.85	121.02	125.37
31	c	511	CLA	CMB-C2B-C1B	-2.85	121.02	125.37
45	10	310	KC2	CAB-C3B-C4B	-2.85	118.01	124.90
31	2	307	CLA	CBC-CAC-C3C	2.85	120.29	112.43
31	0	311	CLA	CMB-C2B-C3B	2.85	133.50	126.59
31	A	403	CLA	CMB-C2B-C3B	2.85	133.50	126.59
43	8	305	A86	O4-C38-O5	-2.85	117.30	122.96
43	13	305	A86	O4-C38-O5	-2.85	117.30	122.96
37	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
42	13	314	KC1	C4D-C3D-C2D	-2.85	103.58	107.30
43	19	303	A86	O1-C20-C19	2.85	115.52	113.38
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
37	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	c	509	CLA	C3B-C4B-NB	-2.85	107.87	110.52
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
31	A	403	CLA	C3B-C4B-NB	-2.84	107.88	110.52
34	A	408	SQD	O8-S-C6	2.84	110.27	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	12	315	CLA	C3B-C4B-NB	-2.84	107.88	110.52
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
37	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
37	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	9	308	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
31	P	607	CLA	CBA-CAA-C2A	-2.84	108.03	114.02
42	9	314	KC1	C3B-C2B-C1B	-2.84	104.36	107.08
31	5	314	CLA	C3B-C4B-NB	-2.84	107.88	110.52
43	9	302	A86	C23-C16-C17	-2.84	104.05	108.98
31	0	314	CLA	C3B-C4B-NB	-2.84	107.88	110.52
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
43	7	301	A86	O4-C34-C35	2.83	114.65	107.59
38	B	621	DGD	C3G-O3G-C1D	2.83	119.28	113.74
38	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
37	F	102	LMG	O6-C1-O1	-2.83	103.26	109.97
41	v	201	HEM	CBA-CAA-C2A	2.83	120.50	112.63
41	v	201	HEM	C4A-NA-C1A	2.83	108.12	105.35
31	10	309	CLA	CMB-C2B-C3B	2.83	133.45	126.59
38	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
45	0	310	KC2	C1D-CHD-C4C	-2.83	119.62	126.34
43	16	301	A86	C3-C4-C5	-2.83	117.68	123.47
31	10	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	16	313	CLA	CMB-C2B-C3B	2.83	133.44	126.59
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	409	PL9	C7-C3-C2	-2.83	119.58	123.30
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
37	D	404	LMG	C4-C3-C2	2.82	115.75	110.82
43	3	305	A86	C25-C24-C1	-2.82	118.49	126.42
31	3	312	CLA	CHB-C1B-NB	2.82	127.25	124.26
31	b	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
42	10	315	KC1	CBD-CHA-C4D	-2.82	102.39	109.14
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	613	CLA	CMB-C2B-C1B	-2.82	121.07	125.37
43	13	304	A86	C41-C32-C40	-2.82	99.87	108.53
41	V	201	HEM	C4A-NA-C1A	2.82	108.11	105.35
43	15	304	A86	C34-O4-C38	2.82	123.15	117.90
42	17	314	KC1	CHD-C1D-C2D	2.82	135.20	127.24
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
37	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
43	17	301	A86	O4-C38-O5	-2.82	117.36	122.96
45	14	310	KC2	CHD-C1D-C2D	2.82	135.19	127.24
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
41	V	201	HEM	CBA-CAA-C2A	2.82	120.45	112.63
31	C	508	CLA	C2A-C1A-CHA	2.82	128.78	123.86
31	16	312	CLA	CHC-C4B-NB	2.82	127.24	124.26
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
31	10	317	CLA	CHB-C1B-NB	2.81	127.24	124.26
31	0	313	CLA	CHB-C4A-NA	2.81	128.40	124.51
43	2	304	A86	C28-C27-C26	-2.81	118.98	122.92
38	h	102	DGD	C1E-O6E-C5E	2.81	119.21	113.69
42	10	315	KC1	C1D-CHD-C4C	-2.81	119.67	126.34
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
42	P	609	KC1	CHD-C1D-C2D	2.81	135.18	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	z	101	CLA	C3B-C4B-NB	-2.81	107.91	110.52
43	16	303	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
45	13	309	KC2	C1D-CHD-C4C	-2.81	119.68	126.34
43	1	320	A86	O1-C15-C20	-2.81	56.65	59.40
42	p	609	KC1	CHD-C1D-C2D	2.81	135.17	127.24
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
31	p	602	CLA	CHB-C1B-NB	2.81	127.23	124.26
31	4	307	CLA	CHB-C1B-NB	2.81	127.23	124.26
43	14	301	A86	O4-C38-O5	-2.81	117.39	122.96
31	D	405	CLA	CMC-C2C-C1C	2.81	129.31	125.04
35	A	409	PL9	C7-C3-C2	-2.81	119.61	123.30
31	b	614	CLA	CMB-C2B-C1B	-2.81	121.10	125.37
42	4	313	KC1	C1A-NA-C4A	-2.80	105.44	106.71
31	c	503	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
31	3	308	CLA	CHB-C1B-NB	2.80	127.23	124.26
31	17	310	CLA	CMB-C2B-C3B	2.80	133.38	126.59
36	8	316	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	b	606	CLA	C1-C2-C3	-2.80	121.20	126.04
31	Z	101	CLA	C3B-C4B-NB	-2.80	107.92	110.52
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
31	w	203	CLA	C3B-C4B-NB	-2.80	107.92	110.52
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
45	0	310	KC2	CHD-C1D-C2D	2.80	135.14	127.24

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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	C	503	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
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	12	316	CLA	C3B-C4B-NB	-2.80	107.92	110.52
31	5	314	CLA	CHB-C4A-NA	2.80	128.38	124.51
37	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
45	18	310	KC2	C3A-C4A-NA	2.79	113.62	110.57
45	18	310	KC2	CAD-C3D-C2D	-2.79	138.41	144.44
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
31	7	315	CLA	C3B-C4B-NB	-2.79	107.92	110.52
31	10	311	CLA	C3B-C4B-NB	-2.79	107.92	110.52
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
43	8	304	A86	C3-C4-C5	-2.79	117.76	123.47
31	d	405	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	313	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
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
45	5	310	KC2	CHD-C4C-NC	2.79	128.43	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	3	314	KC1	CHD-C1D-C2D	2.79	135.10	127.24
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
31	P	602	CLA	CHB-C1B-NB	2.78	127.20	124.26
43	17	306	A86	C4-C3-C2	-2.78	117.77	123.47
37	d	404	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	308	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
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
37	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	8	313	CLA	CAA-CBA-CGA	2.78	121.38	113.25
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
31	0	307	CLA	C3B-C4B-NB	-2.78	107.94	110.52
41	v	201	HEM	C1C-CHC-C4B	-2.78	120.06	126.06
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
42	4	313	KC1	C4D-C3D-CAD	2.78	109.29	107.42
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
42	14	313	KC1	CHD-C1D-C2D	2.78	135.08	127.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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
35	D	407	PL9	C7-C8-C9	-2.77	122.18	126.79
31	18	307	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
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
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	C	513	CLA	CMB-C2B-C3B	2.77	133.29	126.59
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	407	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	12	307	CLA	C2B-C1B-NB	2.76	112.08	110.23
31	B	604	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
31	c	511	CLA	C3B-C4B-NB	-2.76	107.95	110.52
42	8	314	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	c	506	CLA	CMB-C2B-C3B	2.76	133.28	126.59
31	14	307	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
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	315	CLA	CHB-C4A-NA	2.76	128.33	124.51
42	7	314	KC1	CMB-C2B-C1B	2.76	129.57	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
43	11	302	A86	C7-C6-C5	-2.76	119.06	122.92
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
37	D	404	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
43	1	302	A86	C40-C32-C33	2.75	121.41	109.05
31	18	307	CLA	C3B-C4B-NB	-2.75	107.96	110.52
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	301	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
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
43	0	301	A86	C8-C6-C5	2.75	123.16	118.94
31	4	314	CLA	CHB-C1B-NB	2.75	127.16	124.26
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
31	C	506	CLA	CMB-C2B-C3B	2.74	133.24	126.59
43	6	307	A86	C-C1-C24	2.74	122.40	118.08
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
31	3	312	CLA	CHC-C4B-NB	2.74	127.16	124.26
34	a	408	SQD	O6-C1-C2	2.74	112.58	108.30
45	2	310	KC2	CAD-C3D-C2D	-2.74	138.52	144.44
43	9	304	A86	O1-C15-C20	-2.74	56.72	59.40
31	18	314	CLA	C3B-C4B-NB	-2.74	107.97	110.52
34	L	102	SQD	C4-C3-C2	2.74	115.61	110.82
31	18	312	CLA	CMB-C2B-C1B	-2.74	121.19	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	1	314	KC1	C4B-C3B-C2B	-2.74	104.50	106.75
31	14	309	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
43	14	301	A86	C41-C32-C31	-2.74	108.02	110.47
45	3	309	KC2	CMD-C2D-C3D	2.74	133.32	125.93
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	c	513	CLA	CMB-C2B-C3B	2.74	133.22	126.59
31	p	603	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
43	8	302	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
31	a	403	CLA	CHB-C1B-NB	2.73	127.15	124.26
38	C	520	DGD	CDB-CCB-CBB	-2.73	100.55	114.42
41	V	201	HEM	C1C-CHC-C4B	-2.73	120.16	126.06
43	13	302	A86	O1-C20-C19	2.73	115.44	113.38
31	c	512	CLA	CHC-C4B-NB	2.73	127.15	124.26
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	C	512	CLA	CHC-C4B-NB	2.73	127.15	124.26
31	B	607	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
31	9	312	CLA	CHB-C4A-NA	2.73	128.29	124.51
31	2	311	CLA	CHB-C1B-NB	2.73	127.15	124.26
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
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
31	C	511	CLA	C3B-C4B-NB	-2.73	107.98	110.52
38	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	14	312	CLA	CHA-C1A-NA	-2.73	120.15	126.40
31	3	315	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
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
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	17	312	CLA	C3B-C4B-NB	-2.72	107.99	110.52
37	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
45	16	309	KC2	C3B-C2B-C1B	-2.72	104.47	107.08
41	v	201	HEM	CHD-C1D-ND	2.72	127.38	124.42
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
31	b	608	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
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
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	6	314	CLA	C2B-C1B-NB	-2.72	108.41	110.23
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	305	A86	C23-C16-C17	2.72	113.70	108.98
31	11	312	CLA	C3B-C4B-NB	-2.71	108.00	110.52
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	305	A86	C20-C19-C18	-2.71	107.38	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	311	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
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
31	12	308	CLA	CMB-C2B-C3B	2.71	133.16	126.59
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
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	6	313	CLA	C3B-C4B-NB	-2.71	108.00	110.52
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
38	h	102	DGD	CDB-CCB-CBB	-2.71	100.68	114.42
31	c	508	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	c	514	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	c	509	CLA	CMD-C2D-C3D	2.71	133.84	127.61
45	16	309	KC2	O2D-CGD-O1D	-2.71	118.55	123.84
31	8	312	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
31	18	311	CLA	C3B-C4B-NB	-2.71	108.00	110.52
31	p	606	CLA	CMB-C2B-C1B	-2.70	121.25	125.37
38	H	102	DGD	CDB-CCB-CBB	-2.70	100.70	114.42
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	605	CLA	CHB-C4A-NA	2.70	128.25	124.51
31	0	311	CLA	C3B-C4B-NB	-2.70	108.01	110.52
34	8	301	SQD	O48-C23-O10	-2.70	116.78	123.59
38	B	621	DGD	C5B-C4B-C3B	-2.70	100.72	114.42
45	8	309	KC2	O2D-CGD-O1D	-2.70	118.56	123.84
42	8	314	KC1	C3A-C4A-NA	2.70	113.52	110.57
31	0	313	CLA	CAC-C3C-C4C	2.70	128.31	124.81
31	14	307	CLA	CHB-C1B-NB	2.70	127.11	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	W	202	CLA	C3B-C4B-NB	-2.70	108.01	110.52
45	18	308	KC2	CMD-C2D-C1D	-2.70	121.26	125.37
31	B	606	CLA	C3A-C2A-C1A	2.70	105.38	101.34
43	16	302	A86	O1-C15-C20	-2.69	56.77	59.40
31	P	604	CLA	CHB-C1B-NB	2.69	127.11	124.26
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
45	5	310	KC2	C2D-C1D-ND	-2.69	108.43	110.23
43	12	302	A86	C4-C3-C2	-2.69	117.96	123.47
45	6	310	KC2	C3B-C2B-C1B	-2.69	104.50	107.08
45	4	310	KC2	CAD-C3D-C2D	-2.69	138.63	144.44
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
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
31	C	514	CLA	C3B-C4B-NB	-2.69	108.02	110.52
45	1	309	KC2	C2A-C1A-CHA	-2.69	118.54	127.44
31	P	606	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
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
37	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
37	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
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	16	312	CLA	C3B-C4B-NB	-2.68	108.03	110.52
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	313	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	17	305	A86	C-C1-C2	-2.68	119.17	122.92
31	B	603	CLA	CHC-C4B-NB	2.68	127.09	124.26
43	0	306	A86	C9-C8-C6	-2.68	118.89	126.42
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	311	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
45	8	309	KC2	CAC-C3C-C2C	-2.68	119.78	128.60
43	8	305	A86	C3-C4-C5	-2.68	117.99	123.47
31	14	314	CLA	CHB-C1B-NB	2.68	127.09	124.26
31	4	309	CLA	CMB-C2B-C3B	2.68	133.07	126.59
41	V	201	HEM	CHD-C1D-ND	2.68	127.33	124.42
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	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
37	d	409	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	305	A86	O4-C34-C35	2.67	114.25	107.59
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	0	313	CLA	CHC-C4B-NB	2.67	127.09	124.26
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
31	2	312	CLA	CMB-C2B-C3B	2.67	133.06	126.59
43	16	303	A86	C41-C32-C31	-2.67	108.08	110.47
42	0	315	KC1	C4C-C3C-C2C	-2.67	103.00	106.90
38	c	519	DGD	CDB-CCB-CBB	-2.67	100.87	114.42
43	16	306	A86	C9-C8-C6	-2.67	118.92	126.42
31	1	308	CLA	C3B-C4B-NB	-2.67	108.04	110.52
43	6	305	A86	C20-C19-C18	-2.67	107.47	112.75
31	0	312	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
31	a	406	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
31	14	311	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
45	19	309	KC2	C2A-C3A-C4A	2.67	108.47	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	10	313	CLA	CHC-C4B-NB	2.67	127.08	124.26
31	A	406	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
43	17	301	A86	C34-O4-C38	-2.67	112.93	117.90
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	313	CLA	CHC-C4B-NB	2.67	127.08	124.26
31	7	308	CLA	CHB-C1B-NB	2.67	127.08	124.26
43	13	301	A86	O4-C34-C35	2.67	114.23	107.59
45	16	309	KC2	CAC-C3C-C4C	2.66	136.89	124.47
43	0	304	A86	C4-C5-C6	-2.66	123.51	127.31
45	15	308	KC2	O2D-CGD-O1D	-2.66	118.63	123.84
31	13	310	CLA	CHB-C4A-NA	2.66	128.19	124.51
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
37	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	14	313	KC1	CED-O2D-CGD	2.66	121.95	115.94
32	D	403	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	A	403	CLA	CHB-C1B-NB	2.66	127.07	124.26
42	5	313	KC1	CGD-CBD-CAD	-2.66	102.13	110.73
31	b	605	CLA	C3B-C2B-C1B	2.66	110.37	107.16
43	11	304	A86	O1-C20-C19	2.66	115.38	113.38
38	C	519	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
42	15	317	KC1	C2D-C1D-ND	-2.66	108.45	110.23
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	312	CLA	CAA-C2A-C3A	-2.65	105.51	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	1	314	KC1	C2D-C1D-ND	-2.65	108.45	110.23
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	402	CLA	O2D-CGD-CBD	2.65	115.98	111.27
44	p	612	DD6	C32-C31-C36	-2.65	118.89	122.63
37	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	304	A86	C41-C32-C31	2.65	112.84	110.47
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
37	D	409	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
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	403	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
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	B	603	CLA	C3B-C4B-NB	-2.64	108.06	110.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	19	312	CLA	CHB-C4A-NA	2.64	128.17	124.51
43	5	302	A86	C26-C25-C24	-2.64	114.97	123.22
31	C	508	CLA	C3B-C4B-NB	-2.64	108.06	110.52
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
31	b	604	CLA	C3B-C4B-NB	-2.64	108.06	110.52
43	3	302	A86	O4-C34-C35	2.64	114.17	107.59
38	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	c	510	CLA	CMB-C2B-C3B	2.64	132.98	126.59
45	13	311	KC2	C1D-CHD-C4C	-2.64	120.08	126.34
31	B	612	CLA	CMB-C2B-C3B	2.64	132.98	126.59
31	b	613	CLA	CMB-C2B-C3B	2.64	132.98	126.59
31	16	307	CLA	C3A-C2A-C1A	2.64	105.29	101.34
38	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	305	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	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
45	11	309	KC2	CHD-C1D-C2D	2.63	134.68	127.24
31	C	510	CLA	CMB-C2B-C3B	2.63	132.97	126.59
43	6	306	A86	C9-C8-C6	-2.63	119.02	126.42
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
31	P	603	CLA	CHB-C1B-NB	2.63	127.05	124.26
31	p	604	CLA	CHB-C1B-NB	2.63	127.05	124.26
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	8	307	CLA	C3B-C4B-NB	-2.63	108.07	110.52
31	p	603	CLA	CMD-C2D-C3D	2.63	133.67	127.61
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	316	CLA	C1D-ND-C4D	-2.63	104.47	106.33
34	8	301	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
37	K	101	LMG	O3-C3-C2	-2.63	104.27	110.35
37	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	311	KC2	C3A-C4A-NA	2.63	113.44	110.57
38	c	520	DGD	O2D-C2D-C1D	-2.63	103.67	110.05
31	B	603	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	D	402	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	311	KC2	CAB-C3B-C4B	-2.62	118.56	124.90
31	b	604	CLA	CHC-C4B-NB	2.62	127.03	124.26
33	c	515	BCR	C11-C10-C9	-2.62	123.56	127.31
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	405	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	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
31	11	307	CLA	C3B-C4B-NB	-2.62	108.08	110.52
33	Y	101	BCR	C38-C26-C27	-2.62	108.58	113.62
43	0	303	A86	O4-C34-C35	-2.62	101.07	107.59
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	b	613	CLA	C3B-C4B-NB	-2.62	108.08	110.52
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
42	5	313	KC1	C1D-CHD-C4C	-2.62	120.13	126.34
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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
31	6	314	CLA	CMB-C2B-C3B	2.61	132.92	126.59
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
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
37	n	701	LMG	O7-C10-O9	-2.61	117.39	123.70
31	d	405	CLA	CBC-CAC-C3C	2.61	119.63	112.43
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	310	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
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	302	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	302	A86	C25-C24-C1	-2.61	119.09	126.42
38	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	307	CLA	O2D-CGD-CBD	2.61	115.90	111.27
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
31	13	308	CLA	CMB-C2B-C3B	2.61	132.90	126.59
43	16	306	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
31	19	307	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	312	CLA	CHB-C1B-NB	2.60	127.01	124.26
31	17	312	CLA	CHB-C1B-NB	2.60	127.01	124.26
31	12	312	CLA	C2A-C1A-CHA	2.60	128.41	123.86
43	16	304	A86	C4-C3-C2	-2.60	118.14	123.47
31	8	313	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
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
31	12	313	CLA	CHB-C1B-C2B	-2.60	119.89	127.24
43	12	306	A86	O3-C36-C37	-2.60	104.76	109.39
37	B	620	LMG	C38-C37-C36	-2.60	101.22	114.42
31	7	313	CLA	CMB-C2B-C3B	2.60	132.89	126.59
43	0	303	A86	C20-C19-C18	2.60	117.89	112.75
38	1	318	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
37	d	404	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	317	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
38	C	519	DGD	O3E-C3E-C2E	-2.60	104.35	110.35
38	c	519	DGD	O3E-C3E-C2E	-2.60	104.35	110.35
45	16	309	KC2	CBC-CAC-C3C	-2.60	114.71	127.62
37	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	P	604	CLA	CMB-C2B-C3B	2.59	132.87	126.59
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
43	8	302	A86	C20-C19-C18	-2.59	107.62	112.75
42	p	609	KC1	CAC-C3C-C4C	2.59	128.17	124.81
37	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
31	b	615	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	0	313	CLA	C3A-C2A-C1A	2.59	105.22	101.34
31	17	315	CLA	C3B-C4B-NB	-2.59	108.11	110.52
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
37	D	409	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
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	16	311	KC2	CAD-C3D-C2D	-2.59	138.85	144.44
45	14	310	KC2	CGD-CBD-CAD	-2.59	102.35	110.73
42	1	314	KC1	CHD-C1D-C2D	2.59	134.54	127.24
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	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
31	B	604	CLA	C3B-C2B-C1B	2.59	110.28	107.16
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	311	KC2	O2D-CGD-O1D	-2.58	118.79	123.84
37	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
37	F	102	LMG	O3-C3-C2	-2.58	104.38	110.35
43	7	302	A86	C9-C10-C11	-2.58	119.02	126.61
37	d	409	LMG	C9-C8-C7	-2.58	105.68	111.79
43	16	305	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
43	4	306	A86	C8-C6-C5	-2.58	114.98	118.94
43	8	302	A86	C3-C4-C5	-2.58	118.19	123.47
37	J	101	LMG	O6-C1-O1	-2.58	103.86	109.97
31	3	316	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	8	307	CLA	C3A-C2A-C1A	2.58	105.20	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	10	307	CLA	CHB-C1B-C2B	-2.58	119.95	127.24
33	B	617	BCR	C11-C10-C9	-2.58	123.63	127.31
45	15	308	KC2	C3A-C4A-NA	2.58	113.39	110.57
31	B	605	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	c	507	CLA	C3B-C4B-NB	-2.58	108.12	110.52
31	p	604	CLA	CMB-C2B-C3B	2.58	132.83	126.59
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	610	CLA	CMB-C2B-C1B	-2.58	121.45	125.37
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
31	d	405	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
43	14	305	A86	C20-C19-C18	2.57	117.84	112.75
43	4	305	A86	C28-C27-C26	-2.57	119.32	122.92
31	p	603	CLA	CHB-C1B-NB	2.57	126.98	124.26
31	2	315	CLA	CHD-C4C-NC	2.57	128.26	124.20
43	8	306	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	17	308	CLA	CHB-C1B-NB	2.57	126.98	124.26
31	B	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	18	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
43	5	302	A86	C3-C4-C5	-2.57	118.21	123.47
31	19	315	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	19	308	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
37	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
31	b	615	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	19	310	CLA	CMB-C2B-C3B	2.57	132.81	126.59
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
43	16	301	A86	O4-C38-O5	-2.57	117.86	122.96
31	5	309	CLA	CMB-C2B-C1B	-2.57	121.46	125.37
31	B	606	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	0	312	CLA	CAC-C3C-C4C	-2.57	121.48	124.81
31	8	312	CLA	O2D-CGD-O1D	-2.57	118.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	9	314	KC1	C2B-C1B-NB	2.57	112.00	110.10
43	3	302	A86	C7-C6-C5	-2.57	119.33	122.92
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
31	B	608	CLA	CMB-C2B-C3B	2.56	132.80	126.59
33	B	619	BCR	C20-C21-C22	-2.56	123.65	127.31
31	B	614	CLA	C3B-C4B-NB	-2.56	108.14	110.52
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	6	309	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
38	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
31	B	614	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
43	5	303	A86	C25-C24-C1	-2.56	119.22	126.42
31	p	601	CLA	C3B-C4B-NB	-2.56	108.14	110.52
31	11	308	CLA	C3B-C4B-NB	-2.56	108.14	110.52
31	11	316	CLA	C3B-C4B-NB	-2.56	108.14	110.52
31	15	312	CLA	CHC-C4B-NB	2.56	126.97	124.26
33	f	101	BCR	C27-C26-C25	2.56	126.45	122.73
37	w	201	LMG	O2-C2-C1	-2.56	103.83	110.05
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
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
37	n	701	LMG	O6-C1-O1	-2.56	103.92	109.97
45	12	309	KC2	CAD-C3D-C2D	-2.56	138.92	144.44
33	C	515	BCR	C2-C1-C6	2.56	114.42	110.48
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	308	CLA	CAC-C3C-C4C	2.56	128.13	124.81
42	p	609	KC1	CAD-C3D-C2D	-2.56	138.92	144.44
31	16	313	CLA	C3D-C4D-CHA	-2.56	106.88	112.72
31	11	310	CLA	C1-C2-C3	-2.56	122.62	126.75
45	6	312	KC2	CAD-C3D-C2D	-2.56	138.92	144.44
31	8	308	CLA	CHB-C1B-NB	2.56	126.96	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	603	CLA	CHC-C1C-NC	2.55	128.08	124.20
38	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
42	5	313	KC1	CAD-C3D-C2D	2.55	149.95	144.44
43	11	320	A86	C17-C16-C15	2.55	111.77	109.16
45	14	308	KC2	O2D-CGD-O1D	-2.55	118.85	123.84
31	D	402	CLA	C1-C2-C3	-2.55	121.63	126.04
37	11	317	LMG	O7-C10-O9	-2.55	117.54	123.70
31	14	309	CLA	CMB-C2B-C3B	2.55	132.76	126.59
35	D	407	PL9	C40-C39-C41	2.55	119.56	115.27
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
31	P	601	CLA	C3B-C4B-NB	-2.55	108.15	110.52
43	0	304	A86	C10-C9-C8	-2.55	115.27	123.22
38	C	519	DGD	O3G-C1D-C2D	-2.55	104.33	108.30
31	B	606	CLA	CHB-C1B-NB	2.55	126.95	124.26
43	16	304	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
37	14	316	LMG	O7-C10-C11	2.55	116.99	111.50
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	D	405	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
31	19	315	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
38	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	8	313	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
38	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	B	609	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	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	307	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
37	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	A	403	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
31	d	402	CLA	C1-C2-C3	-2.54	121.65	126.04
31	17	307	CLA	C2D-C1D-ND	-2.54	108.23	110.10
31	6	316	CLA	C3B-C4B-NB	-2.54	108.16	110.52
34	10	320	SQD	C44-O6-C1	2.54	118.70	113.74
31	b	607	CLA	C3C-C4C-NC	-2.54	107.73	110.57
45	2	310	KC2	CHD-C1D-C2D	2.54	134.40	127.24
31	p	605	CLA	CAA-C2A-C3A	-2.54	110.18	116.10
43	16	304	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
37	p	614	LMG	O3-C3-C2	-2.54	104.49	110.35
35	d	407	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	7	307	CLA	C3B-C4B-NB	-2.53	108.17	110.52
37	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	16	304	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	507	CLA	C3B-C4B-NB	-2.53	108.17	110.52
42	P	609	KC1	CAD-C3D-C2D	-2.53	138.98	144.44
31	b	609	CLA	CMB-C2B-C3B	2.53	132.72	126.59
31	c	512	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	8	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
43	11	303	A86	C19-C18-C17	-2.53	105.89	110.77
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
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
31	12	307	CLA	CHB-C1B-C2B	-2.53	120.10	127.24
45	18	308	KC2	CAC-C3C-C2C	-2.53	120.28	128.60
37	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
31	c	510	CLA	CHD-C1D-ND	-2.53	122.13	124.45
37	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	B	610	CLA	CHB-C1B-NB	2.53	126.93	124.26
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
37	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	405	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
31	b	607	CLA	CHB-C1B-NB	2.52	126.93	124.26
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
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
31	b	611	CLA	CHB-C1B-NB	2.52	126.93	124.26
43	4	302	A86	O1-C15-C20	-2.52	56.93	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	316	LHG	C11-C10-C9	-2.52	101.64	114.42
31	p	603	CLA	CGD-CBD-CAD	-2.52	102.58	110.73
31	11	315	CLA	CHB-C1B-NB	2.52	126.92	124.26
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	b	614	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
31	3	310	CLA	CMB-C2B-C3B	2.52	132.68	126.59
43	8	303	A86	C25-C24-C1	-2.52	119.35	126.42
31	D	405	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
33	c	516	BCR	C29-C30-C25	2.52	114.35	110.48
31	b	602	CLA	CHB-C1B-NB	2.52	126.92	124.26
37	d	404	LMG	O6-C1-O1	-2.52	104.02	109.97
43	3	301	A86	C7-C6-C8	2.52	122.04	118.08
43	16	303	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
37	B	620	LMG	O6-C1-C2	-2.51	105.03	110.35
31	15	307	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
42	15	317	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	306	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	408	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	304	A86	C40-C32-C31	-2.51	108.22	110.47
43	6	304	A86	O2-C18-C17	-2.51	104.81	109.80
31	9	310	CLA	CMB-C2B-C3B	2.51	132.67	126.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	308	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
31	b	609	CLA	CHB-C1B-NB	2.51	126.91	124.26
31	16	313	CLA	C2B-C1B-NB	-2.51	108.55	110.23
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	16	310	CLA	CMB-C2B-C1B	-2.50	121.55	125.37
31	b	616	CLA	C2A-C1A-CHA	2.50	128.24	123.86
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
37	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
41	E	101	HEM	C1B-NB-C4B	2.50	107.66	105.07
31	C	511	CLA	CMB-C2B-C3B	2.50	132.65	126.59
31	c	511	CLA	CMB-C2B-C3B	2.50	132.65	126.59
43	8	303	A86	C12-C11-C13	2.50	120.23	116.02
31	9	315	CLA	C3B-C4B-NB	-2.50	108.19	110.52
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
38	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	408	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	304	A86	C14-C15-C16	2.50	128.33	118.75
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
37	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
37	5	316	LMG	O3-C3-C2	-2.50	104.57	110.35
38	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
31	B	611	CLA	CMB-C2B-C3B	2.50	132.64	126.59
43	8	306	A86	C22-C16-C17	-2.50	104.64	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	313	CLA	C4D-C3D-CAD	2.50	111.04	108.10
31	P	610	CLA	C3B-C4B-NB	-2.50	108.20	110.52
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
45	1	311	KC2	CHD-C1D-C2D	2.50	134.29	127.24
43	0	303	A86	O2-C18-C17	-2.50	104.84	109.80
37	b	621	LMG	O6-C1-C2	-2.50	105.07	110.35
31	7	307	CLA	CHB-C1B-NB	2.49	126.90	124.26
43	7	305	A86	C26-C25-C24	-2.49	115.43	123.22
38	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
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
31	6	313	CLA	CHB-C1B-NB	2.49	126.89	124.26
43	12	301	A86	O-C13-C14	-2.49	116.60	121.66
45	14	308	KC2	CGD-CBD-CAD	-2.49	102.67	110.73
31	b	607	CLA	CBA-CAA-C2A	2.49	121.22	113.86
38	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
45	8	311	KC2	CAD-C3D-C2D	-2.49	139.06	144.44
31	d	402	CLA	CMB-C2B-C3B	2.49	132.62	126.59
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
31	b	606	CLA	C3B-C4B-NB	-2.49	108.20	110.52
43	11	305	A86	C25-C24-C1	-2.49	119.42	126.42
31	9	307	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
42	15	317	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	304	A86	O3-C36-C37	-2.49	104.97	109.39
37	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	312	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
31	15	313	CLA	CHB-C1B-NB	2.49	126.89	124.26
31	D	402	CLA	CMB-C2B-C3B	2.49	132.61	126.59
37	B	620	LMG	C40-C39-C38	-2.48	101.81	114.42
42	8	314	KC1	CAD-C3D-C2D	-2.48	139.08	144.44
38	C	519	DGD	O5D-C6D-C5D	-2.48	104.45	109.05
31	P	610	CLA	CMB-C2B-C3B	2.48	132.60	126.59
31	b	605	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
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
31	6	309	CLA	CHB-C1B-NB	2.48	126.89	124.26
43	16	303	A86	C3-C4-C5	-2.48	118.39	123.47
31	12	310	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
43	11	319	A86	O1-C15-C20	-2.48	56.97	59.40
43	10	318	A86	C4-C3-C2	-2.48	118.39	123.47
31	p	610	CLA	CMB-C2B-C3B	2.48	132.60	126.59
31	B	608	CLA	CHB-C1B-NB	2.48	126.88	124.26
43	6	303	A86	C4-C3-C2	-2.48	118.39	123.47
37	15	315	LMG	O3-C3-C2	-2.48	104.61	110.35
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	304	A86	C9-C10-C11	-2.48	119.31	126.61
31	B	604	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
43	11	319	A86	O4-C34-C35	2.48	113.77	107.59
43	16	304	A86	C10-C9-C8	-2.48	115.48	123.22
43	16	304	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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	402	CLA	CHD-C1D-ND	-2.48	122.18	124.45
31	7	313	CLA	CHB-C1B-C2B	-2.48	120.25	127.24
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
31	5	309	CLA	CMB-C2B-C3B	2.48	132.58	126.59
45	5	310	KC2	C2A-C3A-C4A	2.47	108.32	106.49
31	1	308	CLA	CHB-C1B-NB	2.47	126.88	124.26
31	16	308	CLA	CHB-C1B-NB	2.47	126.88	124.26
38	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	5	314	CLA	CHB-C1B-NB	2.47	126.88	124.26
31	0	313	CLA	O2D-CGD-CBD	2.47	115.66	111.27
31	B	601	CLA	CHB-C1B-NB	2.47	126.88	124.26
31	C	504	CLA	C2A-C1A-CHA	2.47	128.18	123.86
31	16	315	CLA	C3B-C4B-NB	-2.47	108.22	110.52
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
31	3	307	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
37	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
31	10	314	CLA	C3B-C4B-NB	-2.47	108.22	110.52
37	m	101	LMG	O2-C2-C1	-2.47	104.04	110.05
31	b	612	CLA	CMB-C2B-C3B	2.47	132.57	126.59
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
31	3	316	CLA	CHC-C4B-NB	2.47	126.87	124.26
45	1	309	KC2	C2D-C1D-ND	-2.47	108.58	110.23
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	10	316	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	15	309	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
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
42	4	313	KC1	CHD-C1D-C2D	2.47	134.21	127.24
31	9	312	CLA	C3B-C4B-NB	-2.47	108.23	110.52
38	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	16	310	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
33	c	516	BCR	C11-C10-C9	-2.47	123.79	127.31
31	5	309	CLA	C3B-C4B-NB	-2.47	108.23	110.52
35	A	409	PL9	O1-C4-C3	-2.47	118.00	120.72
31	3	313	CLA	CHB-C1B-C2B	-2.46	120.28	127.24
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	2	309	CLA	CMB-C2B-C3B	2.46	132.55	126.59
31	10	314	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
31	b	614	CLA	C3B-C4B-NB	-2.46	108.23	110.52
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
38	w	204	DGD	C3G-C2G-C1G	-2.46	105.97	111.79
31	p	610	CLA	C3B-C4B-NB	-2.46	108.23	110.52
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
38	C	520	DGD	C3G-C2G-C1G	-2.46	105.97	111.79
45	14	308	KC2	C1D-CHD-C4C	-2.46	120.51	126.34
31	b	602	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	311	CLA	CHB-C1B-NB	2.46	126.86	124.26
31	13	316	CLA	CAA-C2A-C1A	-2.46	103.92	111.97
31	a	404	CLA	CMB-C2B-C3B	2.46	132.54	126.59
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	403	PHO	O2D-CGD-CBD	2.46	114.11	111.00
31	P	607	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
31	9	313	CLA	CMB-C2B-C3B	2.45	132.53	126.59
37	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
31	0	309	CLA	CHB-C1B-NB	2.45	126.86	124.26
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
43	9	305	A86	C40-C32-C31	2.45	112.67	110.47
31	19	312	CLA	C3B-C4B-NB	-2.45	108.24	110.52
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
37	B	620	LMG	C6-C5-C4	-2.45	107.26	113.00
43	19	304	A86	C9-C8-C6	-2.45	119.53	126.42
31	b	607	CLA	C3B-C4B-NB	-2.45	108.24	110.52
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	5	307	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
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
37	w	201	LMG	C6-C5-C4	-2.45	107.27	113.00
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	7	309	KC2	CBC-CAC-C3C	-2.45	115.44	127.62
43	P	611	A86	C35-C34-C33	2.45	114.14	109.88
37	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
45	12	311	KC2	CHD-C1D-C2D	2.45	134.15	127.24
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
37	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
37	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
37	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	408	LHG	C5-O7-C7	-2.44	111.78	117.79
43	1	306	A86	O4-C38-O5	-2.44	118.11	122.96
31	12	316	CLA	CHB-C1B-NB	2.44	126.84	124.26
43	12	305	A86	O3-C36-C37	-2.44	105.05	109.39
38	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
31	8	313	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
43	8	303	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
38	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	7	312	CLA	CHC-C4B-NB	2.44	126.84	124.26
31	10	311	CLA	CHB-C1B-NB	2.44	126.84	124.26
31	A	404	CLA	CMB-C2B-C3B	2.44	132.50	126.59
31	0	316	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
37	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
38	c	520	DGD	C3G-C2G-C1G	-2.44	106.02	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	B	613	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	C	502	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
34	8	301	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
37	W	201	LMG	C6-C5-C4	-2.44	107.30	113.00
37	b	621	LMG	C6-C5-C4	-2.44	107.30	113.00
37	b	621	LMG	O6-C1-O1	-2.44	104.20	109.97
31	15	306	CLA	CAC-C3C-C2C	-2.44	123.36	127.53
37	4	316	LMG	O7-C10-O9	-2.44	117.82	123.70
31	1	321	CLA	CHB-C1B-C2B	-2.44	120.36	127.24
37	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	403	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	c	504	CLA	C2A-C1A-CHA	2.43	128.11	123.86
31	19	308	CLA	CMB-C2B-C3B	2.43	132.48	126.59
42	6	315	KC1	C3A-C4A-NA	2.43	113.23	110.57
37	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	308	CLA	CAC-C3C-C4C	2.43	127.96	124.81
43	0	301	A86	C7-C6-C5	-2.43	119.52	122.92
31	6	311	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
31	p	602	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
38	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	301	A86	O1-C15-C20	-2.43	57.02	59.40
31	11	313	CLA	CMD-C2D-C3D	2.43	133.20	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	19	311	CLA	C3A-C2A-C1A	2.43	104.98	101.34
45	11	311	KC2	CHD-C1D-C2D	2.43	134.10	127.24
43	p	613	A86	C20-C19-C18	2.43	117.55	112.75
37	C	522	LMG	C38-C37-C36	-2.43	102.10	114.42
35	d	407	PL9	C31-C32-C33	-2.43	103.90	111.88
31	p	606	CLA	CHC-C1C-NC	2.43	127.89	124.20
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	304	A86	C28-C27-C29	2.43	124.55	118.93
37	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
31	16	312	CLA	CHB-C1B-NB	2.43	126.83	124.26
33	f	101	BCR	C35-C13-C14	-2.43	119.52	122.92
37	P	614	LMG	O2-C2-C1	-2.43	104.15	110.05
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	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
31	C	514	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
38	B	621	DGD	C7B-C6B-C5B	-2.42	102.12	114.42
31	2	311	CLA	C3B-C4B-NB	-2.42	108.27	110.52
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	407	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
37	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
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	402	CLA	CHD-C1D-ND	-2.42	122.23	124.45
31	1	312	CLA	C2A-C1A-CHA	2.42	128.09	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	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	408	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
37	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
45	6	310	KC2	CMD-C2D-C1D	2.42	129.05	125.37
31	19	315	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
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
42	16	314	KC1	C3D-C4D-ND	-2.42	106.70	110.17
31	c	502	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
31	b	605	CLA	CHD-C4C-NC	2.42	128.01	124.20
31	10	316	CLA	CMB-C2B-C3B	2.42	132.44	126.59
42	14	313	KC1	C1D-CHD-C4C	-2.42	120.61	126.34
31	15	306	CLA	C3B-C4B-NB	-2.42	108.27	110.52
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	304	A86	C25-C24-C1	-2.41	119.64	126.42
38	11	318	DGD	O3D-C3D-C4D	-2.41	104.77	110.35
31	d	406	CLA	CHB-C1B-NB	2.41	126.81	124.26
31	16	313	CLA	C2A-C3A-C4A	2.41	105.77	101.87
43	8	302	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
31	4	311	CLA	CMB-C2B-C3B	2.41	132.43	126.59
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})
37	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
31	B	608	CLA	C3B-C4B-NB	-2.41	108.28	110.52
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
45	4	308	KC2	C1D-CHD-C4C	-2.41	120.62	126.34
42	P	609	KC1	CGD-CBD-CAD	-2.41	102.93	110.73
43	16	303	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
31	d	402	CLA	CHB-C1B-NB	2.41	126.81	124.26
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
38	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
37	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
37	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
31	19	311	CLA	C3B-C4B-NB	-2.40	108.28	110.52
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
37	N	101	LMG	O8-C28-O10	-2.40	117.52	123.59
31	1	316	CLA	CHC-C4B-NB	2.40	126.80	124.26
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	304	A86	C7-C6-C8	2.40	121.86	118.08
43	10	318	A86	C25-C26-C27	-2.40	123.88	127.31
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
45	18	308	KC2	CBC-CAC-C3C	-2.40	115.67	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	7	313	CLA	CHB-C4A-NA	2.40	127.83	124.51
33	y	101	BCR	C35-C13-C14	-2.40	119.56	122.92
37	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	302	A86	O5-C38-C39	-2.40	116.07	124.81
42	15	317	KC1	C4C-C3C-C2C	-2.40	103.40	106.90
43	10	318	A86	C33-C32-C31	-2.40	106.88	109.21
31	12	307	CLA	C3B-C4B-NB	-2.40	108.29	110.52
31	7	315	CLA	CHB-C1B-NB	2.40	126.80	124.26
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
37	W	201	LMG	O8-C28-O10	-2.40	117.54	123.59
31	14	311	CLA	CHC-C4B-NB	2.40	126.80	124.26
31	A	404	CLA	C3B-C4B-NB	-2.40	108.29	110.52
37	k	101	LMG	C40-C39-C38	-2.40	102.25	114.42
31	A	406	CLA	CMB-C2B-C3B	2.40	132.39	126.59
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	17	311	KC2	CHD-C1D-C2D	2.40	134.00	127.24
45	16	311	KC2	O2D-CGD-O1D	-2.40	119.16	123.84
43	5	302	A86	O1-C20-C19	2.39	115.18	113.38
37	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	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	10	316	CLA	CMB-C2B-C1B	-2.39	121.72	125.37
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
31	9	312	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
31	13	308	CLA	C3B-C4B-NB	-2.39	108.30	110.52
43	12	306	A86	O4-C34-C35	2.39	113.55	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
38	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
45	8	311	KC2	CHD-C1D-C2D	2.39	133.99	127.24
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
31	13	307	CLA	C2D-C1D-ND	-2.39	108.34	110.10
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
38	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
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
31	19	312	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
31	6	311	CLA	CHC-C4B-NB	2.39	126.78	124.26
31	11	316	CLA	CHB-C1B-NB	2.39	126.78	124.26
43	8	304	A86	O4-C38-O5	2.39	127.70	122.96
31	8	313	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
37	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
37	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
31	p	602	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
43	8	302	A86	C9-C10-C11	-2.39	119.59	126.61
31	11	315	CLA	C3B-C4B-NB	-2.39	108.30	110.52
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
38	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	6	308	CLA	CHC-C4B-NB	2.39	126.78	124.26
31	C	504	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
31	c	514	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	309	KC2	CBC-CAC-C3C	-2.38	115.76	127.62
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
31	a	406	CLA	CMB-C2B-C3B	2.38	132.36	126.59
36	D	408	LHG	C11-C10-C9	-2.38	102.33	114.42
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
38	11	318	DGD	C3G-C2G-C1G	-2.38	106.15	111.79
31	C	504	CLA	CMB-C2B-C3B	2.38	132.36	126.59
31	c	504	CLA	CMB-C2B-C3B	2.38	132.36	126.59
37	k	101	LMG	C9-C8-C7	-2.38	106.16	111.79
43	14	305	A86	O2-C18-C17	-2.38	105.07	109.80
37	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
37	d	409	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	408	LHG	C11-C10-C9	-2.38	102.35	114.42
33	b	619	BCR	C31-C1-C6	2.38	114.16	110.30
31	15	309	CLA	C3B-C4B-NB	-2.38	108.31	110.52
45	7	311	KC2	C2A-C3A-C4A	2.38	108.25	106.49
38	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	305	A86	O4-C38-O5	-2.38	118.24	122.96
43	2	304	A86	O1-C15-C20	-2.38	57.08	59.40
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
37	C	522	LMG	O2-C2-C1	-2.38	104.27	110.05
31	14	311	CLA	CMB-C2B-C3B	2.38	132.34	126.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	521	LMG	C40-C39-C38	-2.37	102.37	114.42
31	8	308	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
43	15	303	A86	C4-C3-C2	-2.37	118.61	123.47
37	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
31	D	406	CLA	CHB-C1B-NB	2.37	126.77	124.26
43	5	304	A86	C40-C32-C33	-2.37	98.39	109.05
31	c	513	CLA	C3B-C4B-NB	-2.37	108.31	110.52
43	7	301	A86	C23-C16-C22	-2.37	103.87	107.37
31	b	603	CLA	CMB-C2B-C3B	2.37	132.34	126.59
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
37	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
32	A	405	PHO	C1-C2-C3	-2.37	121.94	126.04
31	P	605	CLA	C3B-C4B-NB	-2.37	108.31	110.52
31	p	605	CLA	C3B-C4B-NB	-2.37	108.31	110.52
37	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	4	307	CLA	CMB-C2B-C3B	2.37	132.33	126.59
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
31	D	402	CLA	CHB-C1B-NB	2.37	126.77	124.26
31	c	508	CLA	CHC-C4B-NB	2.37	126.77	124.26
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
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
37	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
31	P	602	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
37	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
38	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
37	D	409	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	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
38	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	C	505	CLA	CAC-C3C-C4C	2.37	127.88	124.81
38	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
37	14	316	LMG	C3-C4-C5	-2.36	106.02	110.24
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
37	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	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	8	307	CLA	CMB-C2B-C3B	2.36	132.31	126.59
31	12	307	CLA	C3C-C4C-NC	-2.36	107.92	110.57
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	612	CLA	CMD-C2D-C3D	2.36	133.05	127.61
38	c	520	DGD	O3D-C3D-C4D	-2.36	104.89	110.35
31	4	311	CLA	CHC-C4B-NB	2.36	126.76	124.26
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	10	317	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	15	311	CLA	CHA-C1A-NA	-2.36	120.99	126.40
38	C	520	DGD	O6E-C1E-O5D	-2.36	104.38	109.97
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
37	D	409	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
37	c	522	LMG	O2-C2-C1	-2.36	104.32	110.05
31	a	404	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	1	310	CLA	C3B-C4B-NB	-2.36	108.33	110.52
31	C	503	CLA	C2A-C1A-CHA	2.36	127.98	123.86
31	14	315	CLA	C2B-C1B-NB	2.36	111.81	110.23
33	B	619	BCR	C27-C26-C25	2.36	126.16	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	17	309	KC2	C2A-C3A-C4A	2.36	108.23	106.49
42	9	314	KC1	CHD-C1D-C2D	2.36	133.90	127.24
42	11	314	KC1	C1D-CHD-C4C	-2.36	120.75	126.34
31	7	313	CLA	C1-C2-C3	-2.36	122.94	126.75
31	10	317	CLA	CHB-C4A-NA	2.36	127.77	124.51
37	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
42	12	314	KC1	C1D-CHD-C4C	-2.36	120.75	126.34
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	b	613	CLA	CHC-C4B-NB	2.35	126.75	124.26
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
38	1	318	DGD	C5B-C4B-C3B	-2.35	102.48	114.42
31	b	609	CLA	C3B-C4B-NB	-2.35	108.33	110.52
45	12	309	KC2	C1D-CHD-C4C	-2.35	120.76	126.34
37	d	409	LMG	O7-C10-O9	-2.35	118.02	123.70
42	15	317	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
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
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
42	11	314	KC1	CHD-C1D-C2D	2.35	133.87	127.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	604	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
31	2	311	CLA	CHC-C4B-NB	2.35	126.74	124.26
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
41	v	201	HEM	CHA-C1A-C2A	2.35	130.49	125.36
33	b	618	BCR	C15-C14-C13	-2.35	123.96	127.31
38	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
45	2	310	KC2	C2D-C1D-ND	-2.35	108.66	110.23
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
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	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
38	B	621	DGD	C6D-O5D-C1E	2.34	118.32	113.74
31	9	315	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
43	10	305	A86	O-C13-C14	2.34	126.42	121.66
31	B	612	CLA	CHC-C4B-NB	2.34	126.74	124.26
31	18	307	CLA	OBD-CAD-C3D	2.34	134.16	128.52
38	c	520	DGD	O6E-C1E-O5D	-2.34	104.42	109.97
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
41	e	101	HEM	C4A-NA-C1A	2.34	107.64	105.35
37	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	602	CLA	CMB-C2B-C3B	2.34	132.26	126.59
31	11	307	CLA	CHB-C1B-C2B	-2.34	120.62	127.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	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
42	0	315	KC1	C2D-C1D-ND	-2.34	108.66	110.23
31	C	508	CLA	CHC-C4B-NB	2.34	126.73	124.26
41	V	201	HEM	CHA-C1A-C2A	2.34	130.47	125.36
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
31	0	316	CLA	CMB-C2B-C3B	2.34	132.25	126.59
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
42	7	314	KC1	C1D-CHD-C4C	-2.34	120.80	126.34
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	2	306	CLA	CMB-C2B-C3B	2.34	132.25	126.59
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
43	17	302	A86	C20-C19-C18	2.34	117.37	112.75
43	16	302	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
38	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	407	PL9	C8-C7-C3	2.33	118.58	111.98
35	d	407	PL9	C8-C7-C3	2.33	118.58	111.98
31	15	309	CLA	CMB-C2B-C3B	2.33	132.24	126.59
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
31	z	103	CLA	CMB-C2B-C1B	-2.33	121.82	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
42	4	313	KC1	C1D-CHD-C4C	-2.33	120.81	126.34
31	0	312	CLA	CMC-C2C-C1C	-2.33	121.49	125.04
31	8	312	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	304	A86	O4-C38-O5	-2.33	118.34	122.96
31	C	513	CLA	C3B-C4B-NB	-2.33	108.36	110.52
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	303	A86	C19-C18-C17	-2.33	106.28	110.77
37	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
31	13	308	CLA	C3A-C2A-C1A	2.32	104.82	101.34
37	k	101	LMG	C38-C37-C36	-2.32	102.63	114.42
31	16	312	CLA	CHB-C4A-NA	2.32	127.72	124.51
43	12	304	A86	C8-C6-C5	2.32	122.51	118.94
31	W	202	CLA	CHB-C1B-NB	2.32	126.72	124.26
43	6	304	A86	O4-C38-O5	-2.32	118.35	122.96
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
31	z	103	CLA	C3B-C4B-NB	-2.32	108.36	110.52
38	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
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
32	a	405	PHO	C1C-C2C-C3C	-2.32	106.68	108.61
43	9	305	A86	O4-C38-O5	-2.32	118.35	122.96
43	8	306	A86	C4-C3-C2	-2.32	118.72	123.47
37	11	317	LMG	C38-C37-C36	-2.32	102.65	114.42
43	8	304	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	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
42	15	317	KC1	C3D-C4D-ND	-2.32	106.84	110.17
38	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
31	B	603	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
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
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
38	c	520	DGD	O3E-C3E-C2E	-2.31	105.00	110.35
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	9	308	CLA	CMB-C2B-C3B	2.31	132.19	126.59
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
42	19	314	KC1	CHD-C1D-C2D	2.31	133.76	127.24
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
37	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	312	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	406	CLA	O2D-CGD-CBD	2.31	115.37	111.27
36	a	410	LHG	C11-C10-C9	-2.31	102.71	114.42
42	3	314	KC1	C2D-C1D-ND	-2.31	108.69	110.23
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
31	11	310	CLA	C3B-C4B-NB	-2.31	108.38	110.52
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	314	KC1	CAA-C2A-C1A	2.31	135.35	124.75
31	1	313	CLA	CHA-C1A-NA	-2.31	121.12	126.40
31	18	311	CLA	CHC-C4B-NB	2.31	126.70	124.26
32	A	405	PHO	C1C-C2C-C3C	-2.31	106.69	108.61
43	10	302	A86	C25-C24-C1	-2.31	119.94	126.42
42	19	314	KC1	CAD-C3D-C2D	-2.30	139.47	144.44
43	16	303	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
38	11	318	DGD	C5B-C4B-C3B	-2.30	102.73	114.42
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
38	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
42	19	314	KC1	CMD-C2D-C3D	2.30	132.15	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	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	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
37	W	201	LMG	C38-C37-C36	-2.30	102.76	114.42
31	19	313	CLA	CMB-C2B-C3B	2.30	132.15	126.59
45	16	311	KC2	C2B-C1B-NB	2.30	111.80	110.10
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
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
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
37	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	19	310	CLA	C3B-C4B-NB	-2.29	108.39	110.52
43	19	301	A86	C36-C31-C32	2.29	121.97	119.70
37	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
43	1	302	A86	C12-C11-C10	-2.29	117.87	123.42
31	16	313	CLA	CHB-C1B-C2B	-2.29	120.76	127.24
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	406	CLA	CHB-C1B-NB	2.29	126.68	124.26
41	E	101	HEM	C4A-NA-C1A	2.29	107.59	105.35
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
31	b	614	CLA	CMB-C2B-C3B	2.29	132.14	126.59
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	A	406	CLA	CHB-C1B-NB	2.29	126.68	124.26
31	w	203	CLA	CHB-C1B-NB	2.29	126.68	124.26
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
33	C	516	BCR	C30-C25-C26	-2.29	119.39	122.61
31	D	405	CLA	CMD-C2D-C3D	2.29	132.88	127.61
31	w	203	CLA	CAC-C3C-C2C	-2.29	123.61	127.53
43	8	305	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
31	7	312	CLA	C3B-C4B-NB	-2.29	108.39	110.52
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	16	310	CLA	CMB-C2B-C3B	2.29	132.13	126.59
31	18	307	CLA	CMD-C2D-C1D	-2.29	120.68	124.71
31	19	307	CLA	CMB-C2B-C3B	2.29	132.12	126.59
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
45	6	312	KC2	CHD-C1D-C2D	2.28	133.69	127.24
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
45	11	311	KC2	CAD-C3D-C2D	-2.28	139.51	144.44
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
45	18	310	KC2	CHD-C1D-C2D	2.28	133.69	127.24
31	17	307	CLA	C3A-C2A-C1A	2.28	105.51	101.64
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	306	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
31	B	613	CLA	CMB-C2B-C3B	2.28	132.11	126.59
35	D	407	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	406	CLA	O2D-CGD-CBD	2.28	115.32	111.27
36	A	410	LHG	O8-C23-C24	2.28	119.06	111.91
31	12	315	CLA	CHB-C1B-NB	2.28	126.67	124.26
37	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	309	KC2	C3C-C2C-C1C	2.28	108.18	106.49
31	15	307	CLA	C3B-C4B-NB	-2.28	108.40	110.52
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	311	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	403	PHO	C4A-C3A-C2A	-2.28	100.67	102.84
43	11	306	A86	C23-C16-C17	-2.28	105.03	108.98
38	11	318	DGD	C1E-O6E-C5E	2.28	118.15	113.69
37	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
38	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
31	P	606	CLA	C3B-C2B-C1B	-2.27	104.42	107.16
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	407	PL9	C36-C37-C38	-2.27	104.43	111.88
37	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	302	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	302	A86	C41-C32-C40	-2.27	101.57	108.53
31	z	103	CLA	CHB-C4A-NA	2.27	127.65	124.51
37	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
31	17	313	CLA	CHB-C1B-C2B	-2.27	120.84	127.24
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
37	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
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	405	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	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
31	p	606	CLA	C3B-C2B-C1B	-2.26	104.43	107.16
42	9	314	KC1	O2D-CGD-O1D	-2.26	119.42	123.84
31	8	313	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
31	9	311	CLA	C3B-C4B-NB	-2.26	108.42	110.52
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	408	LHG	C27-C26-C25	-2.26	102.96	114.42
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
31	0	316	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
37	M	101	LMG	O3-C3-C2	-2.26	105.13	110.35
31	17	307	CLA	CHB-C1B-NB	2.26	126.65	124.26
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	301	A86	C4-C3-C2	-2.26	118.85	123.47
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
38	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
43	9	305	A86	C10-C9-C8	-2.26	116.18	123.22
37	4	316	LMG	O2-C2-C1	-2.26	104.57	110.05
45	15	310	KC2	C2D-C1D-ND	-2.26	108.72	110.23
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	L	101	LHG	C20-C19-C18	-2.25	102.98	114.42
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
37	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	408	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
31	17	315	CLA	CHB-C1B-NB	2.25	126.64	124.26
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
38	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
31	10	309	CLA	CHB-C1B-NB	2.25	126.64	124.26
37	B	620	LMG	O6-C5-C4	2.25	113.78	109.69
43	8	306	A86	C25-C26-C27	-2.25	124.10	127.31
42	9	314	KC1	C2A-C3A-C4A	2.25	108.16	106.49
31	B	609	CLA	C3B-C4B-NB	-2.25	108.43	110.52
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	17	313	CLA	CMB-C2B-C3B	2.25	132.03	126.59
31	0	307	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
42	7	314	KC1	C1A-NA-C4A	-2.25	105.69	106.71
38	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
31	7	312	CLA	CHB-C1B-NB	2.25	126.64	124.26
45	16	311	KC2	CHD-C1D-C2D	2.25	133.58	127.24
34	8	301	SQD	C45-O47-C7	2.25	123.32	117.79
43	0	301	A86	O-C13-C14	-2.25	117.09	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	b	610	CLA	C3B-C4B-NB	-2.25	108.43	110.52
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
37	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
36	8	316	LHG	C27-C26-C25	-2.24	103.03	114.42
31	B	601	CLA	C2A-C1A-CHA	2.24	127.78	123.86
38	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	305	A86	C4-C3-C2	-2.24	118.88	123.47
31	6	311	CLA	CMB-C2B-C3B	2.24	132.02	126.59
42	10	315	KC1	CAD-C3D-C2D	-2.24	139.60	144.44
31	5	307	CLA	C3B-C4B-NB	-2.24	108.43	110.52
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	303	A86	C26-C25-C24	-2.24	116.22	123.22
33	b	618	BCR	C29-C30-C25	2.24	113.93	110.48
31	13	316	CLA	C3B-C4B-NB	-2.24	108.44	110.52
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
31	14	307	CLA	CMB-C2B-C3B	2.24	132.01	126.59
45	5	310	KC2	C3A-C4A-NA	2.24	113.02	110.57
31	16	315	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
32	D	403	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	18	312	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
31	10	312	CLA	O2D-CGD-CBD	2.24	115.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	d	409	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
42	11	314	KC1	CAD-C3D-C2D	-2.23	139.62	144.44
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
42	3	314	KC1	C3D-C4D-ND	-2.23	106.96	110.17
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
31	13	315	CLA	CHB-C1B-NB	2.23	126.62	124.26
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
42	P	609	KC1	C1D-CHD-C4C	-2.23	121.06	126.34
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
37	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
37	0	317	LMG	O3-C3-C2	-2.23	105.20	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	0	314	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
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
45	16	309	KC2	CAA-CBA-CGA	-2.22	115.84	127.26
31	8	308	CLA	C4-C3-C5	2.22	119.01	115.27
34	8	301	SQD	C13-C12-C11	-2.22	103.15	114.42
31	19	315	CLA	CHB-C1B-NB	2.22	126.61	124.26
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	305	A86	O4-C34-C33	2.22	113.12	107.59
31	6	316	CLA	CHB-C1B-NB	2.22	126.61	124.26
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	408	LHG	C20-C19-C18	-2.22	103.16	114.42
43	8	306	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	302	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	407	PL9	C7-C3-C4	2.22	118.68	116.88
45	8	309	KC2	C2A-C1A-CHA	-2.22	120.11	127.44
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
45	0	310	KC2	CMD-C2D-C3D	2.22	131.92	125.93
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	5	303	A86	C-C1-C2	-2.22	119.82	122.92
31	8	312	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
37	D	409	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
38	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
33	C	515	BCR	C15-C14-C13	-2.21	124.15	127.31
36	d	408	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
37	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
42	p	609	KC1	C1D-CHD-C4C	-2.21	121.10	126.34
37	W	201	LMG	C40-C39-C38	-2.21	103.21	114.42
43	16	304	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
31	19	308	CLA	C3B-C4B-NB	-2.21	108.47	110.52
43	2	302	A86	C7-C6-C5	-2.21	119.83	122.92
41	v	201	HEM	CAC-C3C-C4C	-2.21	119.56	124.90
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
31	B	607	CLA	CHC-C4B-NB	2.21	126.59	124.26
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	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
31	5	312	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
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
37	14	316	LMG	O1-C1-C2	-2.20	104.87	108.30
31	c	502	CLA	CMB-C2B-C3B	2.20	131.92	126.59
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
37	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
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
37	11	317	LMG	O2-C2-C1	-2.20	104.70	110.05
43	8	304	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
37	c	521	LMG	O6-C1-O1	-2.20	104.77	109.97
41	V	201	HEM	CAC-C3C-C4C	-2.20	119.59	124.90
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
31	C	502	CLA	CMB-C2B-C3B	2.20	131.91	126.59
43	11	306	A86	C36-C31-C32	-2.20	117.52	119.70
43	16	304	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	305	A86	C22-C16-C17	-2.20	105.17	108.98
31	1	313	CLA	CMB-C2B-C3B	2.20	131.91	126.59
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	9	307	CLA	CMB-C2B-C3B	2.20	131.91	126.59
31	16	315	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	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	15	309	CLA	CHB-C1B-NB	2.19	126.58	124.26
31	C	514	CLA	CMB-C2B-C3B	2.19	131.90	126.59
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
37	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	0	313	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
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
31	16	310	CLA	CHC-C4B-NB	2.19	126.58	124.26
34	l	101	SQD	O48-C23-O10	-2.19	118.06	123.59
31	p	608	CLA	C3B-C4B-NB	-2.19	108.48	110.52
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	310	CLA	CMB-C2B-C3B	2.19	131.89	126.59
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
43	12	301	A86	C20-C19-C18	2.19	117.08	112.75
31	15	306	CLA	CHB-C1B-NB	2.19	126.57	124.26
31	p	603	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
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	312	CLA	CMB-C2B-C3B	2.19	131.89	126.59
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
31	c	514	CLA	CMB-C2B-C3B	2.19	131.89	126.59
31	C	512	CLA	CHB-C1B-NB	2.19	126.57	124.26
31	2	307	CLA	CHB-C1B-NB	2.19	126.57	124.26
31	5	309	CLA	CHB-C1B-NB	2.19	126.57	124.26
43	11	302	A86	C8-C6-C5	2.19	122.30	118.94
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	1	311	KC2	CAD-C3D-C2D	-2.19	139.72	144.44
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
37	1	301	LMG	O3-C3-C2	-2.19	105.30	110.35
31	8	312	CLA	C3B-C4B-NB	-2.18	108.49	110.52
31	B	606	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
43	8	304	A86	C41-C32-C40	-2.18	101.82	108.53
43	8	303	A86	O-C13-C11	-2.18	116.32	121.15
31	10	308	CLA	CHD-C4C-C3C	2.18	128.05	124.84
42	7	314	KC1	CHD-C1D-C2D	2.18	133.41	127.24
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	307	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
37	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
31	P	603	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
37	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
37	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	315	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
37	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
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
31	13	310	CLA	CHB-C1B-NB	2.18	126.56	124.26
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
38	C	519	DGD	C2G-O2G-C1B	2.18	123.15	117.79
33	F	101	BCR	C11-C10-C9	-2.18	124.20	127.31
37	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	302	A86	C19-C18-C17	-2.17	106.58	110.77
31	4	312	CLA	CAD-C3D-C2D	2.17	151.29	140.80
31	18	306	CLA	CHB-C1B-NB	2.17	126.56	124.26
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
38	w	204	DGD	C5B-C4B-C3B	-2.17	103.39	114.42
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
42	9	314	KC1	CMD-C2D-C3D	2.17	131.79	125.93
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
45	3	311	KC2	CHD-C1D-C2D	2.17	133.37	127.24
43	3	303	A86	O1-C20-C19	2.17	115.01	113.38
31	b	608	CLA	CHC-C4B-NB	2.17	126.55	124.26
31	c	512	CLA	CHB-C1B-NB	2.17	126.55	124.26
31	3	315	CLA	CHB-C1B-NB	2.17	126.55	124.26
42	9	314	KC1	CAD-C3D-C2D	-2.17	139.76	144.44
31	10	311	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
31	5	312	CLA	CHB-C1B-NB	2.17	126.55	124.26
31	16	313	CLA	CHB-C4A-NA	2.17	127.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	303	A86	C41-C32-C33	2.16	118.77	109.05
38	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
37	d	404	LMG	O7-C10-O9	-2.16	118.47	123.70
37	11	301	LMG	O3-C3-C2	-2.16	105.35	110.35
42	14	313	KC1	CAA-CBA-CGA	-2.16	116.14	127.26
31	12	310	CLA	C3B-C4B-NB	-2.16	108.51	110.52
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	306	A86	C9-C10-C11	-2.16	120.25	126.61
31	19	310	CLA	C1-C2-C3	-2.16	122.31	126.04
31	1	310	CLA	CHC-C4B-NB	2.16	126.55	124.26
31	0	311	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
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	2	314	CLA	CHB-C1B-NB	2.16	126.54	124.26
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	302	A86	C28-C27-C26	-2.16	119.90	122.92
43	1	319	A86	C10-C9-C8	-2.16	116.48	123.22
31	9	315	CLA	CHB-C1B-NB	2.16	126.54	124.26
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
45	17	311	KC2	O2D-CGD-O1D	-2.16	119.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
37	P	614	LMG	C3-C4-C5	-2.15	106.39	110.24
31	9	310	CLA	C3B-C4B-NB	-2.15	108.52	110.52
31	2	315	CLA	CHB-C1B-NB	2.15	126.54	124.26
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
37	0	317	LMG	C4-C3-C2	2.15	114.58	110.82
31	2	306	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
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	306	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	312	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	407	PL9	C7-C3-C4	2.15	118.62	116.88
43	13	302	A86	C9-C10-C11	-2.15	120.28	126.61
37	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	3	307	CLA	CHB-C1B-NB	2.15	126.53	124.26
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	313	CLA	C4A-NA-C1A	2.15	107.67	106.71
43	15	302	A86	C3-C4-C5	-2.15	119.07	123.47
37	p	614	LMG	C3-C4-C5	-2.15	106.41	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	19	315	CLA	CMB-C2B-C3B	2.15	131.79	126.59
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	407	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
31	1	316	CLA	C2B-C1B-NB	-2.15	108.79	110.23
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	308	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
38	C	519	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
38	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	314	KC1	O2D-CGD-O1D	-2.14	119.65	123.84
31	13	316	CLA	O2D-CGD-CBD	2.14	115.07	111.27
38	c	519	DGD	C2G-O2G-C1B	2.14	123.06	117.79
31	11	315	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
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
31	11	308	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
31	b	615	CLA	CMB-C2B-C3B	2.14	131.77	126.59
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
37	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
31	19	308	CLA	CHB-C1B-NB	2.14	126.52	124.26
33	C	517	BCR	C11-C10-C9	-2.14	124.26	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	310	CLA	C2A-C1A-CHA	2.14	127.58	123.85
31	p	610	CLA	CHB-C1B-NB	2.14	126.52	124.26
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
31	17	310	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
38	C	519	DGD	O6E-C1E-O5D	-2.14	104.91	109.97
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
31	15	307	CLA	CHB-C1B-NB	2.14	126.52	124.26
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
37	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
38	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
31	P	610	CLA	CHB-C1B-NB	2.13	126.52	124.26
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
45	15	308	KC2	CAD-C3D-C2D	-2.13	139.84	144.44
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
45	5	308	KC2	C3D-C4D-ND	-2.13	107.11	110.17
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
38	c	519	DGD	CAB-C9B-C8B	-2.13	103.61	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	613	CLA	O1D-CGD-CBD	2.13	128.84	124.48
45	2	308	KC2	C1D-CHD-C4C	-2.13	121.29	126.34
37	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
38	C	520	DGD	CBB-CAB-C9B	-2.13	103.62	114.42
38	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
31	b	610	CLA	CHB-C1B-NB	2.13	126.51	124.26
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	407	PL9	C20-C19-C21	2.13	118.85	115.27
38	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
31	9	313	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
43	6	305	A86	C3-C2-C1	-2.13	124.28	127.31
31	15	311	CLA	C4B-CHC-C1C	-2.13	121.30	126.34
45	19	309	KC2	C1D-CHD-C4C	-2.13	121.30	126.34
31	11	313	CLA	C6-C5-C3	-2.13	107.88	113.45
38	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	10	317	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
31	1	307	CLA	CHB-C4A-NA	2.12	127.45	124.51
41	V	201	HEM	C2A-C1A-NA	-2.12	107.77	110.15
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	B	614	CLA	CMB-C2B-C3B	2.12	131.73	126.59
31	9	315	CLA	CMB-C2B-C3B	2.12	131.73	126.59
31	18	309	CLA	C2A-C1A-CHA	2.12	127.57	123.86
45	15	308	KC2	C3D-C4D-ND	-2.12	107.12	110.17
31	c	502	CLA	C7-C6-C5	-2.12	107.60	113.36
45	7	311	KC2	CHD-C1D-C2D	2.12	133.23	127.24
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	4	316	LMG	O8-C28-O10	-2.12	118.24	123.59
38	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
31	P	608	CLA	C3B-C4B-NB	-2.12	108.55	110.52
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
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
37	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
43	8	305	A86	O2-C18-C19	2.12	114.01	109.80
31	10	314	CLA	CHD-C1D-C2D	2.12	129.92	125.48
31	B	609	CLA	CHB-C1B-NB	2.12	126.50	124.26
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	305	A86	C9-C10-C11	-2.12	120.39	126.61
31	b	611	CLA	C3A-C2A-C1A	2.12	104.51	101.34
38	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	315	CLA	CAA-C2A-C3A	-2.12	106.99	112.78
45	14	308	KC2	C3C-C2C-C1C	-2.11	104.92	106.49
38	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	311	KC2	C2B-C1B-NB	2.11	111.66	110.10
31	C	505	CLA	C2D-C1D-ND	-2.11	108.55	110.10
38	c	520	DGD	CBB-CAB-C9B	-2.11	103.69	114.42
31	13	307	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
38	C	518	DGD	C7B-C6B-C5B	-2.11	103.70	114.42
31	c	511	CLA	CHB-C1B-NB	2.11	126.49	124.26
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	b	610	CLA	CMB-C2B-C3B	2.11	131.71	126.59
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
37	1	317	LMG	O3-C3-C2	-2.11	105.47	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	609	CLA	CMB-C2B-C3B	2.11	131.70	126.59
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	305	A86	C4-C5-C6	-2.11	124.30	127.31
43	8	305	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	312	CLA	C2A-C1A-CHA	2.11	127.55	123.86
38	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
42	5	313	KC1	OBD-CAD-C3D	-2.11	123.45	128.52
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	407	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
41	v	201	HEM	C2A-C1A-NA	-2.10	107.80	110.15
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
37	P	614	LMG	C6-C5-C4	-2.10	108.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	606	CLA	CMB-C2B-C3B	2.10	131.68	126.59
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
41	v	201	HEM	C4A-CHB-C1B	-2.10	121.36	126.34
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	407	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
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
43	16	306	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
32	D	403	PHO	OBD-CAD-C3D	2.10	131.46	127.98
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
37	p	614	LMG	C6-C5-C4	-2.10	108.09	113.00
38	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	b	610	CLA	CHC-C4B-NB	2.10	126.47	124.26
31	C	502	CLA	C11-C12-C13	-2.10	109.15	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	303	A86	O4-C38-C39	2.09	114.94	111.09
31	B	603	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
31	3	310	CLA	C3B-C4B-NB	-2.09	108.57	110.52
42	19	314	KC1	C1D-CHD-C4C	-2.09	121.37	126.34
43	1	305	A86	C4-C5-C6	-2.09	124.32	127.31
38	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
38	C	520	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
43	16	302	A86	O-C13-C11	-2.09	116.53	121.15
43	19	304	A86	C36-C31-C32	-2.09	117.62	119.70
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
31	0	314	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
38	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	312	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
41	V	201	HEM	C4A-CHB-C1B	-2.09	121.39	126.34
37	5	316	LMG	C1-O6-C5	2.09	117.78	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	10	307	CLA	O2D-CGD-CBD	2.09	114.98	111.27
42	15	317	KC1	O1D-CGD-CBD	-2.09	120.21	124.48
31	8	310	CLA	C2A-C1A-CHA	2.09	127.51	123.86
43	16	303	A86	C14-C15-C16	2.09	126.74	118.75
37	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
45	9	309	KC2	C1D-CHD-C4C	-2.09	121.39	126.34
31	1	313	CLA	CHB-C1B-C2B	-2.09	121.35	127.24
31	C	511	CLA	CHB-C1B-NB	2.09	126.47	124.26
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
38	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	408	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
38	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	408	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	15	312	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
31	P	606	CLA	CAC-C3C-C4C	2.08	127.51	124.81
38	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
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
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
31	C	507	CLA	CMB-C2B-C3B	2.08	131.63	126.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	19	307	CLA	CHB-C1B-NB	2.08	126.46	124.26
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
38	w	204	DGD	C8B-C7B-C6B	-2.08	103.86	114.42
38	c	520	DGD	CAB-C9B-C8B	-2.08	103.86	114.42
42	8	314	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
38	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
31	c	507	CLA	CMB-C2B-C3B	2.08	131.62	126.59
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
38	W	203	DGD	C7B-C6B-C5B	-2.08	103.88	114.42
38	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
32	d	403	PHO	OBD-CAD-C3D	2.08	131.43	127.98
45	16	311	KC2	O1D-CGD-CBD	-2.08	120.23	124.48
45	5	308	KC2	CAD-C3D-C2D	-2.08	139.96	144.44
43	12	305	A86	O4-C38-O5	-2.08	118.84	122.96
37	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
37	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	C	502	CLA	CHB-C1B-NB	2.08	126.45	124.26
31	2	315	CLA	C2C-C1C-NC	-2.08	108.03	109.97
38	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
31	15	306	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
43	9	305	A86	C3-C4-C5	-2.07	119.23	123.47
31	C	510	CLA	C3C-C4C-NC	-2.07	108.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	307	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
31	b	617	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
38	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
31	c	506	CLA	C3B-C4B-NB	-2.07	108.59	110.52
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
37	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
31	b	617	CLA	C3B-C4B-NB	-2.07	108.59	110.52
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
31	B	616	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
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
37	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
33	c	517	BCR	C30-C25-C26	-2.06	119.71	122.61
31	9	308	CLA	C3B-C4B-NB	-2.06	108.60	110.52
37	D	404	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	620	LMG	C33-C32-C31	-2.06	103.95	114.42
37	B	620	LMG	O2-C2-C1	-2.06	105.03	110.05
37	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
38	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
31	1	307	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
33	Y	101	BCR	C2-C3-C4	-2.06	106.77	111.38
45	8	309	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	308	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
37	15	315	LMG	O8-C28-O10	-2.06	118.39	123.59
31	0	307	CLA	C2A-C1A-CHA	2.06	127.46	123.86
31	16	315	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	306	A86	C34-O4-C38	2.06	121.73	117.90
37	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
38	11	318	DGD	CFB-CEB-CDB	-2.06	103.97	114.42
31	13	307	CLA	CHB-C1B-NB	2.06	126.44	124.26
31	17	312	CLA	CHC-C4B-NB	2.06	126.44	124.26
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
38	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	9	312	CLA	CMB-C2B-C3B	2.06	131.57	126.59
31	D	402	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	303	A86	C21-C20-C19	-2.06	111.97	114.28
31	8	308	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
38	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
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
31	p	603	CLA	CHC-C4B-NB	2.05	126.43	124.26
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
31	5	307	CLA	CHB-C1B-NB	2.05	126.43	124.26
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	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	606	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
31	B	602	CLA	C3A-C2A-C1A	2.05	104.41	101.34
31	8	307	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	p	605	CLA	C3C-C4C-NC	-2.05	108.27	110.57
31	0	312	CLA	CMB-C2B-C3B	2.05	131.56	126.59
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
31	B	616	CLA	C3B-C4B-NB	-2.05	108.61	110.52
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
37	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	b	607	CLA	CHC-C4B-NB	2.05	126.42	124.26
31	5	306	CLA	CHB-C1B-NB	2.05	126.42	124.26
31	13	310	CLA	CHC-C4B-NB	2.05	126.42	124.26
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
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	303	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
38	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	b	607	CLA	CMB-C2B-C3B	2.04	131.53	126.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	8	301	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	303	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
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	c	502	CLA	CHB-C1B-NB	2.04	126.41	124.26
32	D	403	PHO	C1C-C2C-C3C	-2.04	106.92	108.61
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
37	F	102	LMG	O1-C7-C8	-2.04	105.98	110.90
31	d	405	CLA	CHB-C4A-NA	2.04	127.33	124.51
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
37	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	402	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
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	8	301	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	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	0	314	CLA	CMB-C2B-C3B	2.03	131.51	126.59
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	405	CLA	CHB-C4A-NA	2.03	127.32	124.51
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	309	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
32	d	403	PHO	C1C-C2C-C3C	-2.03	106.92	108.61
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	C	506	CLA	C3B-C4B-NB	-2.03	108.63	110.52
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	4	315	CLA	C3B-C4B-NB	-2.03	108.63	110.52
31	19	313	CLA	O1D-CGD-CBD	2.03	128.64	124.48
31	18	311	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
31	C	513	CLA	O2D-CGD-CBD	2.03	114.87	111.27
38	C	520	DGD	C5B-C4B-C3B	-2.03	104.12	114.42
31	B	606	CLA	CHC-C4B-NB	2.03	126.41	124.26
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
37	M	101	LMG	C9-C8-C7	-2.03	106.99	111.79
38	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
45	6	310	KC2	C1D-CHD-C4C	-2.03	121.53	126.34
43	8	304	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	305	A86	O2-C18-C17	2.03	113.83	109.80
31	b	603	CLA	C3A-C2A-C1A	2.03	104.37	101.34
31	P	603	CLA	CHC-C4B-NB	2.03	126.40	124.26
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
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	313	CLA	C3D-C2D-C1D	2.02	108.59	105.83
43	6	307	A86	C10-C9-C8	-2.02	116.90	123.22
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	305	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
37	D	404	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
37	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
38	h	102	DGD	O5E-C6E-C5E	-2.02	104.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	d	407	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
37	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	304	A86	C9-C10-C11	-2.02	120.67	126.61
45	15	308	KC2	CGD-CBD-CAD	-2.02	104.20	110.73
31	18	309	CLA	C3B-C4B-NB	-2.02	108.64	110.52
31	9	308	CLA	CHB-C1B-NB	2.02	126.39	124.26
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
45	1	309	KC2	CMD-C2D-C3D	2.02	131.38	125.93
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
37	Z	102	LMG	O3-C3-C2	-2.02	105.69	110.35
31	d	406	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
43	18	301	A86	C35-C34-C33	-2.01	106.36	109.88
31	P	607	CLA	CHB-C1B-NB	2.01	126.39	124.26
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	305	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	309	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	407	PL9	C11-C12-C13	-2.01	105.27	111.88
31	10	314	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
44	P	612	DD6	C3-C4-C5	-2.01	119.35	123.47
38	H	102	DGD	O5E-C6E-C5E	-2.01	104.39	111.29
31	12	313	CLA	CMB-C2B-C1B	-2.01	122.31	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
31	19	312	CLA	CMB-C2B-C3B	2.01	131.46	126.59
31	18	307	CLA	CMB-C2B-C3B	2.01	131.46	126.59
38	C	518	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
38	c	518	DGD	O5D-C6D-C5D	-2.01	105.33	109.05
31	5	306	CLA	C3B-C4B-NB	-2.01	108.65	110.52
31	b	617	CLA	CHA-C1A-NA	-2.01	121.79	126.40
31	b	612	CLA	O2D-CGD-CBD	2.01	114.84	111.27
37	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
37	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
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	B	609	CLA	CHC-C4B-NB	2.01	126.38	124.26
31	14	311	CLA	CHA-C1A-NA	-2.01	121.80	126.40
38	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
31	7	307	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
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	p	606	CLA	CHC-C4B-NB	-2.01	122.13	124.26
31	5	307	CLA	CMB-C2B-C3B	2.01	131.45	126.59
31	16	308	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	402	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	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	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
38	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	302	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	403	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
42	1	314	KC1	C1D-CHD-C4C	-2.00	121.59	126.34
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
31	8	313	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
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
37	c	522	LMG	O3-C3-C2	-2.00	105.72	110.35
31	8	310	CLA	CHD-C1D-ND	-2.00	122.62	124.45
31	7	313	CLA	C3C-C4C-NC	-2.00	108.33	110.57

There are no chirality outliers.

All (5700) 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
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

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Mol	Chain	Res	Type	Atoms
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	C2B-C3B-CAB-CBB
31	B	605	CLA	C4B-C3B-CAB-CBB
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	C2B-C3B-CAB-CBB
31	B	606	CLA	C4B-C3B-CAB-CBB
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	615	CLA	C4B-C3B-CAB-CBB
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	503	CLA	C2B-C3B-CAB-CBB
31	C	503	CLA	C4B-C3B-CAB-CBB
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	C	508	CLA	C2B-C3B-CAB-CBB
31	C	508	CLA	C4B-C3B-CAB-CBB
31	D	402	CLA	CHA-CBD-CGD-O1D
31	D	402	CLA	CHA-CBD-CGD-O2D
31	D	406	CLA	C2-C3-C5-C6
31	D	406	CLA	C4-C3-C5-C6
31	P	601	CLA	C2B-C3B-CAB-CBB
31	P	601	CLA	C4B-C3B-CAB-CBB
31	P	601	CLA	CHA-CBD-CGD-O1D
31	P	601	CLA	CAD-CBD-CGD-O1D
31	P	601	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	605	CLA	C4B-C3B-CAB-CBB
31	P	606	CLA	C1A-C2A-CAA-CBA
31	P	606	CLA	CBD-CGD-O2D-CED
31	P	607	CLA	C4B-C3B-CAB-CBB
31	P	608	CLA	CBD-CGD-O2D-CED
31	R	101	CLA	C2B-C3B-CAB-CBB
31	R	101	CLA	C4B-C3B-CAB-CBB
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	C2B-C3B-CAB-CBB
31	b	606	CLA	C4B-C3B-CAB-CBB
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	607	CLA	C2B-C3B-CAB-CBB
31	b	607	CLA	C4B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
31	b	616	CLA	C4B-C3B-CAB-CBB
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	503	CLA	C2B-C3B-CAB-CBB
31	c	503	CLA	C4B-C3B-CAB-CBB
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	c	508	CLA	C2B-C3B-CAB-CBB
31	c	508	CLA	C4B-C3B-CAB-CBB
31	d	402	CLA	CHA-CBD-CGD-O1D
31	d	402	CLA	CHA-CBD-CGD-O2D
31	d	406	CLA	C2-C3-C5-C6
31	d	406	CLA	C4-C3-C5-C6
31	p	601	CLA	C2B-C3B-CAB-CBB
31	p	601	CLA	C4B-C3B-CAB-CBB
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	605	CLA	C4B-C3B-CAB-CBB
31	p	606	CLA	C1A-C2A-CAA-CBA
31	p	606	CLA	CBD-CGD-O2D-CED
31	p	607	CLA	C4B-C3B-CAB-CBB
31	p	608	CLA	CBD-CGD-O2D-CED
31	p	608	CLA	O1D-CGD-O2D-CED
31	r	101	CLA	C2B-C3B-CAB-CBB
31	r	101	CLA	C4B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
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	313	CLA	C4B-C3B-CAB-CBB
31	1	316	CLA	C1A-C2A-CAA-CBA
31	1	316	CLA	C2B-C3B-CAB-CBB
31	1	316	CLA	C4B-C3B-CAB-CBB
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	C2B-C3B-CAB-CBB
31	2	307	CLA	C4B-C3B-CAB-CBB
31	2	307	CLA	C2-C3-C5-C6
31	2	307	CLA	C4-C3-C5-C6
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	312	CLA	C2B-C3B-CAB-CBB
31	3	312	CLA	C4B-C3B-CAB-CBB
31	3	313	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	C4B-C3B-CAB-CBB
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	312	CLA	C2B-C3B-CAB-CBB
31	4	312	CLA	C4B-C3B-CAB-CBB
31	4	314	CLA	C2B-C3B-CAB-CBB
31	4	314	CLA	C4B-C3B-CAB-CBB
31	4	315	CLA	C1A-C2A-CAA-CBA
31	4	315	CLA	C4B-C3B-CAB-CBB
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	C4B-C3B-CAB-CBB
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	C2B-C3B-CAB-CBB
31	6	308	CLA	C4B-C3B-CAB-CBB
31	6	308	CLA	CAD-CBD-CGD-O2D
31	6	309	CLA	C2B-C3B-CAB-CBB
31	6	309	CLA	C4B-C3B-CAB-CBB
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	313	CLA	C1A-C2A-CAA-CBA
31	6	313	CLA	C2B-C3B-CAB-CBB
31	6	313	CLA	C4B-C3B-CAB-CBB
31	6	314	CLA	C2B-C3B-CAB-CBB
31	6	314	CLA	CBD-CGD-O2D-CED
31	7	307	CLA	CAD-CBD-CGD-O2D
31	7	308	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	7	308	CLA	C4B-C3B-CAB-CBB
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	308	CLA	C2B-C3B-CAB-CBB
31	8	308	CLA	C4B-C3B-CAB-CBB
31	8	308	CLA	C2-C3-C5-C6
31	8	308	CLA	C4-C3-C5-C6
31	8	310	CLA	CBD-CGD-O2D-CED
31	8	312	CLA	C1A-C2A-CAA-CBA
31	8	312	CLA	CBA-CGA-O2A-C1
31	8	313	CLA	C1A-C2A-CAA-CBA
31	8	313	CLA	C2B-C3B-CAB-CBB
31	8	313	CLA	C4B-C3B-CAB-CBB
31	8	313	CLA	CBD-CGD-O2D-CED
31	8	315	CLA	CHA-CBD-CGD-O1D
31	8	315	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	311	CLA	C2B-C3B-CAB-CBB
31	9	311	CLA	C4B-C3B-CAB-CBB
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	11	313	CLA	C2B-C3B-CAB-CBB
31	11	313	CLA	C4B-C3B-CAB-CBB
31	12	307	CLA	C4B-C3B-CAB-CBB
31	12	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	12	310	CLA	CBD-CGD-O2D-CED
31	12	312	CLA	C2B-C3B-CAB-CBB
31	12	312	CLA	C4B-C3B-CAB-CBB
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	C4B-C3B-CAB-CBB
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
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	C4B-C3B-CAB-CBB
31	14	312	CLA	CBD-CGD-O2D-CED
31	14	314	CLA	C2B-C3B-CAB-CBB
31	14	314	CLA	C4B-C3B-CAB-CBB
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	C4B-C3B-CAB-CBB
31	15	311	CLA	CHA-CBD-CGD-O1D
31	15	311	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	15	312	CLA	C4B-C3B-CAB-CBB
31	15	312	CLA	CBD-CGD-O2D-CED
31	16	307	CLA	C3A-C2A-CAA-CBA
31	16	308	CLA	C2B-C3B-CAB-CBB
31	16	308	CLA	C4B-C3B-CAB-CBB
31	16	308	CLA	C2-C3-C5-C6
31	16	308	CLA	C4-C3-C5-C6
31	16	310	CLA	CBD-CGD-O2D-CED
31	16	312	CLA	C1A-C2A-CAA-CBA
31	16	312	CLA	C2B-C3B-CAB-CBB
31	16	312	CLA	C4B-C3B-CAB-CBB
31	16	313	CLA	C1A-C2A-CAA-CBA
31	16	313	CLA	C2B-C3B-CAB-CBB
31	16	313	CLA	C4B-C3B-CAB-CBB
31	16	313	CLA	CBD-CGD-O2D-CED
31	16	313	CLA	O1D-CGD-O2D-CED
31	16	315	CLA	CHA-CBD-CGD-O1D
31	16	315	CLA	CHA-CBD-CGD-O2D
31	17	307	CLA	CAD-CBD-CGD-O2D
31	17	308	CLA	C2B-C3B-CAB-CBB
31	17	308	CLA	C4B-C3B-CAB-CBB
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	307	CLA	C2B-C3B-CAB-CBB
31	18	307	CLA	C4B-C3B-CAB-CBB
31	18	311	CLA	C4B-C3B-CAB-CBB
31	18	311	CLA	CBD-CGD-O2D-CED
31	18	312	CLA	C1A-C2A-CAA-CBA
31	18	312	CLA	C2B-C3B-CAB-CBB
31	18	312	CLA	C4B-C3B-CAB-CBB
31	18	314	CLA	CHA-CBD-CGD-O1D
31	18	314	CLA	CHA-CBD-CGD-O2D
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	311	CLA	C2B-C3B-CAB-CBB
31	19	311	CLA	C4B-C3B-CAB-CBB
31	19	313	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
34	l	101	SQD	C5-C6-S-O9
34	8	301	SQD	C2-C1-O6-C44
34	8	301	SQD	O5-C5-C6-S
34	8	301	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	408	LHG	O1-C1-C2-C3
36	D	408	LHG	C3-O3-P-O4
36	D	408	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
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	408	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
36	d	408	LHG	C3-O3-P-O4
36	d	408	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	316	LHG	C1-C2-C3-O3
36	8	316	LHG	C3-O3-P-O4
36	8	317	LHG	O1-C1-C2-C3
36	8	317	LHG	C4-O6-P-O3
36	8	317	LHG	C5-C4-O6-P
36	8	317	LHG	O9-C7-O7-C5
36	8	317	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
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

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Mol	Chain	Res	Type	Atoms
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
37	B	620	LMG	O6-C1-O1-C7
37	C	522	LMG	C11-C10-O7-C8
37	D	409	LMG	O9-C10-O7-C8
37	D	409	LMG	C11-C10-O7-C8
37	F	102	LMG	O9-C10-O7-C8
37	F	102	LMG	C11-C10-O7-C8
37	J	101	LMG	C2-C1-O1-C7
37	J	101	LMG	O6-C1-O1-C7
37	b	621	LMG	O6-C1-O1-C7
37	c	521	LMG	C11-C10-O7-C8
37	d	409	LMG	O9-C10-O7-C8
37	d	409	LMG	C11-C10-O7-C8
37	f	102	LMG	O9-C10-O7-C8
37	f	102	LMG	C11-C10-O7-C8
37	j	101	LMG	C2-C1-O1-C7
37	j	101	LMG	O6-C1-O1-C7
37	1	301	LMG	C2-C1-O1-C7
37	1	301	LMG	O6-C1-O1-C7
37	1	301	LMG	O7-C8-C9-O8
37	1	317	LMG	O6-C1-O1-C7
37	4	316	LMG	O9-C10-O7-C8
37	4	316	LMG	C11-C10-O7-C8
37	5	315	LMG	C2-C1-O1-C7
37	5	315	LMG	O6-C1-O1-C7
37	5	316	LMG	C2-C1-O1-C7
37	5	316	LMG	O6-C1-O1-C7
37	11	301	LMG	C2-C1-O1-C7
37	11	301	LMG	O6-C1-O1-C7
37	11	301	LMG	O7-C8-C9-O8
37	11	317	LMG	C2-C1-O1-C7
37	11	317	LMG	O6-C1-O1-C7
37	14	316	LMG	O9-C10-O7-C8
37	14	316	LMG	C11-C10-O7-C8
37	15	314	LMG	C2-C1-O1-C7
37	15	314	LMG	O6-C1-O1-C7
37	15	315	LMG	C2-C1-O1-C7
37	15	315	LMG	O6-C1-O1-C7
37	15	315	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
38	B	621	DGD	C2D-C1D-O3G-C3G
38	B	621	DGD	C2E-C1E-O5D-C6D
38	B	621	DGD	O6E-C1E-O5D-C6D
38	C	520	DGD	C2D-C1D-O3G-C3G
38	C	520	DGD	O6D-C1D-O3G-C3G
38	H	102	DGD	C2E-C1E-O5D-C6D
38	H	102	DGD	O6E-C1E-O5D-C6D
38	W	203	DGD	C2D-C1D-O3G-C3G
38	W	203	DGD	O6D-C1D-O3G-C3G
38	W	203	DGD	O6E-C1E-O5D-C6D
38	b	622	DGD	C2D-C1D-O3G-C3G
38	b	622	DGD	C2E-C1E-O5D-C6D
38	b	622	DGD	O6E-C1E-O5D-C6D
38	c	520	DGD	C2D-C1D-O3G-C3G
38	c	520	DGD	O6D-C1D-O3G-C3G
38	h	102	DGD	C2E-C1E-O5D-C6D
38	h	102	DGD	O6E-C1E-O5D-C6D
38	w	204	DGD	C2D-C1D-O3G-C3G
38	w	204	DGD	O6D-C1D-O3G-C3G
38	w	204	DGD	O6E-C1E-O5D-C6D
38	1	318	DGD	C2B-C1B-O2G-C2G
38	1	318	DGD	O1B-C1B-O2G-C2G
38	1	318	DGD	O1G-C1G-C2G-O2G
38	1	318	DGD	C2D-C1D-O3G-C3G
38	1	318	DGD	O6D-C1D-O3G-C3G
38	1	318	DGD	C2E-C1E-O5D-C6D
38	1	318	DGD	O6E-C1E-O5D-C6D
38	11	318	DGD	C2B-C1B-O2G-C2G
38	11	318	DGD	O1B-C1B-O2G-C2G
38	11	318	DGD	O1G-C1G-C2G-O2G
38	11	318	DGD	C2D-C1D-O3G-C3G
38	11	318	DGD	O6D-C1D-O3G-C3G
38	11	318	DGD	O6E-C1E-O5D-C6D
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	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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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	302	A86	C10-C11-C13-O
43	8	302	A86	O-C13-C14-C15
43	8	302	A86	C11-C13-C14-C15
43	8	302	A86	C13-C14-C15-C16
43	8	303	A86	C13-C14-C15-C16
43	8	303	A86	C13-C14-C15-O1
43	8	304	A86	C33-C34-O4-C38
43	8	304	A86	C39-C38-O4-C34
43	8	305	A86	C33-C34-O4-C38
43	8	305	A86	C39-C38-O4-C34
43	8	306	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
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

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Mol	Chain	Res	Type	Atoms
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
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	301	A86	C10-C11-C13-O
43	16	301	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	16	301	A86	C13-C14-C15-O1
43	16	301	A86	C39-C38-O4-C34
43	16	303	A86	C13-C14-C15-O1
43	16	305	A86	C13-C14-C15-C20
43	16	305	A86	C13-C14-C15-O1
43	16	306	A86	C12-C11-C13-O
43	16	306	A86	C12-C11-C13-C14
43	16	306	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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
45	7	311	KC2	C4C-C3C-CAC-CBC
45	8	309	KC2	C1A-C2A-CAA-CBA
45	8	309	KC2	C3A-C2A-CAA-CBA
45	8	309	KC2	C2B-C3B-CAB-CBB
45	8	309	KC2	C4B-C3B-CAB-CBB
45	8	309	KC2	C2C-C3C-CAC-CBC
45	8	309	KC2	C4C-C3C-CAC-CBC
45	8	309	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	8	311	KC2	C1A-C2A-CAA-CBA
45	8	311	KC2	C3A-C2A-CAA-CBA
45	8	311	KC2	C2B-C3B-CAB-CBB
45	8	311	KC2	C4B-C3B-CAB-CBB
45	8	311	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
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

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Mol	Chain	Res	Type	Atoms
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	309	KC2	C1A-C2A-CAA-CBA
45	16	309	KC2	C3A-C2A-CAA-CBA
45	16	309	KC2	C2B-C3B-CAB-CBB
45	16	309	KC2	C2C-C3C-CAC-CBC
45	16	309	KC2	C4C-C3C-CAC-CBC
45	16	309	KC2	CBD-CGD-O2D-CED
45	16	311	KC2	C1A-C2A-CAA-CBA
45	16	311	KC2	C3A-C2A-CAA-CBA
45	16	311	KC2	C2B-C3B-CAB-CBB
45	16	311	KC2	C4B-C3B-CAB-CBB
45	16	311	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
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

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Mol	Chain	Res	Type	Atoms
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	302	A86	C39-C38-O4-C34
43	8	303	A86	C39-C38-O4-C34
43	8	304	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
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	303	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
43	16	304	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	307	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
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	305	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
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	309	KC2	O1D-CGD-O2D-CED
45	16	309	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	405	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
31	c	509	CLA	CBD-CGD-O2D-CED
31	c	514	CLA	CBD-CGD-O2D-CED
31	d	405	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	307	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	307	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
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

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Mol	Chain	Res	Type	Atoms
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
37	D	409	LMG	O10-C28-O8-C9
37	M	101	LMG	O10-C28-O8-C9
37	d	409	LMG	O10-C28-O8-C9
37	m	101	LMG	O10-C28-O8-C9
38	B	621	DGD	O1A-C1A-O1G-C1G
38	C	519	DGD	O1A-C1A-O1G-C1G
38	b	622	DGD	O1A-C1A-O1G-C1G
38	c	519	DGD	O1A-C1A-O1G-C1G
31	8	312	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	307	CLA	O1D-CGD-O2D-CED
38	H	102	DGD	C4D-C5D-C6D-O5D
38	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	304	A86	C35-C34-O4-C38
43	17	316	A86	C35-C34-O4-C38
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	313	CLA	O1D-CGD-O2D-CED
31	10	317	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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
37	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
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	303	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

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Mol	Chain	Res	Type	Atoms
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	308	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	316	LHG	O10-C23-O8-C6
36	18	315	LHG	O10-C23-O8-C6
37	D	404	LMG	O10-C28-O8-C9
37	W	201	LMG	O10-C28-O8-C9
37	w	201	LMG	O10-C28-O8-C9
38	W	203	DGD	O1A-C1A-O1G-C1G
38	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
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	302	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
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	301	A86	O5-C38-O4-C34
43	16	303	A86	O5-C38-O4-C34
43	16	304	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	310	CLA	O1D-CGD-O2D-CED
43	1	306	A86	O5-C38-O4-C34
43	3	301	A86	O5-C38-O4-C34
43	8	305	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

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Mol	Chain	Res	Type	Atoms
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
37	C	522	LMG	O9-C10-O7-C8
37	D	404	LMG	O9-C10-O7-C8
37	M	101	LMG	O9-C10-O7-C8
37	c	521	LMG	O9-C10-O7-C8
37	m	101	LMG	O9-C10-O7-C8
37	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
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	403	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	a	405	PHO	C3-C5-C6-C7
32	d	403	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	316	LHG	C24-C23-O8-C6
36	18	315	LHG	C24-C23-O8-C6
37	D	404	LMG	C29-C28-O8-C9
37	D	409	LMG	C29-C28-O8-C9
37	d	409	LMG	C29-C28-O8-C9
37	m	101	LMG	C29-C28-O8-C9
37	4	316	LMG	C29-C28-O8-C9
38	B	621	DGD	C2A-C1A-O1G-C1G
38	C	519	DGD	C2A-C1A-O1G-C1G
38	W	203	DGD	C2A-C1A-O1G-C1G
38	b	622	DGD	C2A-C1A-O1G-C1G
38	c	519	DGD	C2A-C1A-O1G-C1G
38	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	310	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
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

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Mol	Chain	Res	Type	Atoms
43	11	305	A86	O5-C38-O4-C34
36	15	316	LHG	O10-C23-O8-C6
38	1	318	DGD	O6D-C5D-C6D-O5D
38	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	314	KC1	CAA-CBA-CGA-O1A
42	8	314	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	309	KC2	CAA-CBA-CGA-O1A
45	8	309	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
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

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Mol	Chain	Res	Type	Atoms
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	313	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	308	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
37	J	101	LMG	C29-C28-O8-C9
37	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
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
37	d	404	LMG	O9-C10-O7-C8
37	1	317	LMG	O9-C10-O7-C8
38	C	519	DGD	O1B-C1B-O2G-C2G
38	c	519	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
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
37	J	101	LMG	O10-C28-O8-C9
37	j	101	LMG	O10-C28-O8-C9
37	1	317	LMG	O10-C28-O8-C9
38	11	318	DGD	O1A-C1A-O1G-C1G
31	10	316	CLA	CBA-CGA-O2A-C1
36	8	317	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	306	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
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	315	CLA	CBD-CGD-O2D-CED
42	17	314	KC1	CBD-CGD-O2D-CED
31	D	405	CLA	O1D-CGD-O2D-CED
31	d	405	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	8	316	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	406	CLA	CBA-CGA-O2A-C1
31	c	506	CLA	CBA-CGA-O2A-C1
31	d	406	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
37	W	201	LMG	C29-C28-O8-C9
37	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
43	8	306	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

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Mol	Chain	Res	Type	Atoms
43	16	302	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	406	CLA	O1A-CGA-O2A-C1
31	d	406	CLA	O1A-CGA-O2A-C1
37	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
37	d	404	LMG	C11-C10-O7-C8
37	1	317	LMG	C11-C10-O7-C8
37	11	317	LMG	C11-C10-O7-C8
38	C	519	DGD	C2B-C1B-O2G-C2G
38	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
43	7	301	A86	O5-C38-O4-C34
43	8	306	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

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Mol	Chain	Res	Type	Atoms
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	302	A86	O5-C38-O4-C34
43	16	305	A86	O5-C38-O4-C34
43	16	306	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
37	J	101	LMG	C11-C12-C13-C14
37	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
37	K	101	LMG	C11-C12-C13-C14
37	k	101	LMG	C11-C12-C13-C14
37	4	316	LMG	C32-C33-C34-C35
37	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
37	14	316	LMG	C29-C28-O8-C9
41	V	201	HEM	C1A-C2A-CAA-CBA
41	v	201	HEM	C1A-C2A-CAA-CBA
31	B	607	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
38	W	203	DGD	O6E-C5E-C6E-O5E
38	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

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Mol	Chain	Res	Type	Atoms
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
37	5	315	LMG	O10-C28-O8-C9
37	15	314	LMG	O10-C28-O8-C9
38	1	318	DGD	O1A-C1A-O1G-C1G
41	V	201	HEM	C3D-CAD-CBD-CGD
41	v	201	HEM	C3D-CAD-CBD-CGD
37	11	317	LMG	C29-C30-C31-C32
31	14	311	CLA	O1A-CGA-O2A-C1
37	P	614	LMG	O6-C5-C6-O5
37	p	614	LMG	O6-C5-C6-O5
38	H	102	DGD	O6E-C5E-C6E-O5E
38	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
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

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Mol	Chain	Res	Type	Atoms
31	4	309	CLA	O1D-CGD-O2D-CED
31	4	307	CLA	O1A-CGA-O2A-C1
34	l	101	SQD	O10-C23-O48-C46
37	0	317	LMG	O10-C28-O8-C9
37	C	522	LMG	O6-C1-O1-C7
37	c	521	LMG	O6-C1-O1-C7
37	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
37	1	317	LMG	C29-C28-O8-C9
38	11	318	DGD	C2A-C1A-O1G-C1G
31	c	509	CLA	O1D-CGD-O2D-CED
31	9	311	CLA	CBA-CGA-O2A-C1
38	B	621	DGD	O6D-C5D-C6D-O5D
38	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
37	D	404	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
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

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Mol	Chain	Res	Type	Atoms
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
37	J	101	LMG	O9-C10-O7-C8
37	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
37	5	315	LMG	C29-C28-O8-C9
37	15	315	LMG	C29-C28-O8-C9
38	C	520	DGD	C2A-C1A-O1G-C1G
38	c	520	DGD	C2A-C1A-O1G-C1G
38	1	318	DGD	C2A-C1A-O1G-C1G
36	18	316	LHG	C24-C23-O8-C6
38	C	518	DGD	O6E-C5E-C6E-O5E
38	c	518	DGD	O6E-C5E-C6E-O5E
31	b	609	CLA	CBD-CGD-O2D-CED
37	4	316	LMG	C4-C5-C6-O5
31	10	316	CLA	O1A-CGA-O2A-C1
33	B	618	BCR	C13-C14-C15-C16
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

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Mol	Chain	Res	Type	Atoms
37	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
37	14	316	LMG	C4-C5-C6-O5
38	H	102	DGD	C4E-C5E-C6E-O5E
38	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	309	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
37	P	614	LMG	C4-C5-C6-O5
37	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
31	13	316	CLA	C5-C6-C7-C8
31	9	308	CLA	C3-C5-C6-C7
38	C	520	DGD	C1A-C2A-C3A-C4A
38	c	520	DGD	C1A-C2A-C3A-C4A
37	C	522	LMG	C2-C1-O1-C7
37	c	521	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
37	1	317	LMG	C2-C1-O1-C7
38	11	318	DGD	C2E-C1E-O5D-C6D
37	B	620	LMG	O7-C8-C9-O8
37	K	101	LMG	O7-C8-C9-O8
37	b	621	LMG	O7-C8-C9-O8
37	k	101	LMG	O7-C8-C9-O8
37	5	316	LMG	O7-C8-C9-O8
36	18	316	LHG	C12-C13-C14-C15
31	19	313	CLA	O1A-CGA-O2A-C1
37	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
31	19	308	CLA	C6-C7-C8-C9
41	V	201	HEM	C3A-C2A-CAA-CBA
41	v	201	HEM	C3A-C2A-CAA-CBA
31	0	308	CLA	O1D-CGD-O2D-CED
31	0	309	CLA	O1D-CGD-O2D-CED
31	5	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	302	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
37	K	101	LMG	O9-C10-O7-C8
37	k	101	LMG	O9-C10-O7-C8
36	A	410	LHG	C7-C8-C9-C10
36	D	408	LHG	C23-C24-C25-C26
36	a	410	LHG	C7-C8-C9-C10
36	d	408	LHG	C23-C24-C25-C26
37	B	620	LMG	C28-C29-C30-C31
37	b	621	LMG	C28-C29-C30-C31
37	d	404	LMG	C10-C11-C12-C13
37	m	101	LMG	C10-C11-C12-C13
37	1	317	LMG	C28-C29-C30-C31
38	H	102	DGD	O6D-C5D-C6D-O5D
38	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
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

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Mol	Chain	Res	Type	Atoms
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	309	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
37	K	101	LMG	C29-C28-O8-C9
37	d	404	LMG	C29-C28-O8-C9
37	k	101	LMG	C29-C28-O8-C9
37	0	317	LMG	C29-C28-O8-C9
37	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
37	W	201	LMG	O6-C5-C6-O5
37	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	316	LHG	C7-C8-C9-C10
38	B	621	DGD	C1A-C2A-C3A-C4A
38	W	203	DGD	C1B-C2B-C3B-C4B
38	b	622	DGD	C1A-C2A-C3A-C4A
38	w	204	DGD	C1B-C2B-C3B-C4B
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

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Mol	Chain	Res	Type	Atoms
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
37	C	522	LMG	C10-C11-C12-C13
37	D	409	LMG	C10-C11-C12-C13
37	D	409	LMG	C28-C29-C30-C31
37	F	102	LMG	C10-C11-C12-C13
37	J	101	LMG	C10-C11-C12-C13
37	M	101	LMG	C10-C11-C12-C13
37	Z	102	LMG	C28-C29-C30-C31
37	c	521	LMG	C10-C11-C12-C13
37	c	522	LMG	C28-C29-C30-C31
37	d	409	LMG	C10-C11-C12-C13
37	d	409	LMG	C28-C29-C30-C31
37	f	102	LMG	C10-C11-C12-C13
37	j	101	LMG	C10-C11-C12-C13
37	m	101	LMG	C28-C29-C30-C31
37	11	317	LMG	C28-C29-C30-C31
37	15	314	LMG	C10-C11-C12-C13
38	C	519	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
38	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	8	301	SQD	C24-C23-O48-C46
37	15	314	LMG	C29-C28-O8-C9
36	D	408	LHG	C32-C33-C34-C35
36	d	408	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	303	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
37	k	101	LMG	C10-C11-C12-C13
38	H	102	DGD	C1A-C2A-C3A-C4A
38	h	102	DGD	C1A-C2A-C3A-C4A
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

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Mol	Chain	Res	Type	Atoms
37	J	101	LMG	C11-C10-O7-C8
37	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
37	N	101	LMG	O10-C28-O8-C9
38	C	520	DGD	O1A-C1A-O1G-C1G
38	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
37	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
38	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
31	b	611	CLA	O1A-CGA-O2A-C1
34	8	301	SQD	O5-C1-O6-C44
37	W	201	LMG	O6-C1-O1-C7
38	C	519	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
38	C	520	DGD	O6E-C1E-O5D-C6D
38	c	519	DGD	O6E-C1E-O5D-C6D
38	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
37	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	408	LHG	O2-C2-C3-O3
36	d	408	LHG	O2-C2-C3-O3
36	18	315	LHG	O9-C7-O7-C5
38	B	621	DGD	O1B-C1B-O2G-C2G
38	W	203	DGD	C4E-C5E-C6E-O5E
38	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
37	11	317	LMG	C29-C28-O8-C9
31	18	314	CLA	C2C-C3C-CAC-CBC
37	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
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

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Mol	Chain	Res	Type	Atoms
31	9	308	CLA	C13-C15-C16-C17
37	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	316	LHG	C8-C7-O7-C5
38	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	402	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	402	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	408	LHG	C3-O3-P-O6
36	D	408	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	408	LHG	C3-O3-P-O6
36	d	408	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	316	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
37	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

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Mol	Chain	Res	Type	Atoms
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
38	W	203	DGD	C4D-C5D-C6D-O5D
38	w	204	DGD	C4D-C5D-C6D-O5D
31	7	315	CLA	O1D-CGD-O2D-CED
36	D	408	LHG	C1-C2-C3-O3
36	d	408	LHG	C1-C2-C3-O3
34	8	301	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
38	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
37	Z	102	LMG	C29-C28-O8-C9
37	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
36	b	623	LHG	C25-C26-C27-C28
37	J	101	LMG	C17-C18-C19-C20
37	4	316	LMG	C36-C37-C38-C39
36	5	317	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
36	15	316	LHG	C8-C7-O7-C5
37	M	101	LMG	C11-C10-O7-C8
37	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	408	LHG	C9-C10-C11-C12
36	d	408	LHG	C9-C10-C11-C12
36	4	317	LHG	C14-C15-C16-C17
36	14	317	LHG	C12-C13-C14-C15
37	D	404	LMG	C30-C31-C32-C33
37	D	409	LMG	C31-C32-C33-C34
37	D	409	LMG	C32-C33-C34-C35
37	J	101	LMG	C30-C31-C32-C33
37	d	409	LMG	C31-C32-C33-C34
37	d	409	LMG	C32-C33-C34-C35
37	j	101	LMG	C17-C18-C19-C20
37	j	101	LMG	C30-C31-C32-C33
37	0	317	LMG	C11-C12-C13-C14
37	14	316	LMG	C16-C17-C18-C19
38	B	621	DGD	C6B-C7B-C8B-C9B
38	H	102	DGD	C6A-C7A-C8A-C9A
38	c	518	DGD	C2B-C3B-C4B-C5B
38	1	318	DGD	C2B-C3B-C4B-C5B
31	C	507	CLA	C16-C17-C18-C20
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

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Mol	Chain	Res	Type	Atoms
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	8	301	SQD	C24-C25-C26-C27
36	B	622	LHG	C29-C30-C31-C32
36	D	408	LHG	C31-C32-C33-C34
36	b	623	LHG	C29-C30-C31-C32
36	d	408	LHG	C31-C32-C33-C34
37	C	522	LMG	C18-C19-C20-C21
37	D	404	LMG	C11-C12-C13-C14
37	c	521	LMG	C16-C17-C18-C19
37	c	521	LMG	C18-C19-C20-C21
37	c	521	LMG	C31-C32-C33-C34
37	1	317	LMG	C29-C30-C31-C32
37	4	316	LMG	C16-C17-C18-C19
37	11	317	LMG	C14-C15-C16-C17
37	15	315	LMG	C33-C34-C35-C36
38	C	518	DGD	C2B-C3B-C4B-C5B
38	H	102	DGD	CBA-CCA-CDA-CEA
38	b	622	DGD	C5A-C6A-C7A-C8A
38	h	102	DGD	C6A-C7A-C8A-C9A
38	h	102	DGD	CBA-CCA-CDA-CEA
34	L	102	SQD	O49-C7-O47-C45
34	l	101	SQD	O49-C7-O47-C45
38	b	622	DGD	O1B-C1B-O2G-C2G
45	12	309	KC2	CAA-CBA-CGA-O2A
31	19	312	CLA	C15-C16-C17-C18
32	D	403	PHO	C2C-C3C-CAC-CBC
32	d	403	PHO	C2C-C3C-CAC-CBC
34	8	301	SQD	C11-C12-C13-C14
37	C	522	LMG	C31-C32-C33-C34
37	w	201	LMG	C37-C38-C39-C40
37	1	317	LMG	C14-C15-C16-C17
37	14	316	LMG	C36-C37-C38-C39
37	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
34	a	408	SQD	C18-C19-C20-C21
36	18	316	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	C	522	LMG	C16-C17-C18-C19
37	W	201	LMG	C37-C38-C39-C40
38	B	621	DGD	C5A-C6A-C7A-C8A
38	C	519	DGD	C2B-C3B-C4B-C5B
38	C	519	DGD	CBB-CCB-CDB-CEB
38	C	520	DGD	CCA-CDA-CEA-CFA
38	c	519	DGD	C2B-C3B-C4B-C5B
38	c	519	DGD	CBB-CCB-CDB-CEB
38	c	520	DGD	CCA-CDA-CEA-CFA
38	11	318	DGD	C7B-C8B-C9B-CAB
37	J	101	LMG	C4-C5-C6-O5
37	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	316	LHG	C11-C12-C13-C14
36	14	317	LHG	C15-C16-C17-C18
37	5	315	LMG	C16-C17-C18-C19
37	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
37	B	620	LMG	C2-C1-O1-C7
37	D	404	LMG	C2-C1-O1-C7
37	P	614	LMG	C2-C1-O1-C7
37	Z	102	LMG	C2-C1-O1-C7
37	b	621	LMG	C2-C1-O1-C7
37	c	522	LMG	C2-C1-O1-C7
37	d	404	LMG	C2-C1-O1-C7
37	p	614	LMG	C2-C1-O1-C7
38	C	519	DGD	C2E-C1E-O5D-C6D
38	C	520	DGD	C2E-C1E-O5D-C6D
38	c	519	DGD	C2E-C1E-O5D-C6D
38	c	520	DGD	C2E-C1E-O5D-C6D
37	f	102	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	A	408	SQD	C34-C35-C36-C37
37	4	316	LMG	C31-C32-C33-C34
37	14	316	LMG	C12-C13-C14-C15
38	C	520	DGD	C5B-C6B-C7B-C8B
38	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	316	LHG	C27-C28-C29-C30
36	18	315	LHG	C27-C28-C29-C30
37	J	101	LMG	C16-C17-C18-C19
37	j	101	LMG	C16-C17-C18-C19
37	4	316	LMG	C12-C13-C14-C15
38	C	518	DGD	C2A-C3A-C4A-C5A
38	C	519	DGD	CAB-CBB-CCB-CDB
38	b	622	DGD	C5B-C6B-C7B-C8B
38	c	518	DGD	C2A-C3A-C4A-C5A
38	c	519	DGD	CAB-CBB-CCB-CDB
38	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	302	A86	C33-C34-O4-C38
43	12	301	A86	C35-C34-O4-C38
37	1	317	LMG	C10-C11-C12-C13
34	l	101	SQD	C15-C16-C17-C18
37	B	620	LMG	C30-C31-C32-C33
37	b	621	LMG	C31-C32-C33-C34
37	d	404	LMG	C30-C31-C32-C33
38	B	621	DGD	C4B-C5B-C6B-C7B
38	H	102	DGD	C7A-C8A-C9A-CAA
38	H	102	DGD	C4B-C5B-C6B-C7B
38	h	102	DGD	C4B-C5B-C6B-C7B
38	1	318	DGD	C7B-C8B-C9B-CAB
31	B	616	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
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
37	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
37	B	620	LMG	C31-C32-C33-C34
37	15	314	LMG	C30-C31-C32-C33
38	C	520	DGD	CAB-CBB-CCB-CDB
38	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
37	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
37	F	102	LMG	C30-C31-C32-C33
37	f	102	LMG	C30-C31-C32-C33
37	5	316	LMG	C33-C34-C35-C36
37	10	319	LMG	C11-C12-C13-C14
37	14	316	LMG	C15-C16-C17-C18
38	H	102	DGD	CCA-CDA-CEA-CFA
38	c	520	DGD	CAB-CBB-CCB-CDB
37	J	101	LMG	C28-C29-C30-C31
37	W	201	LMG	C28-C29-C30-C31
37	j	101	LMG	C28-C29-C30-C31
37	w	201	LMG	C28-C29-C30-C31
37	11	317	LMG	C10-C11-C12-C13
37	15	315	LMG	C28-C29-C30-C31
34	A	411	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	i	101	SQD	C27-C28-C29-C30
34	10	320	SQD	C11-C12-C13-C14
36	D	408	LHG	C27-C28-C29-C30
36	L	101	LHG	C27-C28-C29-C30
36	d	408	LHG	C27-C28-C29-C30
36	l	102	LHG	C27-C28-C29-C30
36	w	202	LHG	C27-C28-C29-C30
37	C	522	LMG	C37-C38-C39-C40
37	F	102	LMG	C16-C17-C18-C19
37	K	101	LMG	C32-C33-C34-C35
37	W	201	LMG	C30-C31-C32-C33
37	b	621	LMG	C30-C31-C32-C33
37	c	521	LMG	C12-C13-C14-C15
37	c	521	LMG	C37-C38-C39-C40
37	d	404	LMG	C32-C33-C34-C35
37	f	102	LMG	C16-C17-C18-C19
37	k	101	LMG	C32-C33-C34-C35
37	w	201	LMG	C30-C31-C32-C33
37	1	317	LMG	C30-C31-C32-C33
37	4	316	LMG	C33-C34-C35-C36
38	B	621	DGD	CBB-CCB-CDB-CEB
38	C	519	DGD	C3B-C4B-C5B-C6B
38	C	520	DGD	C5A-C6A-C7A-C8A
38	H	102	DGD	C3A-C4A-C5A-C6A
38	b	622	DGD	C6B-C7B-C8B-C9B
38	c	519	DGD	C3B-C4B-C5B-C6B
38	c	520	DGD	C5A-C6A-C7A-C8A
38	h	102	DGD	C5A-C6A-C7A-C8A
38	h	102	DGD	CCA-CDA-CEA-CFA
37	M	101	LMG	O6-C5-C6-O5
31	B	601	CLA	C4B-C3B-CAB-CBB
31	B	603	CLA	C4B-C3B-CAB-CBB
31	C	505	CLA	C4B-C3B-CAB-CBB
31	C	512	CLA	C4B-C3B-CAB-CBB
31	D	406	CLA	C4B-C3B-CAB-CBB
31	Z	101	CLA	C4B-C3B-CAB-CBB
31	b	602	CLA	C4B-C3B-CAB-CBB
31	b	604	CLA	C4B-C3B-CAB-CBB
31	c	505	CLA	C4B-C3B-CAB-CBB
31	c	512	CLA	C4B-C3B-CAB-CBB
31	d	406	CLA	C4B-C3B-CAB-CBB
31	0	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	1	307	CLA	C4B-C3B-CAB-CBB
31	2	306	CLA	C4B-C3B-CAB-CBB
31	2	311	CLA	C4B-C3B-CAB-CBB
31	3	308	CLA	C4B-C3B-CAB-CBB
31	3	313	CLA	C4B-C3B-CAB-CBB
31	6	314	CLA	C4B-C3B-CAB-CBB
31	7	312	CLA	C4B-C3B-CAB-CBB
31	8	312	CLA	C4B-C3B-CAB-CBB
31	10	307	CLA	C4B-C3B-CAB-CBB
31	10	313	CLA	C4B-C3B-CAB-CBB
31	13	316	CLA	C4B-C3B-CAB-CBB
31	14	315	CLA	C4B-C3B-CAB-CBB
31	15	306	CLA	C4B-C3B-CAB-CBB
31	17	312	CLA	C4B-C3B-CAB-CBB
31	B	615	CLA	C16-C17-C18-C19
31	B	615	CLA	C16-C17-C18-C20
31	b	616	CLA	C16-C17-C18-C19
37	D	404	LMG	O6-C1-O1-C7
37	P	614	LMG	O6-C1-O1-C7
37	d	404	LMG	O6-C1-O1-C7
37	p	614	LMG	O6-C1-O1-C7
38	B	621	DGD	O6D-C1D-O3G-C3G
38	C	518	DGD	O6D-C1D-O3G-C3G
38	c	518	DGD	O6D-C1D-O3G-C3G
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
37	W	201	LMG	C18-C19-C20-C21
37	w	201	LMG	C18-C19-C20-C21
37	4	316	LMG	C13-C14-C15-C16
38	H	102	DGD	C5A-C6A-C7A-C8A
38	H	102	DGD	C8A-C9A-CAA-CBA
38	h	102	DGD	C3A-C4A-C5A-C6A
38	h	102	DGD	C8A-C9A-CAA-CBA
31	16	315	CLA	O1D-CGD-O2D-CED
34	B	623	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	b	601	SQD	C12-C13-C14-C15
36	D	408	LHG	C16-C17-C18-C19
36	a	410	LHG	C26-C27-C28-C29
36	d	408	LHG	C16-C17-C18-C19
37	5	315	LMG	C12-C13-C14-C15
38	B	621	DGD	C8B-C9B-CAB-CBB
38	c	520	DGD	C6A-C7A-C8A-C9A
34	8	301	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	408	LHG	C13-C14-C15-C16
36	a	410	LHG	C11-C10-C9-C8
36	d	408	LHG	C13-C14-C15-C16
37	1	317	LMG	C15-C16-C17-C18
37	5	315	LMG	C30-C31-C32-C33
37	15	315	LMG	C31-C32-C33-C34
38	C	519	DGD	C6A-C7A-C8A-C9A
38	C	520	DGD	C6A-C7A-C8A-C9A
38	H	102	DGD	C9A-CAA-CBA-CCA
38	c	519	DGD	C6A-C7A-C8A-C9A
38	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
37	F	102	LMG	C29-C28-O8-C9
37	K	101	LMG	C29-C30-C31-C32
37	k	101	LMG	C29-C30-C31-C32
38	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

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Mol	Chain	Res	Type	Atoms
31	A	403	CLA	C3A-C2A-CAA-CBA
31	C	507	CLA	C3A-C2A-CAA-CBA
31	D	405	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	405	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	312	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
31	16	312	CLA	C3A-C2A-CAA-CBA
31	17	312	CLA	C3A-C2A-CAA-CBA
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
37	W	201	LMG	C11-C12-C13-C14
37	c	521	LMG	C19-C20-C21-C22
37	w	201	LMG	C11-C12-C13-C14
37	5	316	LMG	C31-C32-C33-C34
38	C	520	DGD	C2B-C3B-C4B-C5B
38	W	203	DGD	C6A-C7A-C8A-C9A
38	c	520	DGD	C2B-C3B-C4B-C5B
43	16	301	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

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Mol	Chain	Res	Type	Atoms
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
37	d	404	LMG	C11-C12-C13-C14
37	1	317	LMG	C31-C32-C33-C34
37	4	316	LMG	C15-C16-C17-C18
38	B	621	DGD	C5B-C6B-C7B-C8B
31	8	310	CLA	C3-C5-C6-C7
34	10	320	SQD	C44-C45-C46-O48
37	1	301	LMG	O9-C10-O7-C8
37	11	301	LMG	O9-C10-O7-C8
31	19	308	CLA	CBD-CGD-O2D-CED
37	C	522	LMG	C12-C13-C14-C15
37	C	522	LMG	C19-C20-C21-C22
38	C	519	DGD	C2A-C3A-C4A-C5A
38	b	622	DGD	C3B-C4B-C5B-C6B
38	c	519	DGD	C2A-C3A-C4A-C5A
31	D	402	CLA	C3-C5-C6-C7
31	d	402	CLA	C3-C5-C6-C7
36	d	408	LHG	C14-C15-C16-C17
31	B	605	CLA	C15-C16-C17-C18
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	408	LHG	C14-C15-C16-C17
36	L	101	LHG	C12-C13-C14-C15
36	l	102	LHG	C12-C13-C14-C15
37	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

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Mol	Chain	Res	Type	Atoms
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
37	14	316	LMG	C18-C19-C20-C21
38	W	203	DGD	C3A-C4A-C5A-C6A
38	w	204	DGD	C3A-C4A-C5A-C6A
38	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	408	LHG	C25-C26-C27-C28
36	d	408	LHG	C25-C26-C27-C28
37	J	101	LMG	C31-C32-C33-C34
37	j	101	LMG	C31-C32-C33-C34
31	B	615	CLA	C2B-C3B-CAB-CBB
31	C	505	CLA	C2B-C3B-CAB-CBB
31	C	512	CLA	C2B-C3B-CAB-CBB
31	D	406	CLA	C2B-C3B-CAB-CBB
31	P	602	CLA	C2B-C3B-CAB-CBB
31	P	605	CLA	C2B-C3B-CAB-CBB
31	P	606	CLA	C2B-C3B-CAB-CBB
31	P	607	CLA	C2B-C3B-CAB-CBB
31	Z	101	CLA	C2B-C3B-CAB-CBB
31	b	602	CLA	C2B-C3B-CAB-CBB
31	b	616	CLA	C2B-C3B-CAB-CBB
31	c	505	CLA	C2B-C3B-CAB-CBB
31	c	512	CLA	C2B-C3B-CAB-CBB
31	d	406	CLA	C2B-C3B-CAB-CBB
31	p	602	CLA	C2B-C3B-CAB-CBB
31	p	605	CLA	C2B-C3B-CAB-CBB
31	p	606	CLA	C2B-C3B-CAB-CBB
31	p	607	CLA	C2B-C3B-CAB-CBB
31	0	308	CLA	C2B-C3B-CAB-CBB
31	1	307	CLA	C2B-C3B-CAB-CBB
31	1	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	2	306	CLA	C2B-C3B-CAB-CBB
31	2	311	CLA	C2B-C3B-CAB-CBB
31	3	308	CLA	C2B-C3B-CAB-CBB
31	3	313	CLA	C2B-C3B-CAB-CBB
31	3	316	CLA	C2B-C3B-CAB-CBB
31	4	315	CLA	C2B-C3B-CAB-CBB
31	5	312	CLA	C2B-C3B-CAB-CBB
31	8	312	CLA	C2B-C3B-CAB-CBB
31	10	313	CLA	C2B-C3B-CAB-CBB
31	12	307	CLA	C2B-C3B-CAB-CBB
31	13	312	CLA	C2B-C3B-CAB-CBB
31	13	316	CLA	C2B-C3B-CAB-CBB
31	14	312	CLA	C2B-C3B-CAB-CBB
31	14	315	CLA	C2B-C3B-CAB-CBB
31	15	306	CLA	C2B-C3B-CAB-CBB
31	15	311	CLA	C2B-C3B-CAB-CBB
31	15	312	CLA	C2B-C3B-CAB-CBB
31	17	312	CLA	C2B-C3B-CAB-CBB
31	18	311	CLA	C2B-C3B-CAB-CBB
31	B	613	CLA	C10-C11-C12-C13
31	b	614	CLA	C10-C11-C12-C13
31	14	309	CLA	C13-C15-C16-C17
36	L	101	LHG	C16-C17-C18-C19
37	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
37	M	101	LMG	C32-C33-C34-C35
37	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	408	LHG	C15-C16-C17-C18
36	L	101	LHG	C24-C25-C26-C27
36	d	408	LHG	C15-C16-C17-C18
36	l	102	LHG	C24-C25-C26-C27
37	K	101	LMG	C38-C39-C40-C41
37	K	101	LMG	C39-C40-C41-C42
37	j	101	LMG	C19-C20-C21-C22
37	k	101	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
37	k	101	LMG	C39-C40-C41-C42
37	11	317	LMG	C15-C16-C17-C18
37	Z	102	LMG	O9-C10-O7-C8
37	c	522	LMG	O9-C10-O7-C8
38	W	203	DGD	O1B-C1B-O2G-C2G
38	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
37	J	101	LMG	C19-C20-C21-C22
38	C	518	DGD	C3A-C4A-C5A-C6A
38	C	520	DGD	CBA-CCA-CDA-CEA
38	W	203	DGD	CAB-CBB-CCB-CDB
38	c	518	DGD	C3A-C4A-C5A-C6A
38	c	520	DGD	CBA-CCA-CDA-CEA
38	w	204	DGD	CAB-CBB-CCB-CDB
37	j	101	LMG	O6-C5-C6-O5
31	W	202	CLA	O1A-CGA-O2A-C1
31	w	203	CLA	O1A-CGA-O2A-C1
37	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
37	D	404	LMG	C10-C11-C12-C13
31	8	308	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

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Mol	Chain	Res	Type	Atoms
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
37	d	404	LMG	C12-C13-C14-C15
37	11	317	LMG	C31-C32-C33-C34
38	C	518	DGD	C6B-C7B-C8B-C9B
38	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
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
37	K	101	LMG	C11-C10-O7-C8
37	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
37	J	101	LMG	O6-C5-C6-O5
38	C	520	DGD	O6E-C5E-C6E-O5E
38	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
37	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

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Mol	Chain	Res	Type	Atoms
37	K	101	LMG	O6-C5-C6-O5
37	M	101	LMG	C33-C34-C35-C36
38	W	203	DGD	C2B-C3B-C4B-C5B
38	w	204	DGD	C2B-C3B-C4B-C5B
31	4	309	CLA	C4-C3-C5-C6
31	8	310	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
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	405	CLA	C2C-C3C-CAC-CBC
31	d	405	CLA	C2C-C3C-CAC-CBC
37	1	317	LMG	C34-C35-C36-C37
31	D	405	CLA	C8-C10-C11-C12
31	b	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	617	CLA	C15-C16-C17-C18
31	d	405	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	305	A86	C35-C34-O4-C38
37	k	101	LMG	O6-C5-C6-O5
38	11	318	DGD	O6E-C5E-C6E-O5E
36	D	408	LHG	O9-C7-O7-C5
36	Z	103	LHG	O9-C7-O7-C5
36	d	408	LHG	O9-C7-O7-C5
36	z	102	LHG	O9-C7-O7-C5
37	n	701	LMG	C29-C28-O8-C9
34	l	101	SQD	C32-C33-C34-C35
38	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
37	B	620	LMG	C33-C34-C35-C36
37	15	314	LMG	C15-C16-C17-C18
34	8	301	SQD	C26-C27-C28-C29
37	k	101	LMG	C15-C16-C17-C18
38	C	518	DGD	C1A-C2A-C3A-C4A
38	c	518	DGD	C1A-C2A-C3A-C4A
38	1	318	DGD	C1A-C2A-C3A-C4A
37	K	101	LMG	C15-C16-C17-C18
37	4	316	LMG	C18-C19-C20-C21
37	5	315	LMG	C15-C16-C17-C18
42	1	314	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
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
37	D	404	LMG	C32-C33-C34-C35
37	d	409	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
38	b	622	DGD	O6D-C1D-O3G-C3G
34	a	408	SQD	C28-C29-C30-C31
34	8	301	SQD	C12-C13-C14-C15
36	D	408	LHG	C24-C25-C26-C27
36	d	408	LHG	C24-C25-C26-C27
36	8	316	LHG	C26-C27-C28-C29
37	D	409	LMG	C11-C12-C13-C14
38	H	102	DGD	C3B-C4B-C5B-C6B
38	h	102	DGD	C3B-C4B-C5B-C6B
34	A	408	SQD	C8-C7-O47-C45
34	a	408	SQD	C8-C7-O47-C45
37	N	101	LMG	C11-C10-O7-C8
37	W	201	LMG	C11-C10-O7-C8
37	n	701	LMG	C11-C10-O7-C8
37	w	201	LMG	C11-C10-O7-C8
37	5	315	LMG	C11-C10-O7-C8
37	5	316	LMG	C11-C10-O7-C8
36	A	410	LHG	O6-C4-C5-O7
36	a	410	LHG	O6-C4-C5-O7
37	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

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Mol	Chain	Res	Type	Atoms
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	311	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	309	KC2	C4B-C3B-CAB-CBB
45	16	311	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	316	LHG	O9-C7-O7-C5
43	16	301	A86	C33-C34-O4-C38
43	19	304	A86	C35-C34-O4-C38
37	5	316	LMG	C28-C29-C30-C31
36	8	316	LHG	C14-C15-C16-C17
37	J	101	LMG	C13-C14-C15-C16
37	0	317	LMG	C2-C1-O1-C7
37	10	319	LMG	C2-C1-O1-C7
38	C	518	DGD	C2D-C1D-O3G-C3G
38	c	518	DGD	C2D-C1D-O3G-C3G
34	8	301	SQD	O47-C45-C46-O48
34	10	320	SQD	O47-C45-C46-O48
37	J	101	LMG	O7-C8-C9-O8
37	P	614	LMG	O1-C7-C8-O7
37	j	101	LMG	O7-C8-C9-O8
37	p	614	LMG	O1-C7-C8-O7
36	L	101	LHG	C34-C35-C36-C37
36	l	102	LHG	C34-C35-C36-C37
37	j	101	LMG	C13-C14-C15-C16
38	W	203	DGD	C7A-C8A-C9A-CAA
38	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
37	m	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
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	310	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	407	PL9	C4-C3-C7-C8
35	a	409	PL9	C4-C3-C7-C8
35	d	407	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
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
37	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	312	CLA	C2A-CAA-CBA-CGA
34	8	301	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
38	H	102	DGD	C2B-C3B-C4B-C5B
38	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	317	LHG	C12-C13-C14-C15
37	4	316	LMG	C11-C12-C13-C14
38	B	621	DGD	C3B-C4B-C5B-C6B
38	C	519	DGD	C7A-C8A-C9A-CAA
38	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	402	CLA	C1A-C2A-CAA-CBA
31	D	405	CLA	C1A-C2A-CAA-CBA
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	402	CLA	C1A-C2A-CAA-CBA
31	d	405	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

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Mol	Chain	Res	Type	Atoms
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	308	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
37	W	201	LMG	O9-C10-O7-C8
37	w	201	LMG	O9-C10-O7-C8
37	5	315	LMG	O9-C10-O7-C8
37	10	319	LMG	O9-C10-O7-C8
36	4	317	LHG	C15-C16-C17-C18
37	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
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
37	m	101	LMG	C32-C33-C34-C35
36	8	316	LHG	C23-C24-C25-C26
38	1	318	DGD	O6E-C5E-C6E-O5E
31	C	502	CLA	C3-C5-C6-C7
31	c	502	CLA	C3-C5-C6-C7
37	B	620	LMG	C16-C17-C18-C19
37	b	621	LMG	C16-C17-C18-C19
38	b	622	DGD	C4B-C5B-C6B-C7B
31	8	313	CLA	C5-C6-C7-C8
31	18	307	CLA	C8-C10-C11-C12
31	2	307	CLA	CBA-CGA-O2A-C1
37	B	620	LMG	C29-C28-O8-C9
37	b	621	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
36	z	102	LHG	O6-C4-C5-C6
36	8	317	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
38	1	318	DGD	C5A-C6A-C7A-C8A
36	4	317	LHG	C16-C17-C18-C19
37	b	621	LMG	C33-C34-C35-C36
38	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
37	K	101	LMG	C12-C13-C14-C15
38	1	318	DGD	C5B-C6B-C7B-C8B
37	K	101	LMG	C30-C31-C32-C33
37	b	621	LMG	C34-C35-C36-C37
37	k	101	LMG	C12-C13-C14-C15
37	k	101	LMG	C30-C31-C32-C33
36	D	408	LHG	C30-C31-C32-C33
38	h	102	DGD	CAA-CBA-CCA-CDA
31	B	614	CLA	CBA-CGA-O2A-C1
36	z	102	LHG	C1-C2-C3-O3
37	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	407	PL9	C33-C34-C36-C37
35	d	407	PL9	C33-C34-C36-C37
36	d	408	LHG	C30-C31-C32-C33
37	B	620	LMG	C35-C36-C37-C38
38	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
37	b	621	LMG	C17-C18-C19-C20
37	d	404	LMG	C34-C35-C36-C37
37	m	101	LMG	C12-C13-C14-C15
37	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
37	B	620	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	C	507	CLA	C15-C16-C17-C18
31	c	507	CLA	C15-C16-C17-C18
37	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	8	301	SQD	O6-C44-C45-C46
34	8	301	SQD	C44-C45-C46-O48
34	10	320	SQD	O6-C44-C45-C46
36	8	316	LHG	C4-C5-C6-O8
36	8	317	LHG	C4-C5-C6-O8
37	C	522	LMG	C7-C8-C9-O8
37	D	409	LMG	O1-C7-C8-C9
37	F	102	LMG	C32-C33-C34-C35
37	P	614	LMG	O1-C7-C8-C9
37	c	521	LMG	C7-C8-C9-O8
37	d	409	LMG	O1-C7-C8-C9
37	f	102	LMG	C32-C33-C34-C35
37	p	614	LMG	O1-C7-C8-C9
37	1	301	LMG	O1-C7-C8-C9
37	11	301	LMG	O1-C7-C8-C9
37	11	317	LMG	C7-C8-C9-O8
37	15	315	LMG	C7-C8-C9-O8
38	B	621	DGD	O1G-C1G-C2G-C3G
38	C	518	DGD	O1G-C1G-C2G-C3G
38	C	519	DGD	C1G-C2G-C3G-O3G
38	W	203	DGD	C1G-C2G-C3G-O3G
38	b	622	DGD	O1G-C1G-C2G-C3G
38	c	518	DGD	O1G-C1G-C2G-C3G
38	c	519	DGD	C1G-C2G-C3G-O3G
38	w	204	DGD	C1G-C2G-C3G-O3G
38	1	318	DGD	C1G-C2G-C3G-O3G
38	11	318	DGD	C1G-C2G-C3G-O3G
34	A	408	SQD	C11-C12-C13-C14
34	i	101	SQD	C9-C10-C11-C12
37	W	201	LMG	C29-C30-C31-C32
37	w	201	LMG	C29-C30-C31-C32
37	5	315	LMG	C17-C18-C19-C20
38	C	520	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
38	C	520	DGD	CDB-CEB-CFB-CGB
38	c	520	DGD	CDA-CEA-CFA-CGA
38	c	520	DGD	CDB-CEB-CFB-CGB
37	K	101	LMG	O10-C28-O8-C9
38	C	519	DGD	C5D-C6D-O5D-C1E
38	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
37	M	101	LMG	C15-C16-C17-C18
37	11	317	LMG	C37-C38-C39-C40
37	15	314	LMG	C31-C32-C33-C34
37	15	315	LMG	C29-C30-C31-C32
38	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
37	15	314	LMG	C17-C18-C19-C20
37	15	315	LMG	C34-C35-C36-C37
36	L	101	LHG	C23-C24-C25-C26
36	l	102	LHG	C23-C24-C25-C26
37	K	101	LMG	C28-C29-C30-C31
37	k	101	LMG	C28-C29-C30-C31
37	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
37	K	101	LMG	C40-C41-C42-C43
37	k	101	LMG	C40-C41-C42-C43
37	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	408	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
36	d	408	LHG	O1-C1-C2-O2
36	4	317	LHG	O1-C1-C2-O2
36	8	317	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
37	B	620	LMG	C14-C15-C16-C17
37	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
38	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
37	J	101	LMG	C18-C19-C20-C21
37	K	101	LMG	C35-C36-C37-C38
37	j	101	LMG	C18-C19-C20-C21
31	c	513	CLA	CBD-CGD-O2D-CED
37	B	620	LMG	C34-C35-C36-C37
37	b	621	LMG	C14-C15-C16-C17
37	k	101	LMG	C35-C36-C37-C38
38	11	318	DGD	CFB-CGB-CHB-CIB
31	9	308	CLA	C5-C6-C7-C8
33	b	618	BCR	C20-C21-C22-C37
38	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
37	N	101	LMG	C11-C12-C13-C14
37	0	317	LMG	C12-C13-C14-C15
31	B	609	CLA	C2-C3-C5-C6
31	W	202	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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
37	15	314	LMG	O6-C5-C6-O5
34	A	408	SQD	C11-C10-C9-C8
34	a	408	SQD	C11-C10-C9-C8
37	B	620	LMG	C36-C37-C38-C39
31	C	513	CLA	CBD-CGD-O2D-CED
31	D	406	CLA	CBD-CGD-O2D-CED
31	d	406	CLA	CBD-CGD-O2D-CED
31	D	402	CLA	C13-C15-C16-C17
31	b	617	CLA	C8-C10-C11-C12
31	d	402	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
31	2	307	CLA	C2C-C3C-CAC-CBC
37	1	301	LMG	C34-C35-C36-C37
37	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
37	C	522	LMG	C9-C8-O7-C10
37	c	521	LMG	C9-C8-O7-C10
38	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
37	K	101	LMG	C31-C32-C33-C34
36	14	317	LHG	C24-C23-O8-C6
37	k	101	LMG	C31-C32-C33-C34
34	A	408	SQD	C25-C26-C27-C28
37	c	521	LMG	C22-C23-C24-C25
37	14	316	LMG	C35-C36-C37-C38
38	c	520	DGD	C4B-C5B-C6B-C7B
31	16	308	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

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Mol	Chain	Res	Type	Atoms
34	a	408	SQD	C25-C26-C27-C28
38	C	520	DGD	C4B-C5B-C6B-C7B
34	A	408	SQD	C24-C25-C26-C27
37	d	409	LMG	C12-C13-C14-C15
36	z	102	LHG	O2-C2-C3-O3
37	D	409	LMG	C12-C13-C14-C15
36	D	408	LHG	C7-C8-C9-C10
36	d	408	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
38	W	203	DGD	C2E-C1E-O5D-C6D
38	w	204	DGD	C2E-C1E-O5D-C6D
36	8	316	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
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
37	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
37	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

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Mol	Chain	Res	Type	Atoms
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
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
38	W	203	DGD	C8A-C9A-CAA-CBA
38	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

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Mol	Chain	Res	Type	Atoms
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
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
37	P	614	LMG	C29-C30-C31-C32
37	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
37	11	317	LMG	C34-C35-C36-C37
33	C	516	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
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	317	LHG	C11-C10-C9-C8
37	F	102	LMG	C18-C19-C20-C21
37	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
37	b	621	LMG	C35-C36-C37-C38
37	m	101	LMG	C33-C34-C35-C36
37	10	319	LMG	C12-C13-C14-C15
31	b	615	CLA	O1A-CGA-O2A-C1
37	J	101	LMG	C37-C38-C39-C40
37	j	101	LMG	C37-C38-C39-C40
37	14	316	LMG	C30-C31-C32-C33
31	b	603	CLA	C10-C11-C12-C13
31	B	614	CLA	O1A-CGA-O2A-C1
37	M	101	LMG	C13-C14-C15-C16
31	P	602	CLA	C4B-C3B-CAB-CBB
31	P	603	CLA	C4B-C3B-CAB-CBB
31	p	602	CLA	C4B-C3B-CAB-CBB
31	p	603	CLA	C4B-C3B-CAB-CBB
31	z	101	CLA	C4B-C3B-CAB-CBB
31	0	314	CLA	C4B-C3B-CAB-CBB
31	1	321	CLA	C4B-C3B-CAB-CBB
31	8	315	CLA	C4B-C3B-CAB-CBB
31	10	314	CLA	C4B-C3B-CAB-CBB
31	11	310	CLA	C4B-C3B-CAB-CBB
31	13	307	CLA	C4B-C3B-CAB-CBB
31	18	314	CLA	C4B-C3B-CAB-CBB
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
38	W	203	DGD	C1A-C2A-C3A-C4A
38	w	204	DGD	C1A-C2A-C3A-C4A
38	11	318	DGD	C1A-C2A-C3A-C4A
37	N	101	LMG	C29-C28-O8-C9
33	C	516	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
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
38	11	318	DGD	C9B-CAB-CBB-CCB
31	1	308	CLA	C13-C15-C16-C17
42	12	314	KC1	CAA-CBA-CGA-O1A
38	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
37	D	409	LMG	C33-C34-C35-C36
38	H	102	DGD	C6B-C7B-C8B-C9B
38	H	102	DGD	CAB-CBB-CCB-CDB
38	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
37	d	409	LMG	C33-C34-C35-C36
37	n	701	LMG	C11-C12-C13-C14
38	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	313	CLA	C3A-C2A-CAA-CBA
31	12	310	CLA	C3A-C2A-CAA-CBA
31	14	315	CLA	C3A-C2A-CAA-CBA
36	D	408	LHG	C28-C29-C30-C31
36	L	101	LHG	C28-C29-C30-C31
36	a	410	LHG	C27-C28-C29-C30
36	d	408	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
37	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
38	b	622	DGD	CDB-CEB-CFB-CGB
31	9	312	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
41	V	201	HEM	C2A-CAA-CBA-CGA
41	v	201	HEM	C2A-CAA-CBA-CGA
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
37	b	621	LMG	C29-C30-C31-C32
37	5	316	LMG	C29-C30-C31-C32
31	C	511	CLA	C13-C15-C16-C17
31	D	405	CLA	C15-C16-C17-C18
31	c	511	CLA	C13-C15-C16-C17
31	d	405	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
37	B	620	LMG	O1-C7-C8-C9
37	B	620	LMG	C7-C8-C9-O8
37	D	404	LMG	O1-C7-C8-C9
37	J	101	LMG	O1-C7-C8-C9
37	J	101	LMG	C7-C8-C9-O8
37	K	101	LMG	C7-C8-C9-O8
37	b	621	LMG	O1-C7-C8-C9
37	b	621	LMG	C7-C8-C9-O8
37	d	404	LMG	O1-C7-C8-C9
37	j	101	LMG	O1-C7-C8-C9
37	j	101	LMG	C7-C8-C9-O8
37	k	101	LMG	C7-C8-C9-O8
37	1	301	LMG	C7-C8-C9-O8
37	1	317	LMG	C7-C8-C9-O8
37	5	316	LMG	O1-C7-C8-C9
37	5	316	LMG	C7-C8-C9-O8
37	11	301	LMG	C7-C8-C9-O8
37	15	315	LMG	O1-C7-C8-C9
38	C	518	DGD	C1G-C2G-C3G-O3G
38	c	518	DGD	C1G-C2G-C3G-O3G
38	1	318	DGD	O1G-C1G-C2G-C3G
37	15	314	LMG	O9-C10-O7-C8
38	W	203	DGD	C5A-C6A-C7A-C8A
38	w	204	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
31	1	313	CLA	C8-C10-C11-C12
38	H	102	DGD	O2G-C1B-C2B-C3B
38	h	102	DGD	O2G-C1B-C2B-C3B
36	B	622	LHG	C26-C27-C28-C29
37	M	101	LMG	C35-C36-C37-C38
37	m	101	LMG	C15-C16-C17-C18
31	B	613	CLA	C3-C5-C6-C7
31	b	614	CLA	C3-C5-C6-C7
37	4	316	LMG	C10-C11-C12-C13
36	b	623	LHG	C26-C27-C28-C29
37	B	620	LMG	C22-C23-C24-C25
37	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
37	B	620	LMG	C18-C19-C20-C21
37	b	621	LMG	C18-C19-C20-C21
36	L	101	LHG	C4-O6-P-O3
36	l	102	LHG	C4-O6-P-O3
38	c	518	DGD	O1A-C1A-O1G-C1G
37	15	315	LMG	O6-C5-C6-O5
31	p	607	CLA	C2C-C3C-CAC-CBC
37	W	201	LMG	C14-C15-C16-C17
37	w	201	LMG	C14-C15-C16-C17
38	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
31	19	308	CLA	C5-C6-C7-C8
34	i	101	SQD	C10-C11-C12-C13
36	8	316	LHG	C11-C10-C9-C8
37	1	317	LMG	C17-C18-C19-C20
38	11	318	DGD	CCB-CDB-CEB-CFB
34	A	411	SQD	C10-C11-C12-C13
32	A	405	PHO	O1D-CGD-O2D-CED
38	C	518	DGD	O1A-C1A-O1G-C1G
45	18	310	KC2	C3A-C2A-CAA-CBA
31	14	309	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C2B-C3B-CAB-CBB
31	B	603	CLA	C2B-C3B-CAB-CBB
31	P	603	CLA	C2B-C3B-CAB-CBB
31	b	604	CLA	C2B-C3B-CAB-CBB
31	p	603	CLA	C2B-C3B-CAB-CBB
31	z	101	CLA	C2B-C3B-CAB-CBB
31	1	321	CLA	C2B-C3B-CAB-CBB
31	7	312	CLA	C2B-C3B-CAB-CBB
31	10	307	CLA	C2B-C3B-CAB-CBB
31	13	307	CLA	C2B-C3B-CAB-CBB
37	j	101	LMG	C21-C22-C23-C24
31	6	309	CLA	O1A-CGA-O2A-C1
31	16	308	CLA	O1A-CGA-O2A-C1
37	P	614	LMG	O10-C28-O8-C9
37	p	614	LMG	O10-C28-O8-C9
37	J	101	LMG	C21-C22-C23-C24
37	1	317	LMG	C37-C38-C39-C40
34	L	102	SQD	O47-C45-C46-O48
34	8	301	SQD	O6-C44-C45-O47
36	L	101	LHG	O7-C5-C6-O8
36	l	102	LHG	O7-C5-C6-O8
36	8	317	LHG	O7-C5-C6-O8
37	B	620	LMG	O1-C7-C8-O7
37	D	404	LMG	O1-C7-C8-O7
37	D	409	LMG	O7-C8-C9-O8
37	J	101	LMG	O1-C7-C8-O7
37	b	621	LMG	O1-C7-C8-O7
37	d	409	LMG	O7-C8-C9-O8
37	j	101	LMG	O1-C7-C8-O7
37	11	317	LMG	O1-C7-C8-O7
37	11	317	LMG	O7-C8-C9-O8
38	C	518	DGD	O1G-C1G-C2G-O2G
38	C	518	DGD	O2G-C2G-C3G-O3G
38	C	519	DGD	O2G-C2G-C3G-O3G
38	C	520	DGD	O1G-C1G-C2G-O2G
38	W	203	DGD	O1G-C1G-C2G-O2G
38	c	518	DGD	O1G-C1G-C2G-O2G
38	c	518	DGD	O2G-C2G-C3G-O3G
38	c	519	DGD	O2G-C2G-C3G-O3G
38	c	520	DGD	O1G-C1G-C2G-O2G
38	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
37	K	101	LMG	O6-C1-O1-C7
37	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	302	A86	C10-C11-C13-C14
43	8	304	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	301	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	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
37	14	316	LMG	C33-C34-C35-C36
38	H	102	DGD	CDA-CEA-CFA-CGA
38	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	407	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	308	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
38	W	203	DGD	C4B-C5B-C6B-C7B
38	w	204	DGD	C4B-C5B-C6B-C7B
38	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
38	C	520	DGD	CAA-CBA-CCA-CDA
38	c	518	DGD	C3B-C4B-C5B-C6B
38	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
37	11	317	LMG	C13-C14-C15-C16
38	C	518	DGD	C3B-C4B-C5B-C6B
43	13	303	A86	C7-C6-C8-C9
35	D	407	PL9	C47-C48-C49-C50
38	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	307	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
37	11	317	LMG	C17-C18-C19-C20
31	18	314	CLA	O1D-CGD-O2D-CED
38	C	519	DGD	O6E-C5E-C6E-O5E
36	D	408	LHG	C10-C11-C12-C13
36	d	408	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	317	LHG	C15-C16-C17-C18
43	3	301	A86	C33-C34-O4-C38
34	i	101	SQD	C30-C31-C32-C33
37	1	317	LMG	C35-C36-C37-C38
31	19	307	CLA	O1A-CGA-O2A-C1
34	L	102	SQD	C31-C32-C33-C34
37	M	101	LMG	C30-C31-C32-C33
36	D	408	LHG	O6-C4-C5-C6
36	d	408	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	308	CLA	C11-C10-C8-C7
31	16	308	CLA	C12-C13-C15-C16
31	19	313	CLA	C11-C12-C13-C15
32	A	405	PHO	C2-C3-C5-C6
32	D	403	PHO	C6-C7-C8-C10
32	a	405	PHO	C2-C3-C5-C6
32	d	403	PHO	C6-C7-C8-C10
43	18	305	A86	C24-C25-C26-C27
31	D	405	CLA	C16-C17-C18-C19
31	d	405	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
37	D	404	LMG	C34-C35-C36-C37
31	1	321	CLA	C12-C13-C15-C16
31	14	306	CLA	C12-C13-C15-C16
37	D	404	LMG	C13-C14-C15-C16
37	m	101	LMG	C11-C12-C13-C14
38	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	307	CLA	CAD-CBD-CGD-O2D
31	8	310	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	307	CLA	CAD-CBD-CGD-O2D
31	16	310	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
37	d	404	LMG	C9-C8-O7-C10
38	B	621	DGD	C3G-C2G-O2G-C1B
38	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
37	0	317	LMG	O6-C1-O1-C7
37	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
37	C	522	LMG	O1-C7-C8-C9
37	c	521	LMG	O1-C7-C8-C9
37	m	101	LMG	O1-C7-C8-C9
37	15	314	LMG	O1-C7-C8-C9
38	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	302	A86	C12-C11-C13-O
43	8	303	A86	C12-C11-C13-O
43	8	304	A86	C12-C11-C13-O
43	8	305	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
43	8	306	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	303	A86	C12-C11-C13-O
43	16	304	A86	C12-C11-C13-O
43	16	305	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
37	d	404	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
37	0	317	LMG	O6-C5-C6-O5
31	12	313	CLA	C2C-C3C-CAC-CBC
38	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	314	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
38	w	204	DGD	C4A-C5A-C6A-C7A
31	5	309	CLA	C6-C7-C8-C10
31	8	313	CLA	C6-C7-C8-C9
31	14	309	CLA	C16-C17-C18-C19
37	D	409	LMG	C30-C31-C32-C33
37	Z	102	LMG	C30-C31-C32-C33
37	d	409	LMG	C30-C31-C32-C33
37	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
37	15	315	LMG	O10-C28-O8-C9
38	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
37	B	620	LMG	C29-C30-C31-C32
37	11	317	LMG	C19-C20-C21-C22
38	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
37	C	522	LMG	O7-C8-C9-O8
37	D	409	LMG	O1-C7-C8-O7
37	c	521	LMG	O1-C7-C8-O7
37	c	521	LMG	O7-C8-C9-O8
37	d	404	LMG	O1-C7-C8-O7
37	d	409	LMG	O1-C7-C8-O7
37	1	317	LMG	O7-C8-C9-O8
37	5	316	LMG	O1-C7-C8-O7
37	15	314	LMG	O1-C7-C8-O7
37	15	315	LMG	O1-C7-C8-O7
38	B	621	DGD	O2G-C2G-C3G-O3G
38	b	622	DGD	O2G-C2G-C3G-O3G
38	1	318	DGD	O2G-C2G-C3G-O3G
37	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	303	A86	C10-C11-C13-O
43	8	304	A86	C10-C11-C13-O
43	8	305	A86	C10-C11-C13-O
43	8	306	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	302	A86	C10-C11-C13-O
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	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
37	W	201	LMG	C39-C40-C41-C42
37	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
38	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
37	Z	102	LMG	C29-C30-C31-C32
31	b	613	CLA	C3-C5-C6-C7
38	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
37	w	201	LMG	C12-C13-C14-C15
43	19	302	A86	C35-C34-O4-C38
37	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
37	15	315	LMG	C10-C11-C12-C13
38	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	8	301	SQD	C11-C10-C9-C8
31	D	406	CLA	O1D-CGD-O2D-CED
31	d	406	CLA	O1D-CGD-O2D-CED
43	3	303	A86	C33-C34-O4-C38
43	10	302	A86	C33-C34-O4-C38
36	8	317	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
37	m	101	LMG	C34-C35-C36-C37
31	D	406	CLA	C3-C5-C6-C7
31	d	406	CLA	C3-C5-C6-C7
36	Z	103	LHG	C2-C3-O3-P
36	z	102	LHG	C2-C3-O3-P
38	c	519	DGD	C5B-C6B-C7B-C8B
38	1	318	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
31	P	606	CLA	C4B-C3B-CAB-CBB
31	P	608	CLA	C4B-C3B-CAB-CBB
31	W	202	CLA	C4B-C3B-CAB-CBB
31	p	606	CLA	C4B-C3B-CAB-CBB
31	p	608	CLA	C4B-C3B-CAB-CBB
31	w	203	CLA	C4B-C3B-CAB-CBB
31	2	314	CLA	C4B-C3B-CAB-CBB
31	5	306	CLA	C4B-C3B-CAB-CBB
31	7	315	CLA	C4B-C3B-CAB-CBB
31	8	307	CLA	C4B-C3B-CAB-CBB
31	10	308	CLA	C4B-C3B-CAB-CBB
31	11	307	CLA	C4B-C3B-CAB-CBB
31	17	315	CLA	C4B-C3B-CAB-CBB
36	A	410	LHG	C3-O3-P-O5
36	A	410	LHG	C4-O6-P-O4
36	D	408	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	408	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	317	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
38	c	520	DGD	C1B-C2B-C3B-C4B
38	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
37	W	201	LMG	C4-C5-C6-O5
37	w	201	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
38	C	520	DGD	C3B-C4B-C5B-C6B
31	B	605	CLA	C13-C15-C16-C17
38	C	520	DGD	C1B-C2B-C3B-C4B
38	c	520	DGD	C3B-C4B-C5B-C6B
41	E	101	HEM	C2A-CAA-CBA-CGA
41	e	101	HEM	C2A-CAA-CBA-CGA
37	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
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
37	5	316	LMG	O10-C28-O8-C9
37	14	316	LMG	C37-C38-C39-C40
31	9	308	CLA	O1D-CGD-O2D-CED
37	1	301	LMG	C31-C32-C33-C34
37	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

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Mol	Chain	Res	Type	Atoms
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	408	LHG	O6-C4-C5-O7
36	d	408	LHG	O6-C4-C5-O7
36	z	102	LHG	O6-C4-C5-O7
34	L	102	SQD	C33-C34-C35-C36
32	D	403	PHO	C8-C10-C11-C12
32	d	403	PHO	C8-C10-C11-C12
37	F	102	LMG	C17-C18-C19-C20
37	F	102	LMG	C29-C30-C31-C32
37	f	102	LMG	C29-C30-C31-C32
31	10	307	CLA	CBD-CGD-O2D-CED
37	f	102	LMG	C17-C18-C19-C20
37	1	317	LMG	C32-C33-C34-C35
37	14	316	LMG	C17-C18-C19-C20
38	c	519	DGD	CCA-CDA-CEA-CFA
37	c	522	LMG	C11-C10-O7-C8
37	1	301	LMG	C11-C10-O7-C8
37	11	301	LMG	C11-C10-O7-C8
36	l	102	LHG	C15-C16-C17-C18
37	W	201	LMG	C36-C37-C38-C39
37	w	201	LMG	C36-C37-C38-C39
38	C	519	DGD	CCA-CDA-CEA-CFA
38	c	518	DGD	C7B-C8B-C9B-CAB
37	f	102	LMG	O10-C28-O8-C9
36	L	101	LHG	C15-C16-C17-C18
37	c	522	LMG	C29-C30-C31-C32
38	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

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Mol	Chain	Res	Type	Atoms
31	1	308	CLA	C5-C6-C7-C8
37	1	317	LMG	O1-C7-C8-C9
37	10	319	LMG	C29-C30-C31-C32
38	B	621	DGD	C1G-C2G-C3G-O3G
38	b	622	DGD	C1G-C2G-C3G-O3G
37	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
37	C	522	LMG	O1-C7-C8-O7
37	m	101	LMG	O1-C7-C8-O7
37	1	301	LMG	O1-C7-C8-O7
37	1	317	LMG	O1-C7-C8-O7
37	5	315	LMG	O1-C7-C8-O7
37	11	301	LMG	O1-C7-C8-O7
38	B	621	DGD	O1G-C1G-C2G-O2G
38	W	203	DGD	O2G-C2G-C3G-O3G
38	b	622	DGD	O1G-C1G-C2G-O2G
38	w	204	DGD	O2G-C2G-C3G-O3G
38	11	318	DGD	O2G-C2G-C3G-O3G
37	b	621	LMG	C36-C37-C38-C39
38	C	520	DGD	C7A-C8A-C9A-CAA
34	l	101	SQD	C33-C34-C35-C36
37	11	317	LMG	C36-C37-C38-C39
38	c	520	DGD	C7A-C8A-C9A-CAA
37	C	522	LMG	C11-C12-C13-C14
37	4	316	LMG	C37-C38-C39-C40
43	13	306	A86	C35-C34-O4-C38
36	8	317	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

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Mol	Chain	Res	Type	Atoms
43	5	318	A86	C13-C14-C15-C20
43	7	303	A86	C13-C14-C15-C20
43	8	304	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
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
37	F	102	LMG	C12-C13-C14-C15
37	f	102	LMG	C12-C13-C14-C15
38	H	102	DGD	C8B-C9B-CAB-CBB
38	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

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Mol	Chain	Res	Type	Atoms
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	308	CLA	C11-C10-C8-C9
32	D	403	PHO	C6-C7-C8-C9
32	d	403	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
37	b	621	LMG	C19-C20-C21-C22
31	2	307	CLA	C3-C5-C6-C7
31	4	312	CLA	CAA-CBA-CGA-O2A
31	11	307	CLA	C2C-C3C-CAC-CBC
37	D	404	LMG	C33-C34-C35-C36
38	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	308	CLA	C5-C6-C7-C8
37	B	620	LMG	C19-C20-C21-C22
37	F	102	LMG	C31-C32-C33-C34
34	A	408	SQD	C23-C24-C25-C26
34	a	408	SQD	C23-C24-C25-C26
37	c	521	LMG	C15-C16-C17-C18
37	d	404	LMG	C33-C34-C35-C36
37	f	102	LMG	C31-C32-C33-C34
45	13	309	KC2	O1D-CGD-O2D-CED
31	b	615	CLA	C5-C6-C7-C8
37	W	201	LMG	C19-C20-C21-C22
37	w	201	LMG	C19-C20-C21-C22
31	P	608	CLA	C2B-C3B-CAB-CBB
31	p	608	CLA	C2B-C3B-CAB-CBB
31	0	307	CLA	C2B-C3B-CAB-CBB
31	0	314	CLA	C2B-C3B-CAB-CBB
31	0	316	CLA	C2B-C3B-CAB-CBB
31	5	306	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	7	315	CLA	C2B-C3B-CAB-CBB
31	8	315	CLA	C2B-C3B-CAB-CBB
31	10	314	CLA	C2B-C3B-CAB-CBB
31	10	316	CLA	C2B-C3B-CAB-CBB
31	11	307	CLA	C2B-C3B-CAB-CBB
31	11	310	CLA	C2B-C3B-CAB-CBB
31	13	310	CLA	C2B-C3B-CAB-CBB
31	17	315	CLA	C2B-C3B-CAB-CBB
31	18	314	CLA	C2B-C3B-CAB-CBB
31	19	313	CLA	C2B-C3B-CAB-CBB
43	8	302	A86	C35-C34-O4-C38
43	16	302	A86	C35-C34-O4-C38
36	D	408	LHG	C33-C34-C35-C36
37	C	522	LMG	C29-C30-C31-C32
37	W	201	LMG	C13-C14-C15-C16
37	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	408	LHG	C33-C34-C35-C36
37	15	314	LMG	C11-C12-C13-C14
38	H	102	DGD	C2A-C3A-C4A-C5A
37	P	614	LMG	C29-C28-O8-C9
36	a	410	LHG	C30-C31-C32-C33
38	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
43	11	319	A86	C35-C34-O4-C38
36	A	410	LHG	C30-C31-C32-C33
36	18	315	LHG	C11-C10-C9-C8
37	J	101	LMG	C12-C13-C14-C15
37	j	101	LMG	C12-C13-C14-C15
37	j	101	LMG	C36-C37-C38-C39
37	4	316	LMG	C35-C36-C37-C38
38	1	318	DGD	C9A-CAA-CBA-CCA
34	8	301	SQD	C44-C45-O47-C7
37	M	101	LMG	C9-C8-O7-C10
37	m	101	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
38	b	622	DGD	C3G-C2G-O2G-C1B
31	4	311	CLA	C2A-CAA-CBA-CGA
31	14	311	CLA	C2A-CAA-CBA-CGA
37	J	101	LMG	C36-C37-C38-C39
37	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
37	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	317	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
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	302	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
43	8	303	A86	C12-C11-C13-C14
43	8	304	A86	C12-C11-C13-C14
43	8	306	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	301	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	17	301	A86	C12-C11-C13-C14
43	17	303	A86	C12-C11-C13-C14
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
37	c	521	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	Z	103	LHG	O6-C4-C5-O7
36	8	317	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	407	PL9	C43-C44-C46-C47
35	d	407	PL9	C43-C44-C46-C47
31	2	314	CLA	O1D-CGD-O2D-CED
37	C	522	LMG	C30-C31-C32-C33
38	c	518	DGD	C4B-C5B-C6B-C7B
43	2	301	A86	C33-C34-O4-C38
37	c	521	LMG	C30-C31-C32-C33
38	C	518	DGD	C4B-C5B-C6B-C7B
31	18	312	CLA	C6-C7-C8-C10
37	15	315	LMG	C11-C10-O7-C8
31	C	511	CLA	C15-C16-C17-C18
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

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Mol	Chain	Res	Type	Atoms
36	15	316	LHG	C3-O3-P-O6
34	A	411	SQD	C24-C25-C26-C27
34	i	101	SQD	C24-C25-C26-C27
37	b	621	LMG	C20-C21-C22-C23
38	c	519	DGD	C4E-C5E-C6E-O5E
31	2	307	CLA	C5-C6-C7-C8
37	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
37	M	101	LMG	O1-C7-C8-C9
37	11	317	LMG	O1-C7-C8-C9
31	p	605	CLA	C2C-C3C-CAC-CBC
37	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
38	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
37	14	316	LMG	C31-C32-C33-C34
43	13	302	A86	C35-C34-O4-C38
38	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
37	W	201	LMG	C15-C16-C17-C18
33	B	617	BCR	C11-C12-C13-C35
33	F	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	f	101	BCR	C36-C18-C19-C20
36	B	622	LHG	C32-C33-C34-C35
37	w	201	LMG	C15-C16-C17-C18
36	5	317	LHG	C2-C3-O3-P
37	5	316	LMG	C11-C12-C13-C14
31	C	513	CLA	O1D-CGD-O2D-CED
43	18	303	A86	C2-C1-C24-C25
37	c	521	LMG	C29-C30-C31-C32
38	C	520	DGD	O1B-C1B-O2G-C2G
38	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
37	15	315	LMG	C11-C12-C13-C14
31	10	317	CLA	CBA-CGA-O2A-C1
31	14	309	CLA	CBA-CGA-O2A-C1
37	1	301	LMG	C29-C30-C31-C32
37	11	301	LMG	C29-C30-C31-C32
38	c	520	DGD	CBB-CCB-CDB-CEB
38	W	203	DGD	O6D-C5D-C6D-O5D
38	w	204	DGD	O6D-C5D-C6D-O5D
31	2	312	CLA	O2A-C1-C2-C3
34	A	408	SQD	C7-C8-C9-C10
37	4	316	LMG	C40-C41-C42-C43
38	C	520	DGD	CBB-CCB-CDB-CEB
31	A	404	CLA	C4B-C3B-CAB-CBB
31	a	404	CLA	C4B-C3B-CAB-CBB
31	0	307	CLA	C4B-C3B-CAB-CBB
31	3	315	CLA	C4B-C3B-CAB-CBB
31	10	316	CLA	C4B-C3B-CAB-CBB
31	12	308	CLA	C4B-C3B-CAB-CBB
31	13	310	CLA	C4B-C3B-CAB-CBB
31	15	309	CLA	C4B-C3B-CAB-CBB
31	19	313	CLA	C4B-C3B-CAB-CBB
31	B	603	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
37	B	620	LMG	O10-C28-C29-C30
33	C	517	BCR	C9-C10-C11-C12
33	C	517	BCR	C19-C20-C21-C22
33	H	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
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	406	CLA	C13-C15-C16-C17
31	d	406	CLA	C13-C15-C16-C17
31	11	308	CLA	C8-C10-C11-C12
37	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
37	M	101	LMG	O1-C7-C8-O7
37	Z	102	LMG	O7-C8-C9-O8
37	c	522	LMG	O7-C8-C9-O8
31	9	310	CLA	C15-C16-C17-C18
36	8	317	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
31	b	617	CLA	C3A-C2A-CAA-CBA
31	8	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
37	D	404	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
37	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
37	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	402	CLA	C14-C13-C15-C16
31	b	603	CLA	C6-C7-C8-C9
31	b	612	CLA	C6-C7-C8-C9
31	d	402	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
37	j	101	LMG	C20-C21-C22-C23
31	10	309	CLA	C10-C11-C12-C13
31	17	308	CLA	C2C-C3C-CAC-CBC
37	J	101	LMG	C20-C21-C22-C23
31	C	510	CLA	O1D-CGD-O2D-CED
34	10	320	SQD	C8-C7-O47-C45
37	D	404	LMG	C7-C8-C9-O8
38	H	102	DGD	O1G-C1G-C2G-C3G
38	h	102	DGD	O1G-C1G-C2G-C3G
44	p	612	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	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
37	d	404	LMG	C35-C36-C37-C38
37	Z	102	LMG	O10-C28-O8-C9
37	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	407	PL9	C2-C3-C7-C8
35	d	407	PL9	C2-C3-C7-C8
36	14	317	LHG	C19-C20-C21-C22
37	w	201	LMG	C40-C41-C42-C43
38	C	520	DGD	C4D-C5D-C6D-O5D
38	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
37	D	404	LMG	C9-C8-O7-C10
38	C	519	DGD	C1G-C2G-O2G-C1B
38	C	519	DGD	C3G-C2G-O2G-C1B
38	c	519	DGD	C1G-C2G-O2G-C1B
38	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
37	W	201	LMG	C40-C41-C42-C43
31	B	601	CLA	C11-C10-C8-C7
31	B	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	b	617	CLA	C6-C7-C8-C10
31	9	308	CLA	C6-C7-C8-C10
36	8	316	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
37	B	620	LMG	O8-C28-C29-C30
37	w	201	LMG	C38-C39-C40-C41
37	4	316	LMG	C38-C39-C40-C41
37	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	308	CLA	C8-C10-C11-C12
31	2	311	CLA	CAA-CBA-CGA-O2A
38	C	518	DGD	C4D-C5D-C6D-O5D
38	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	308	CLA	C10-C11-C12-C13
34	A	411	SQD	C7-C8-C9-C10
31	W	202	CLA	C2B-C3B-CAB-CBB
31	w	203	CLA	C2B-C3B-CAB-CBB
31	2	314	CLA	C2B-C3B-CAB-CBB
31	8	307	CLA	C2B-C3B-CAB-CBB
31	9	313	CLA	C2B-C3B-CAB-CBB
31	12	308	CLA	C2B-C3B-CAB-CBB
34	l	101	SQD	C27-C28-C29-C30
37	4	316	LMG	C39-C40-C41-C42
37	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

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Mol	Chain	Res	Type	Atoms
43	5	318	A86	C13-C14-C15-C16
43	8	305	A86	C13-C14-C15-C16
43	13	306	A86	C13-C14-C15-C16
43	14	303	A86	C13-C14-C15-C16
43	16	301	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	8	301	SQD	C13-C14-C15-C16
38	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
37	11	317	LMG	C16-C17-C18-C19
31	d	402	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	303	A86	C10-C11-C13-C14
43	8	305	A86	C10-C11-C13-C14
43	8	306	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

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Mol	Chain	Res	Type	Atoms
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
43	16	305	A86	C10-C11-C13-C14
43	16	306	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	402	CLA	O1D-CGD-O2D-CED
31	0	311	CLA	C4-C3-C5-C6
35	D	407	PL9	C15-C14-C16-C17
35	d	407	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
38	c	520	DGD	O6D-C5D-C6D-O5D
37	f	102	LMG	C35-C36-C37-C38
43	7	302	A86	C35-C34-O4-C38
31	16	308	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
38	W	203	DGD	C2B-C1B-O2G-C2G
38	w	204	DGD	C2B-C1B-O2G-C2G
42	14	313	KC1	C1A-C2A-CAA-CBA
45	9	309	KC2	C1A-C2A-CAA-CBA
37	C	522	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
37	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
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
38	C	520	DGD	O6D-C5D-C6D-O5D
37	D	409	LMG	C8-C7-O1-C1
37	d	409	LMG	C8-C7-O1-C1
37	m	101	LMG	C8-C7-O1-C1
37	C	522	LMG	C15-C16-C17-C18
37	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
37	1	317	LMG	O8-C28-C29-C30
34	l	101	SQD	C26-C27-C28-C29
37	D	404	LMG	C35-C36-C37-C38
31	r	101	CLA	C2-C1-O2A-CGA
38	W	203	DGD	CBB-CCB-CDB-CEB
38	w	204	DGD	CBB-CCB-CDB-CEB
31	c	512	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	0	316	CLA	C4B-C3B-CAB-CBB
31	1	310	CLA	C4B-C3B-CAB-CBB
31	19	315	CLA	C4B-C3B-CAB-CBB
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
36	8	316	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	407	PL9	C13-C14-C16-C17
35	d	407	PL9	C13-C14-C16-C17
31	R	101	CLA	C2-C1-O2A-CGA
34	L	102	SQD	O47-C7-C8-C9
37	1	301	LMG	O8-C28-C29-C30
37	11	301	LMG	O8-C28-C29-C30
36	Z	103	LHG	C5-C4-O6-P
38	H	102	DGD	O1G-C1G-C2G-O2G
38	h	102	DGD	O1G-C1G-C2G-O2G
37	10	319	LMG	C4-C5-C6-O5
38	11	318	DGD	C8B-C9B-CAB-CBB
37	j	101	LMG	O8-C28-C29-C30
31	15	312	CLA	C2-C1-O2A-CGA
31	B	615	CLA	C13-C15-C16-C17
38	1	318	DGD	C8B-C9B-CAB-CBB
31	3	316	CLA	C16-C17-C18-C20
37	W	201	LMG	C16-C17-C18-C19
38	C	519	DGD	CCB-CDB-CEB-CFB
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
38	c	519	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
31	b	603	CLA	CAA-CBA-CGA-O2A
37	J	101	LMG	O8-C28-C29-C30
38	B	621	DGD	C2G-C1G-O1G-C1A
37	w	201	LMG	C16-C17-C18-C19
35	D	407	PL9	C40-C39-C41-C42
35	d	407	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	312	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	306	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	405	CLA	C4C-C3C-CAC-CBC
31	d	405	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	406	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

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Mol	Chain	Res	Type	Atoms
31	c	511	CLA	CAD-CBD-CGD-O2D
31	d	406	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
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	312	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	317	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	405	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	405	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
37	c	521	LMG	C33-C34-C35-C36
35	D	407	PL9	C45-C44-C46-C47
35	d	407	PL9	C45-C44-C46-C47
31	D	405	CLA	C16-C17-C18-C20
31	d	405	CLA	C16-C17-C18-C20
31	7	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	2	315	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A
31	16	312	CLA	CAA-CBA-CGA-O2A
36	8	316	LHG	O8-C23-C24-C25
37	1	301	LMG	O7-C10-C11-C12
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
36	4	317	LHG	C4-C5-C6-O8
38	C	520	DGD	C1G-C2G-C3G-O3G
38	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	302	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	307	CLA	O1A-CGA-O2A-C1
37	11	301	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	C	509	CLA	C16-C17-C18-C20
31	c	509	CLA	C16-C17-C18-C20
33	C	515	BCR	C18-C19-C20-C21
33	c	515	BCR	C18-C19-C20-C21
36	18	316	LHG	O10-C23-O8-C6
38	H	102	DGD	O1B-C1B-C2B-C3B
38	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
38	C	520	DGD	C8A-C9A-CAA-CBA
31	C	502	CLA	CAA-CBA-CGA-O2A
38	C	518	DGD	O2G-C1B-C2B-C3B
38	c	518	DGD	O2G-C1B-C2B-C3B
31	19	310	CLA	C3-C5-C6-C7
38	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

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Mol	Chain	Res	Type	Atoms
31	b	616	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	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
38	C	519	DGD	C8B-C9B-CAB-CBB
38	c	519	DGD	C8B-C9B-CAB-CBB
34	l	101	SQD	C34-C35-C36-C37
37	11	301	LMG	C33-C34-C35-C36
37	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
37	1	301	LMG	C33-C34-C35-C36
34	A	408	SQD	O6-C44-C45-O47
34	a	408	SQD	O6-C44-C45-O47
37	14	316	LMG	O1-C7-C8-O7
38	C	520	DGD	O2G-C2G-C3G-O3G
38	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	316	LHG	C24-C25-C26-C27
36	8	316	LHG	C25-C26-C27-C28
37	W	201	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
37	w	201	LMG	C34-C35-C36-C37
37	5	316	LMG	O9-C10-O7-C8
31	b	609	CLA	CAA-CBA-CGA-O2A
31	12	316	CLA	CAA-CBA-CGA-O2A
36	B	622	LHG	O8-C23-C24-C25
37	D	404	LMG	O8-C28-C29-C30
38	1	318	DGD	O1G-C1A-C2A-C3A
38	C	518	DGD	C5B-C6B-C7B-C8B
38	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
37	D	404	LMG	C15-C16-C17-C18
37	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	308	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

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C12-C13-C15-C16
31	b	602	CLA	C12-C13-C15-C16
31	9	308	CLA	C11-C10-C8-C7
31	8	313	CLA	C6-C7-C8-C10
37	B	620	LMG	O9-C10-O7-C8
37	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	312	CLA	CAA-CBA-CGA-O1A
31	C	510	CLA	C2B-C3B-CAB-CBB
31	c	510	CLA	C2B-C3B-CAB-CBB
31	1	310	CLA	C2B-C3B-CAB-CBB
31	15	309	CLA	C2B-C3B-CAB-CBB
43	6	307	A86	C33-C34-O4-C38
43	8	304	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	8	301	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
38	C	520	DGD	C2B-C1B-O2G-C2G
38	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
38	C	518	DGD	O1B-C1B-C2B-C3B
38	c	518	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
31	3	313	CLA	C16-C17-C18-C19
31	b	608	CLA	C4-C3-C5-C6
38	11	318	DGD	O2G-C1B-C2B-C3B
31	P	606	CLA	C2C-C3C-CAC-CBC
41	e	101	HEM	CAA-CBA-CGA-O1A
37	4	316	LMG	O10-C28-C29-C30
31	8	313	CLA	CBA-CGA-O2A-C1
31	D	406	CLA	C8-C10-C11-C12
31	d	406	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	406	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	406	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	308	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
38	C	518	DGD	C4E-C5E-C6E-O5E
38	11	318	DGD	C4D-C5D-C6D-O5D
42	13	314	KC1	CAA-CBA-CGA-O1A
37	B	620	LMG	C32-C33-C34-C35
37	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	8	301	SQD	O10-C23-C24-C25
36	C	521	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
36	w	202	LHG	O10-C23-C24-C25
37	m	101	LMG	C30-C31-C32-C33
41	V	201	HEM	CAA-CBA-CGA-O1A
41	v	201	HEM	CAA-CBA-CGA-O1A
38	C	520	DGD	O1G-C1G-C2G-C3G
38	c	520	DGD	O1G-C1G-C2G-C3G
31	P	602	CLA	C8-C10-C11-C12
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	402	CLA	CBD-CGD-O2D-CED
31	d	402	CLA	CBD-CGD-O2D-CED
31	9	311	CLA	CBD-CGD-O2D-CED
38	H	102	DGD	CDB-CEB-CFB-CGB
38	h	102	DGD	CDB-CEB-CFB-CGB
31	C	508	CLA	C16-C17-C18-C20
31	c	508	CLA	C16-C17-C18-C20
37	c	522	LMG	O9-C10-C11-C12
31	C	506	CLA	C13-C15-C16-C17
31	c	506	CLA	C13-C15-C16-C17
38	c	518	DGD	C4E-C5E-C6E-O5E
37	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	316	LHG	O10-C23-C24-C25
36	18	315	LHG	O10-C23-C24-C25
37	5	316	LMG	O10-C28-C29-C30
38	1	318	DGD	O1B-C1B-C2B-C3B
34	b	601	SQD	C17-C18-C19-C20
31	2	315	CLA	C4B-C3B-CAB-CBB
31	10	317	CLA	C4B-C3B-CAB-CBB
31	12	315	CLA	C4B-C3B-CAB-CBB
31	13	308	CLA	C4B-C3B-CAB-CBB
36	B	622	LHG	C3-O3-P-O5
36	b	623	LHG	C3-O3-P-O5
36	15	316	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
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
37	p	614	LMG	C8-C9-O8-C28
38	B	621	DGD	O1B-C1B-C2B-C3B
38	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
38	C	519	DGD	CDB-CEB-CFB-CGB
38	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
37	Z	102	LMG	O9-C10-C11-C12
31	p	604	CLA	CAA-CBA-CGA-O2A
31	8	312	CLA	C2A-CAA-CBA-CGA
31	11	308	CLA	C2A-CAA-CBA-CGA
31	8	313	CLA	O1A-CGA-O2A-C1
38	c	519	DGD	CDB-CEB-CFB-CGB
31	15	307	CLA	C13-C15-C16-C17
38	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	307	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

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Mol	Chain	Res	Type	Atoms
34	i	101	SQD	O5-C5-C6-S
36	14	317	LHG	C6-C5-O7-C7
37	D	404	LMG	C7-C8-O7-C10
42	8	314	KC1	CAD-CBD-CGD-O1D
43	17	305	A86	C26-C27-C29-C30
31	16	312	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
38	11	318	DGD	C5B-C6B-C7B-C8B
31	B	613	CLA	CAA-CBA-CGA-O2A
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
38	c	519	DGD	C4B-C5B-C6B-C7B
38	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
37	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
38	B	621	DGD	O1A-C1A-C2A-C3A
31	b	609	CLA	C13-C15-C16-C17
31	0	316	CLA	C2A-CAA-CBA-CGA
38	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	310	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

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Mol	Chain	Res	Type	Atoms
31	19	310	CLA	CAA-CBA-CGA-O2A
36	w	202	LHG	O8-C23-C24-C25
37	N	101	LMG	O8-C28-C29-C30
37	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
37	W	201	LMG	C10-C11-C12-C13
37	w	201	LMG	C10-C11-C12-C13
31	D	405	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
31	3	313	CLA	C3-C5-C6-C7
37	J	101	LMG	O10-C28-C29-C30
37	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
37	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
37	j	101	LMG	O10-C28-C29-C30
37	14	316	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	k	101	LMG	C37-C38-C39-C40
37	p	614	LMG	C12-C13-C14-C15
43	6	303	A86	C35-C34-O4-C38
43	8	306	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
31	11	310	CLA	CAA-CBA-CGA-O2A
31	15	312	CLA	CAA-CBA-CGA-O2A
31	19	308	CLA	CAA-CBA-CGA-O2A
37	c	521	LMG	O8-C28-C29-C30
37	5	315	LMG	O7-C10-C11-C12
38	11	318	DGD	O1G-C1A-C2A-C3A
37	K	101	LMG	C37-C38-C39-C40
38	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	8	301	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

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Mol	Chain	Res	Type	Atoms
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
37	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
34	b	601	SQD	O49-C7-C8-C9
34	10	320	SQD	O10-C23-C24-C25
38	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

332 monomers are involved in 729 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	18	302	A86	1	0
31	p	602	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	318	DGD	2	0
37	W	201	LMG	3	0
31	A	403	CLA	6	0
31	B	610	CLA	3	0
31	8	308	CLA	4	0
36	a	410	LHG	1	0
31	6	308	CLA	5	0
31	D	406	CLA	3	0
31	11	310	CLA	2	0
31	1	316	CLA	1	0
33	h	101	BCR	4	0
37	10	319	LMG	2	0
31	c	504	CLA	7	0
33	C	516	BCR	2	0
31	C	508	CLA	1	0
37	b	621	LMG	2	0
37	f	102	LMG	5	0
43	13	306	A86	1	0
31	D	405	CLA	7	0
31	9	312	CLA	1	0
45	15	308	KC2	1	0
31	14	311	CLA	1	0
38	H	102	DGD	4	0
31	B	608	CLA	1	0
33	y	101	BCR	5	0
43	15	301	A86	1	0
45	17	309	KC2	1	0
43	1	306	A86	1	0
37	w	201	LMG	4	0
31	10	317	CLA	3	0
31	15	306	CLA	5	0
31	15	312	CLA	4	0
31	z	103	CLA	1	0
31	19	310	CLA	1	0
37	M	101	LMG	6	0
33	b	619	BCR	2	0
45	2	308	KC2	1	0
45	6	310	KC2	1	0
36	D	408	LHG	5	0
36	18	316	LHG	3	0
41	e	101	HEM	2	0
43	5	301	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	603	CLA	6	0
31	3	307	CLA	3	0
31	B	603	CLA	3	0
31	0	314	CLA	1	0
31	12	308	CLA	1	0
31	6	314	CLA	2	0
31	9	310	CLA	2	0
41	E	101	HEM	2	0
31	R	101	CLA	1	0
33	C	515	BCR	1	0
31	5	307	CLA	2	0
31	11	315	CLA	2	0
37	14	316	LMG	5	0
31	10	308	CLA	2	0
34	10	320	SQD	1	0
43	0	301	A86	1	0
34	i	101	SQD	2	0
33	B	618	BCR	3	0
31	13	307	CLA	1	0
43	16	303	A86	1	0
31	B	616	CLA	2	0
31	B	604	CLA	3	0
31	c	503	CLA	6	0
31	b	609	CLA	2	0
33	c	517	BCR	3	0
32	d	403	PHO	3	0
31	1	312	CLA	1	0
31	2	315	CLA	4	0
31	10	314	CLA	1	0
31	C	509	CLA	2	0
43	1	303	A86	1	0
31	a	406	CLA	1	0
37	d	409	LMG	2	0
31	b	617	CLA	3	0
31	14	309	CLA	1	0
31	13	312	CLA	2	0
33	b	618	BCR	2	0
36	14	317	LHG	2	0
33	A	407	BCR	3	0
31	B	602	CLA	7	0
31	p	604	CLA	1	0
31	16	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	k	101	LMG	4	0
31	6	309	CLA	2	0
31	5	311	CLA	2	0
43	5	304	A86	1	0
31	15	311	CLA	2	0
31	C	502	CLA	4	0
43	14	303	A86	1	0
31	1	310	CLA	2	0
40	d	401	BCT	1	0
31	7	307	CLA	4	0
31	17	308	CLA	2	0
36	L	101	LHG	5	0
31	2	312	CLA	3	0
31	w	203	CLA	3	0
31	12	310	CLA	3	0
43	18	305	A86	4	0
36	18	315	LHG	1	0
41	v	201	HEM	3	0
31	16	310	CLA	1	0
43	15	305	A86	1	0
43	9	305	A86	2	0
31	c	507	CLA	3	0
31	C	511	CLA	3	0
34	B	623	SQD	7	0
31	c	509	CLA	3	0
43	5	302	A86	1	0
43	14	301	A86	4	0
45	7	309	KC2	1	0
43	14	302	A86	1	0
31	12	312	CLA	1	0
31	11	313	CLA	4	0
33	B	617	BCR	5	0
31	B	611	CLA	3	0
31	11	307	CLA	2	0
31	13	316	CLA	3	0
31	b	607	CLA	4	0
37	c	521	LMG	2	0
31	10	313	CLA	2	0
31	B	607	CLA	4	0
43	p	613	A86	1	0
43	6	303	A86	1	0
31	B	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	5	315	LMG	2	0
35	D	407	PL9	4	0
38	c	519	DGD	3	0
31	z	101	CLA	2	0
31	b	612	CLA	3	0
37	K	101	LMG	6	0
31	17	313	CLA	2	0
31	a	403	CLA	6	0
31	C	505	CLA	4	0
31	8	312	CLA	4	0
38	h	102	DGD	4	0
35	d	407	PL9	5	0
31	5	312	CLA	3	0
31	W	202	CLA	3	0
31	7	308	CLA	2	0
37	C	522	LMG	3	0
31	16	315	CLA	1	0
31	2	306	CLA	5	0
37	4	316	LMG	5	0
37	5	316	LMG	3	0
44	p	612	DD6	3	0
37	D	409	LMG	1	0
31	18	306	CLA	3	0
31	8	310	CLA	1	0
31	9	307	CLA	1	0
45	19	309	KC2	1	0
31	1	315	CLA	1	0
31	b	602	CLA	2	0
31	13	313	CLA	2	0
32	D	403	PHO	2	0
31	c	510	CLA	3	0
31	b	606	CLA	2	0
31	7	313	CLA	4	0
31	3	313	CLA	5	0
31	B	615	CLA	5	0
37	P	614	LMG	1	0
33	Y	101	BCR	6	0
31	P	606	CLA	4	0
34	a	408	SQD	3	0
31	A	404	CLA	2	0
37	N	101	LMG	1	0
31	P	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	w	202	LHG	1	0
31	c	502	CLA	4	0
31	A	406	CLA	1	0
31	0	309	CLA	1	0
43	15	303	A86	1	0
33	f	101	BCR	3	0
31	D	402	CLA	4	0
31	3	308	CLA	2	0
31	6	316	CLA	1	0
31	1	313	CLA	8	0
31	4	309	CLA	1	0
31	5	314	CLA	1	0
37	d	404	LMG	2	0
37	B	620	LMG	3	0
33	B	619	BCR	2	0
36	B	622	LHG	1	0
31	b	610	CLA	1	0
43	17	303	A86	1	0
38	C	518	DGD	1	0
37	0	317	LMG	2	0
38	C	520	DGD	2	0
31	14	306	CLA	4	0
45	9	309	KC2	1	0
33	c	516	BCR	1	0
31	16	313	CLA	3	0
43	10	301	A86	1	0
31	B	614	CLA	4	0
45	18	308	KC2	1	0
37	m	101	LMG	3	0
45	5	308	KC2	1	0
31	C	512	CLA	2	0
31	11	312	CLA	2	0
37	p	614	LMG	2	0
31	5	306	CLA	3	0
31	C	504	CLA	7	0
34	b	601	SQD	9	0
43	4	304	A86	1	0
43	5	303	A86	1	0
43	11	302	A86	1	0
31	19	308	CLA	4	0
31	1	308	CLA	7	0
36	A	410	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	P	613	A86	1	0
37	j	101	LMG	4	0
31	0	313	CLA	1	0
31	B	612	CLA	2	0
31	C	503	CLA	6	0
31	18	311	CLA	3	0
40	D	401	BCT	1	0
43	17	302	A86	1	0
31	b	613	CLA	2	0
33	a	407	BCR	2	0
31	P	601	CLA	3	0
31	b	615	CLA	4	0
31	c	505	CLA	6	0
31	p	606	CLA	4	0
38	b	622	DGD	12	0
37	11	317	LMG	4	0
31	c	511	CLA	3	0
34	A	408	SQD	3	0
31	C	510	CLA	2	0
35	a	409	PL9	2	0
36	P	615	LHG	1	0
34	l	101	SQD	6	0
31	d	405	CLA	8	0
31	19	313	CLA	1	0
42	4	313	KC1	1	0
33	H	101	BCR	3	0
31	19	307	CLA	1	0
31	7	312	CLA	2	0
31	5	309	CLA	1	0
31	14	312	CLA	3	0
45	8	309	KC2	1	0
31	c	508	CLA	1	0
45	10	310	KC2	1	0
31	12	307	CLA	2	0
43	7	301	A86	1	0
31	B	606	CLA	5	0
31	b	608	CLA	5	0
42	8	314	KC1	1	0
31	18	312	CLA	1	0
33	b	620	BCR	3	0
36	l	102	LHG	5	0
31	c	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	310	CLA	1	0
37	1	301	LMG	2	0
33	F	101	BCR	2	0
31	a	404	CLA	2	0
35	A	409	PL9	1	0
31	15	307	CLA	4	0
36	p	615	LHG	1	0
36	4	317	LHG	3	0
31	C	506	CLA	1	0
37	F	102	LMG	4	0
33	c	515	BCR	1	0
31	14	314	CLA	1	0
44	P	612	DD6	1	0
31	17	307	CLA	3	0
38	c	518	DGD	1	0
31	b	611	CLA	2	0
37	11	301	LMG	1	0
38	c	520	DGD	2	0
31	B	601	CLA	1	0
31	4	312	CLA	5	0
43	18	303	A86	5	0
37	n	701	LMG	1	0
31	1	321	CLA	3	0
31	2	307	CLA	3	0
32	a	405	PHO	4	0
31	11	316	CLA	1	0
31	b	604	CLA	3	0
43	4	303	A86	2	0
31	p	601	CLA	1	0
31	13	310	CLA	2	0
43	5	305	A86	1	0
31	0	311	CLA	1	0
31	2	309	CLA	2	0
36	C	521	LHG	1	0
38	11	318	DGD	2	0
31	11	308	CLA	2	0
43	15	304	A86	1	0
43	19	305	A86	2	0
34	L	102	SQD	4	0
31	18	309	CLA	3	0
31	d	402	CLA	5	0
45	4	308	KC2	1	0

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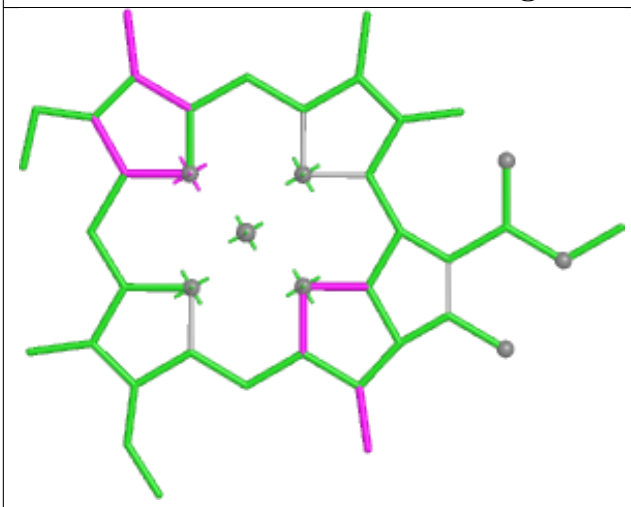
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	16	309	KC2	1	0
31	d	406	CLA	1	0
31	12	313	CLA	1	0
45	3	309	KC2	1	0
31	C	507	CLA	3	0
31	8	307	CLA	2	0
31	6	313	CLA	1	0
31	16	307	CLA	2	0
41	V	201	HEM	4	0
31	3	316	CLA	2	0
31	6	311	CLA	1	0
31	4	314	CLA	1	0
31	0	308	CLA	3	0
31	b	605	CLA	4	0
31	P	602	CLA	2	0
37	1	317	LMG	2	0
34	A	411	SQD	2	0
36	8	316	LHG	1	0
31	19	312	CLA	2	0
31	1	307	CLA	1	0
38	B	621	DGD	6	0
32	A	405	PHO	4	0
31	c	506	CLA	2	0
43	13	301	A86	1	0
31	Z	101	CLA	1	0
38	C	519	DGD	5	0
31	9	308	CLA	3	0
36	d	408	LHG	5	0
34	8	301	SQD	2	0
31	18	307	CLA	2	0
37	J	101	LMG	6	0
36	8	317	LHG	1	0
31	b	616	CLA	5	0
37	15	315	LMG	4	0
31	B	605	CLA	1	0
31	4	311	CLA	1	0

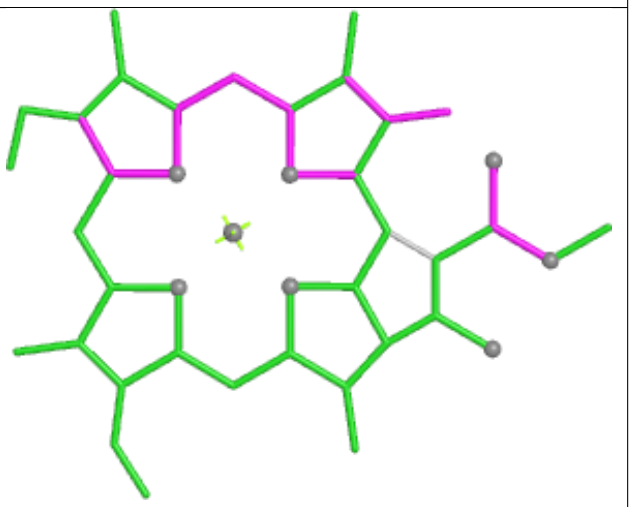
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

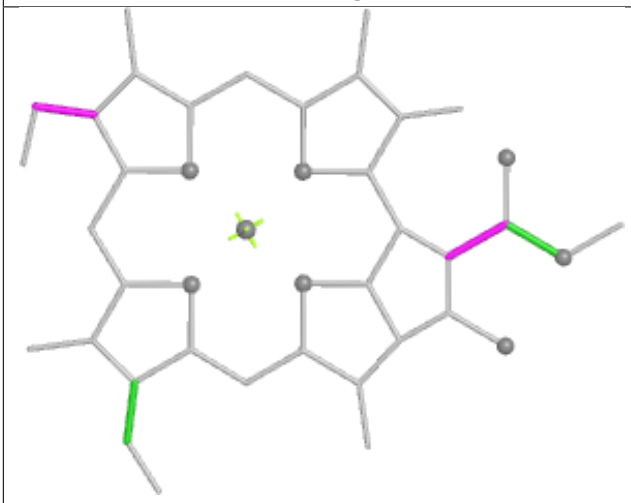
Ligand CLA 12 315



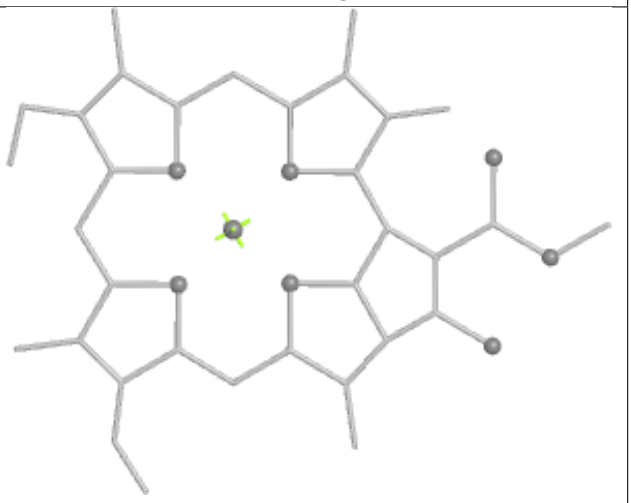
Bond lengths



Bond angles

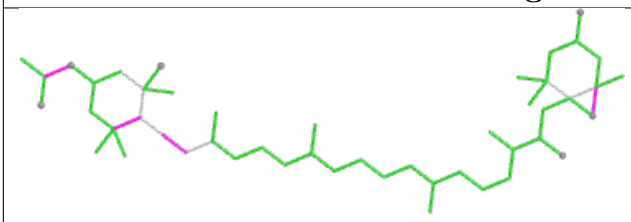


Torsions

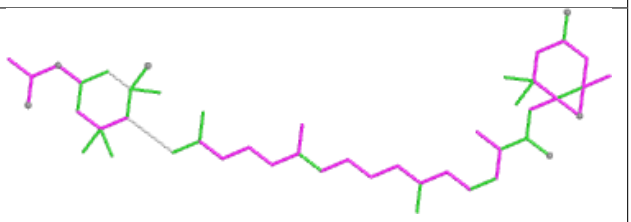


Rings

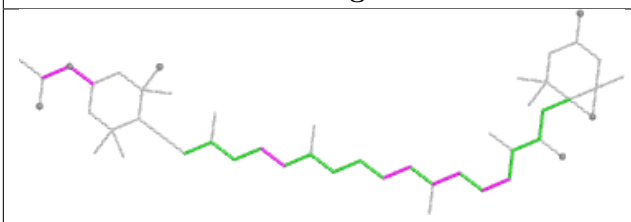
Ligand A86 18 302



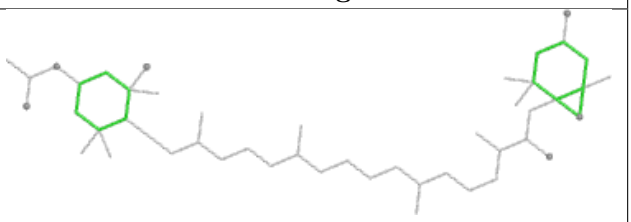
Bond lengths



Bond angles

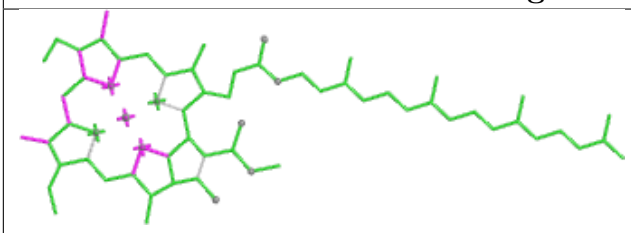


Torsions

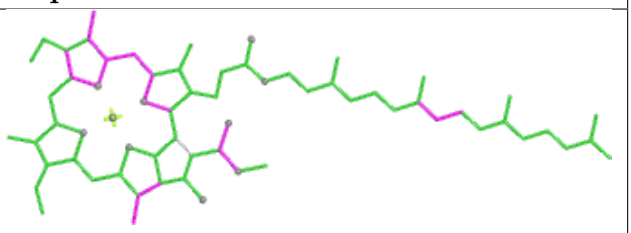


Rings

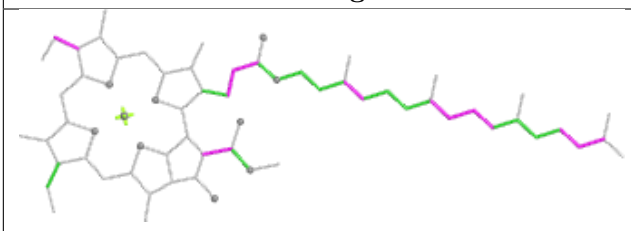
Ligand CLA p 602



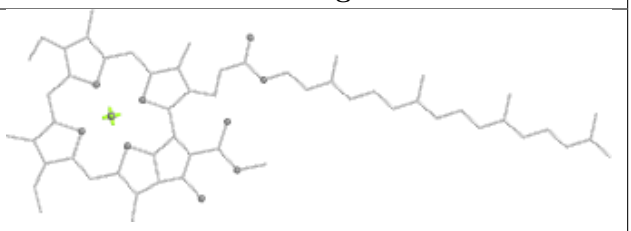
Bond lengths



Bond angles

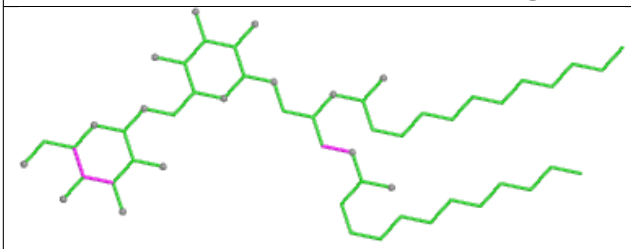


Torsions

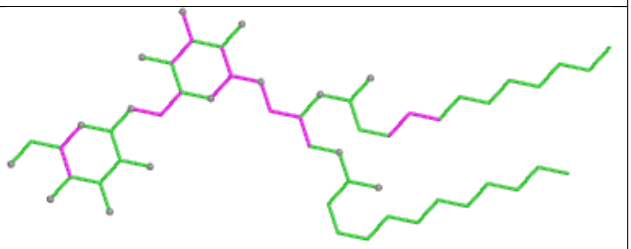


Rings

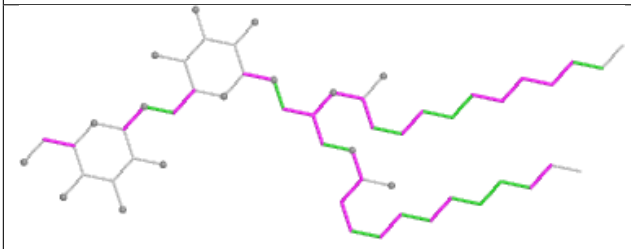
Ligand DGD 1 318



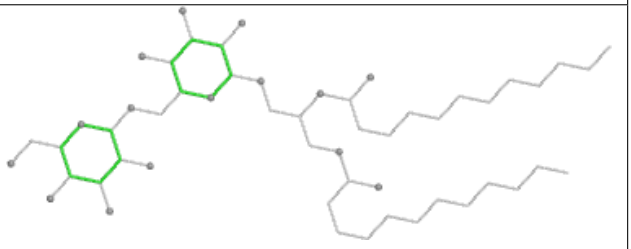
Bond lengths



Bond angles

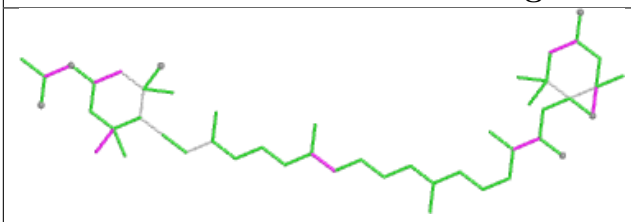


Torsions



Rings

Ligand A86 17 316



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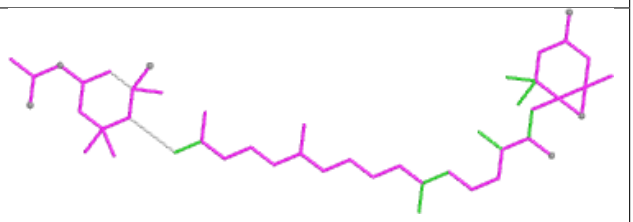

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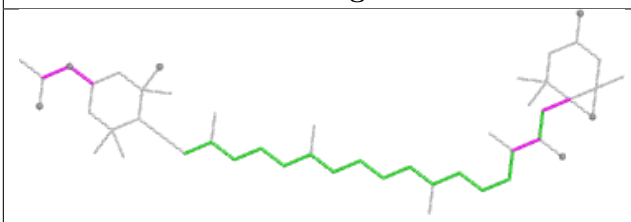

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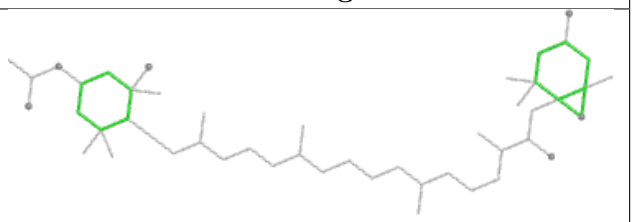
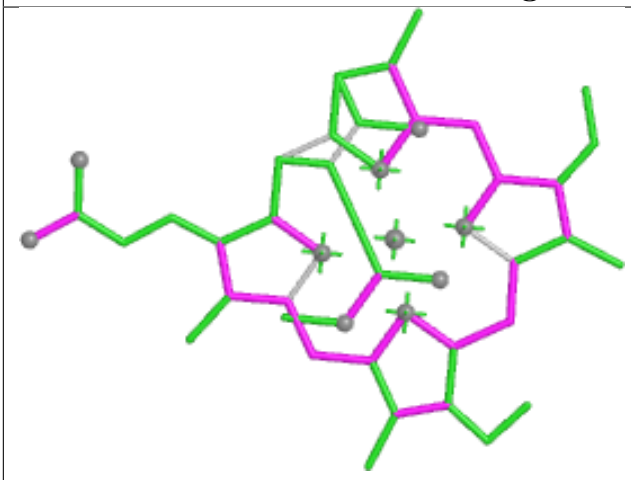


Rings

Ligand KC1 14 313



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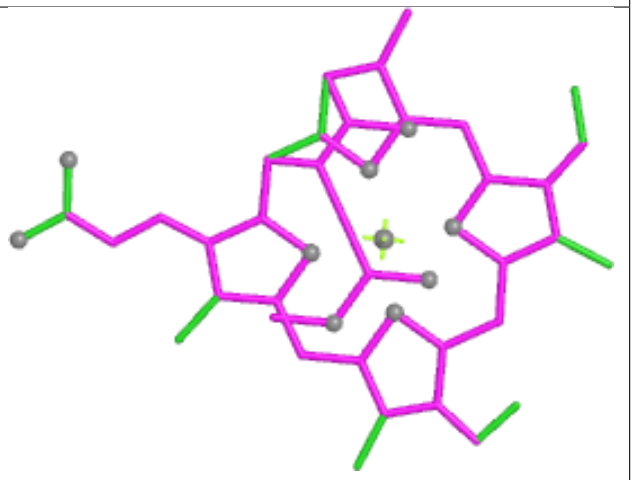

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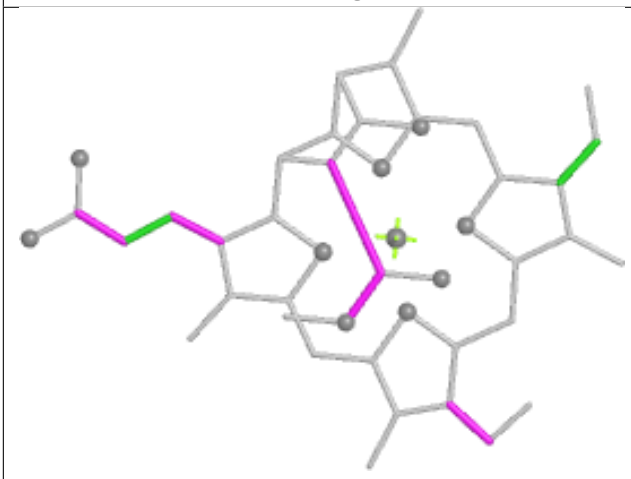

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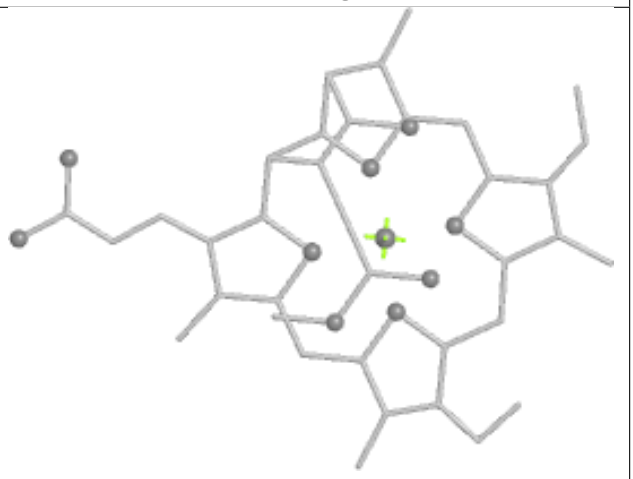
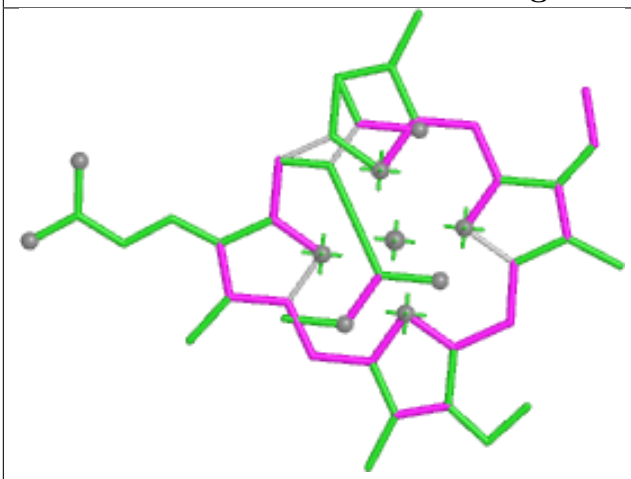


Rings

Ligand KC2 0 310



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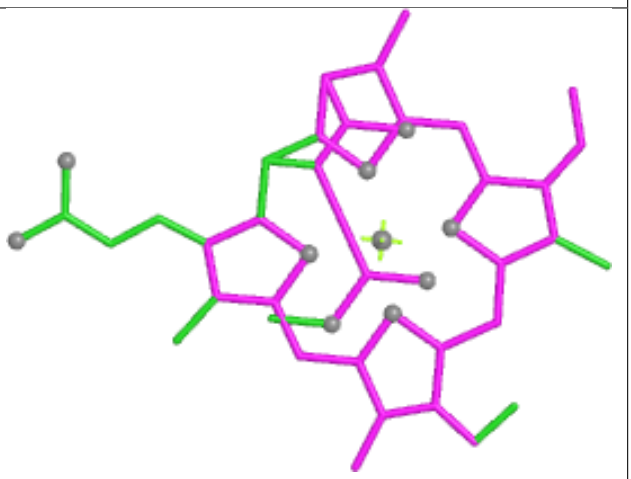

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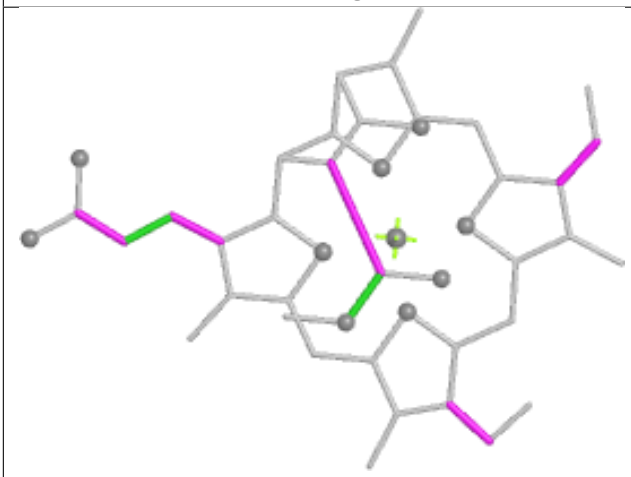

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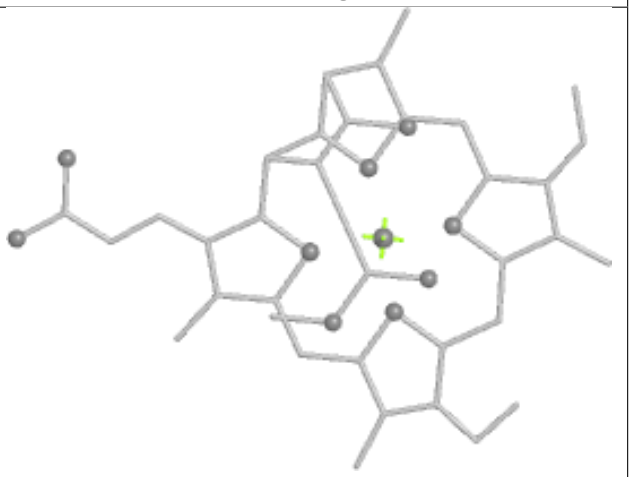
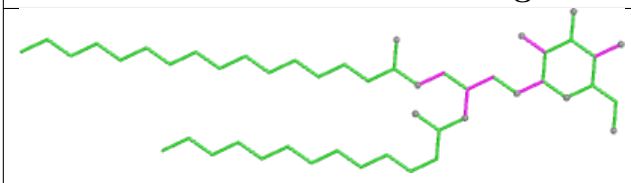


Rings

Ligand LMG W 201



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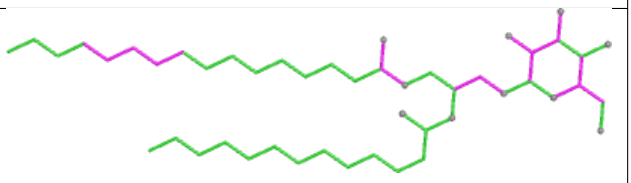

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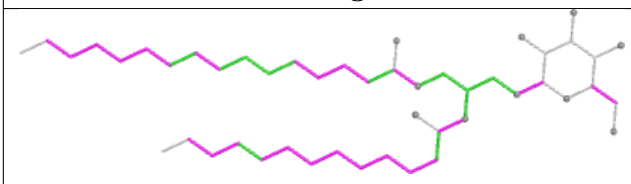

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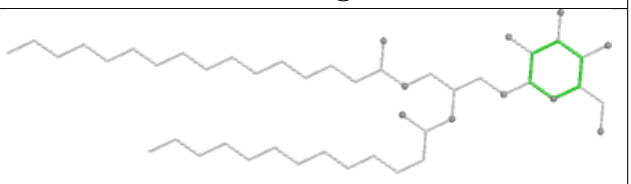
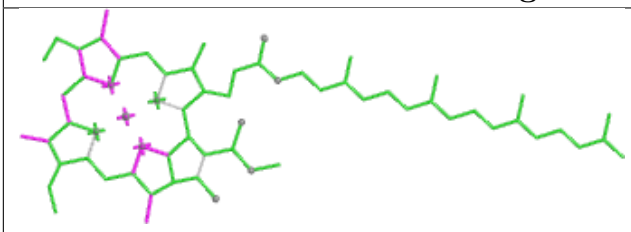


Rings

Ligand CLA 14 307



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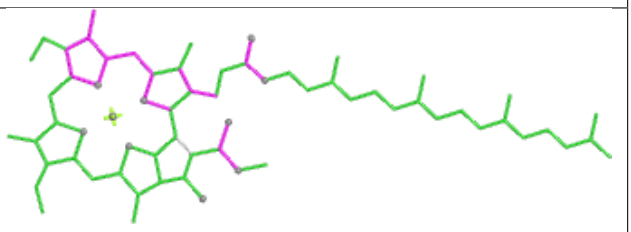

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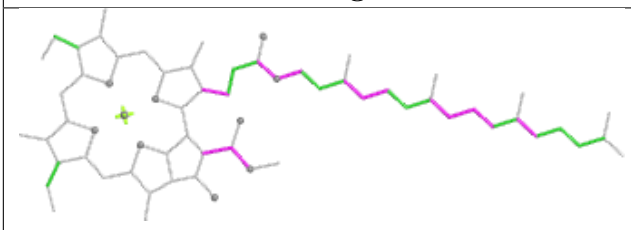

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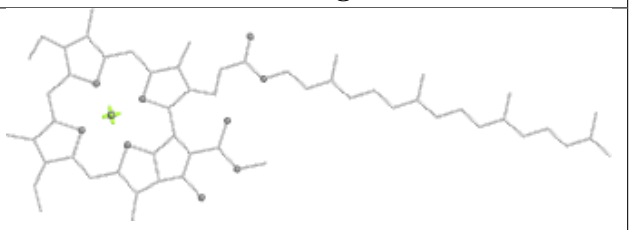
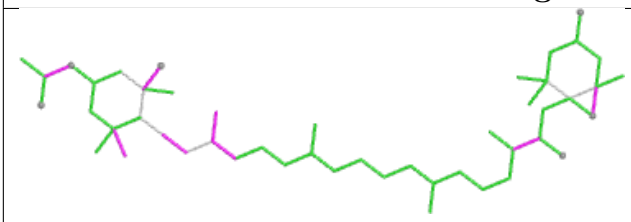


Rings

Ligand A86 0 306



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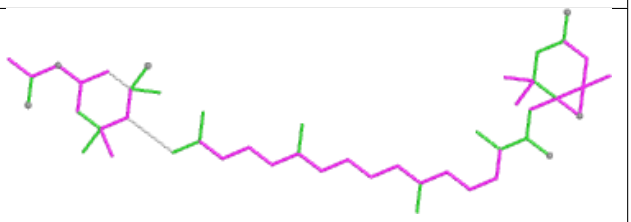

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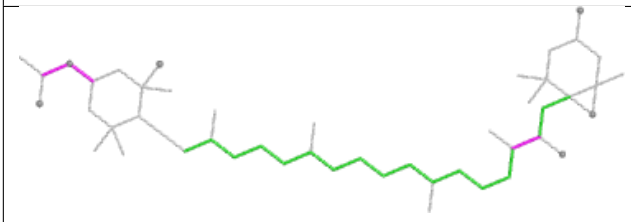

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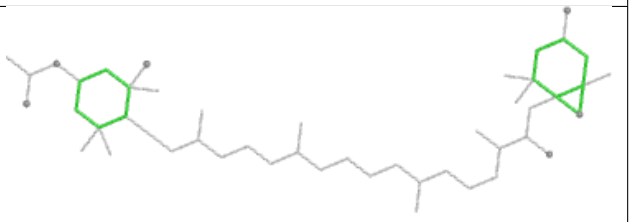
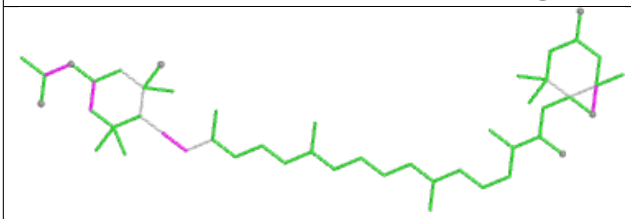


Rings

Ligand A86 6 306



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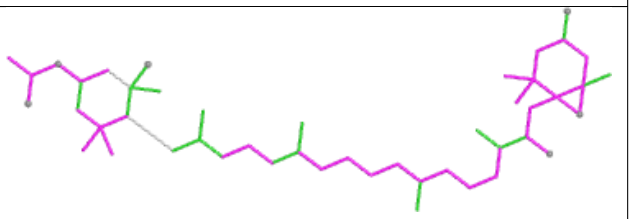

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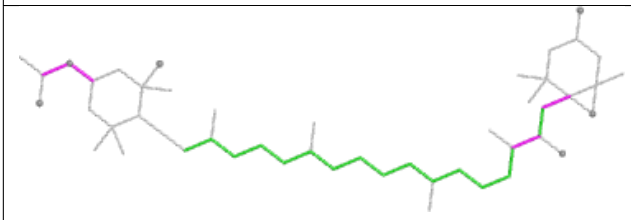

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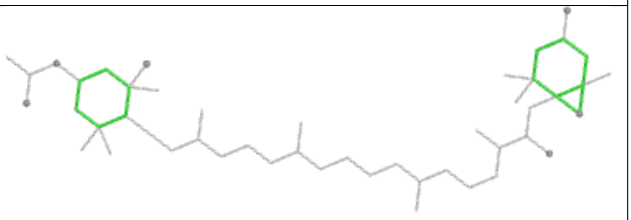
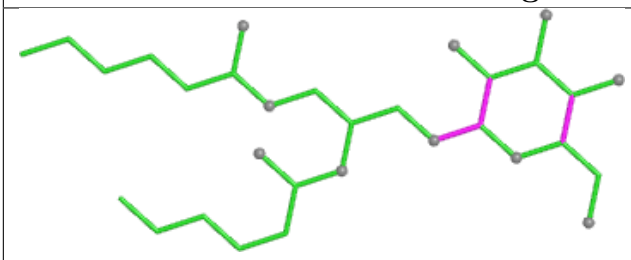


Rings

Ligand LMG Z 102



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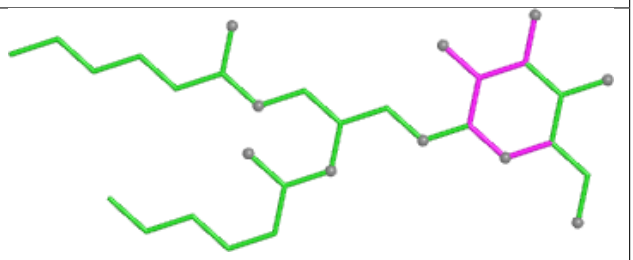

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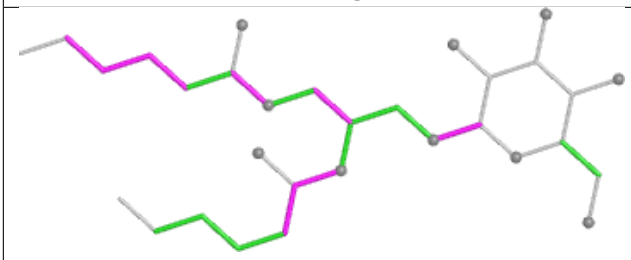

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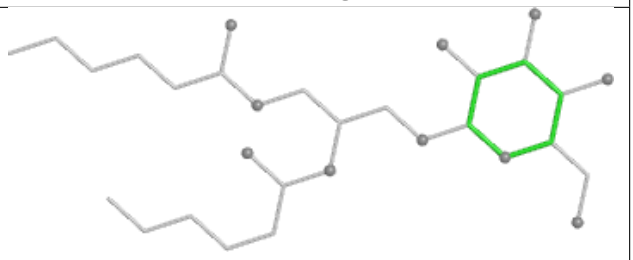
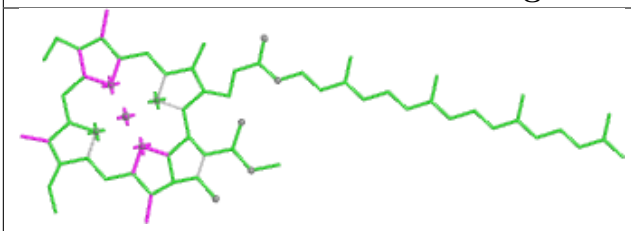


Rings

Ligand CLA A 403



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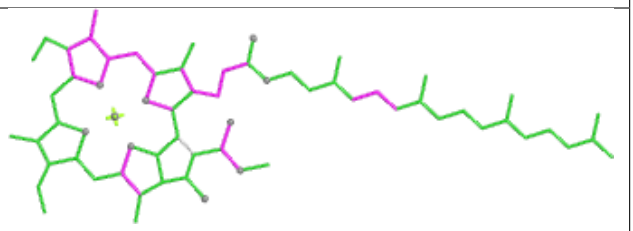
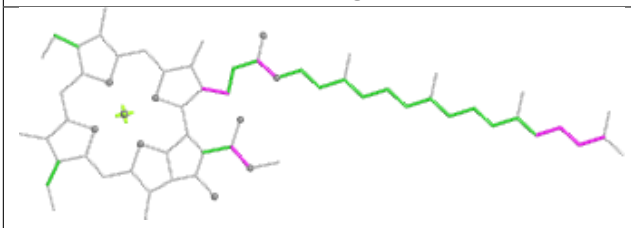


Bond angles



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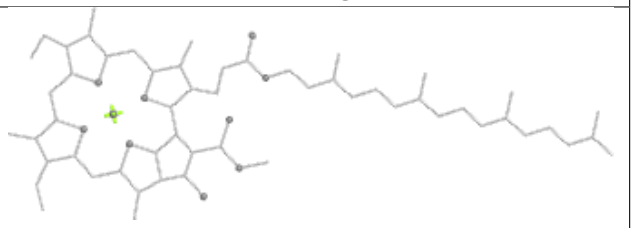
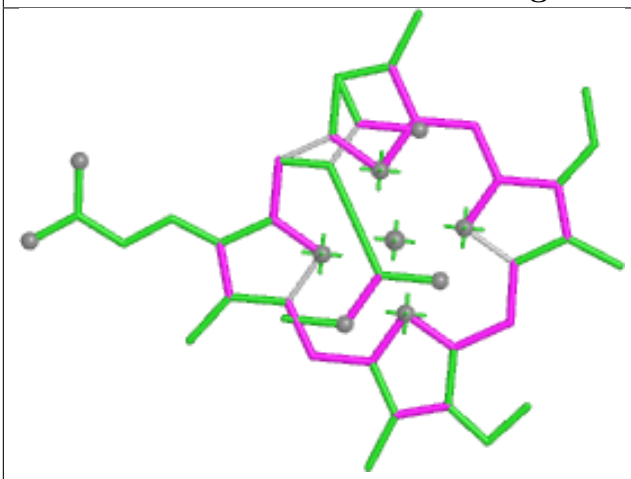


Rings

Ligand KC1 0 315



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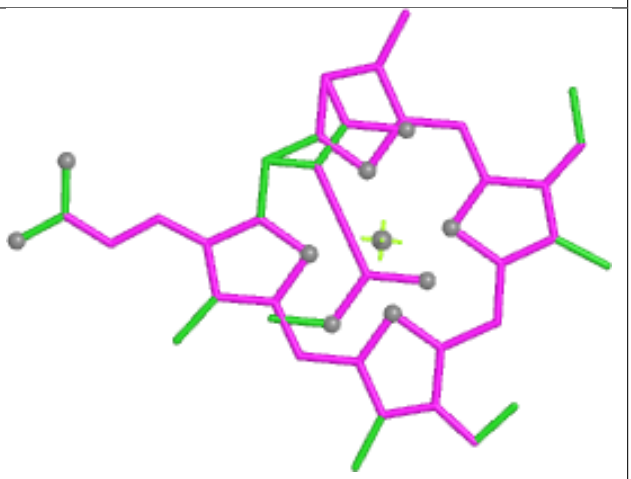
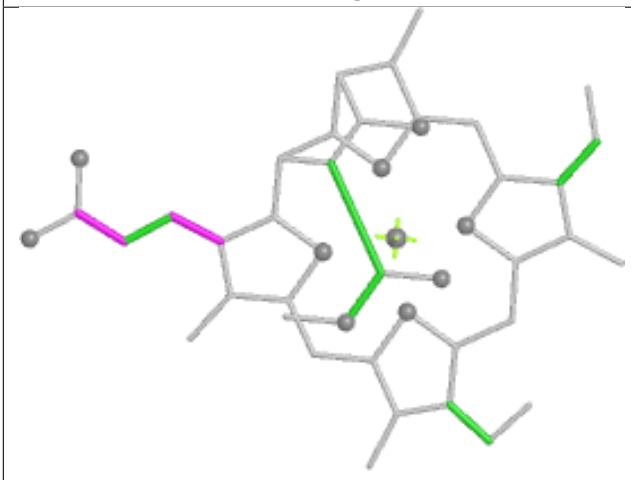


Bond angles



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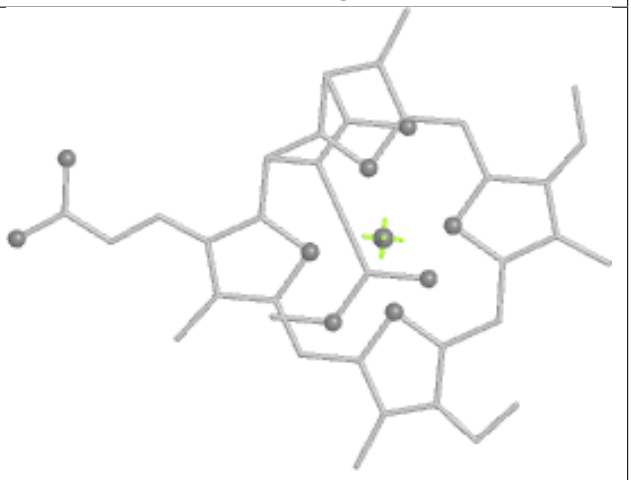
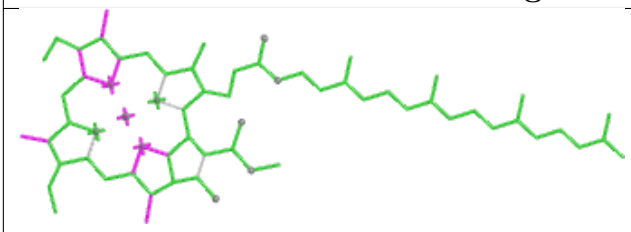


Rings

Ligand CLA B 610



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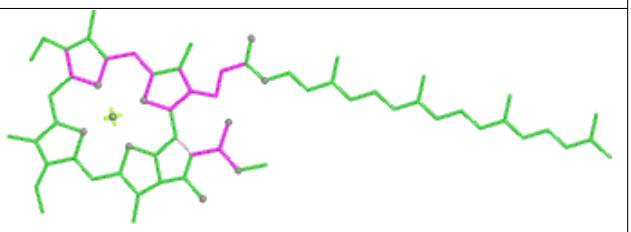
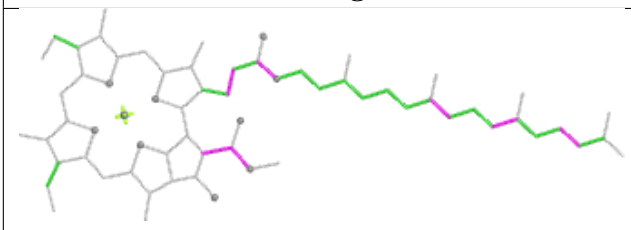


Bond angles



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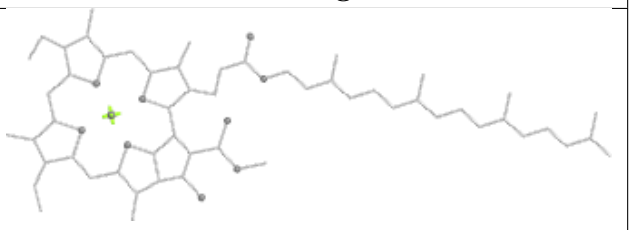
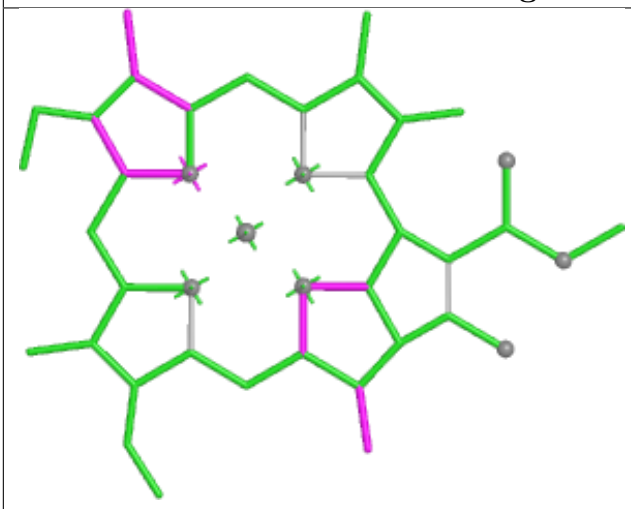


Rings

Ligand CLA 17 315



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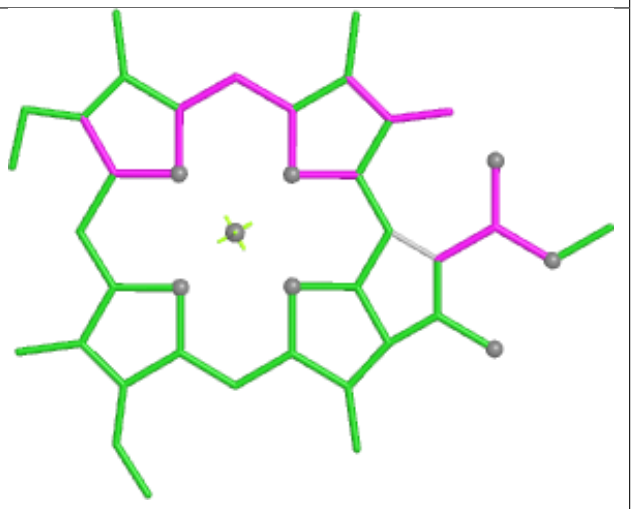
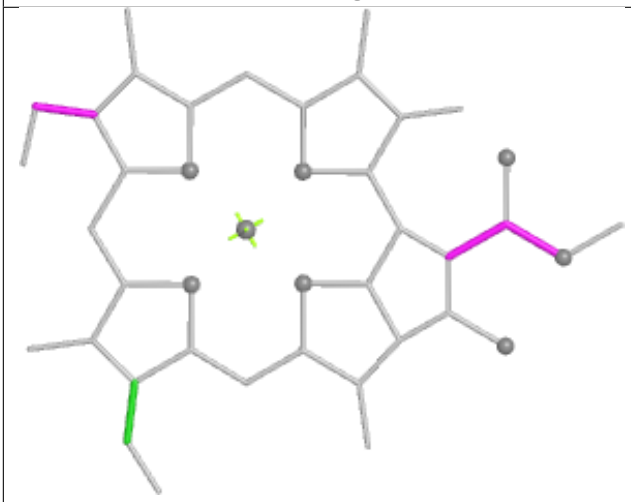


Bond angles



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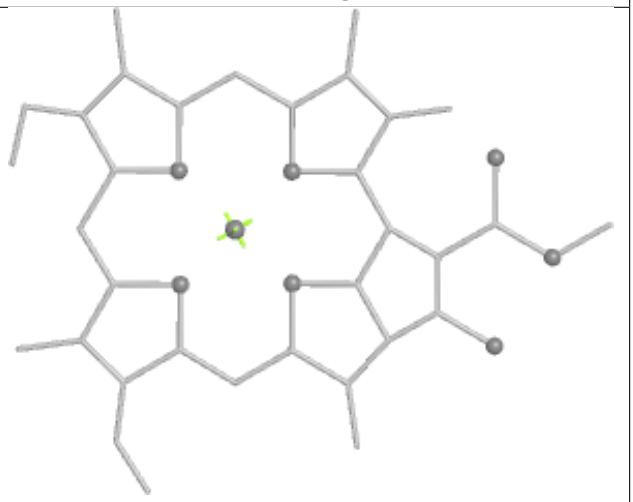
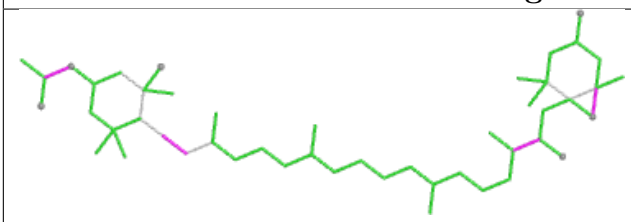


Rings

Ligand A86 12 305



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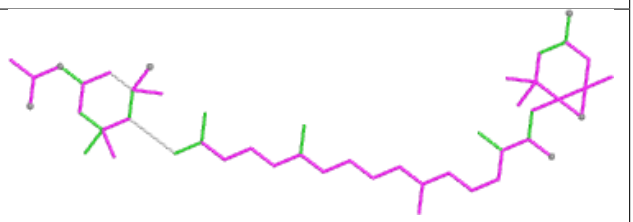
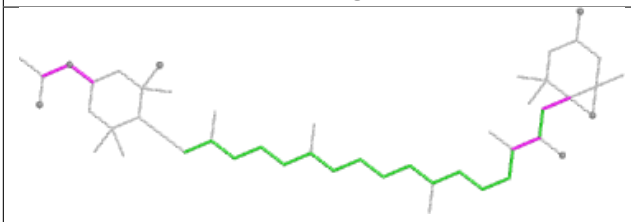


Bond angles



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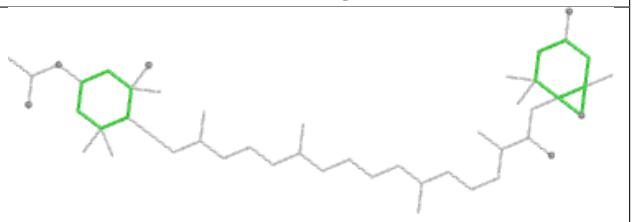
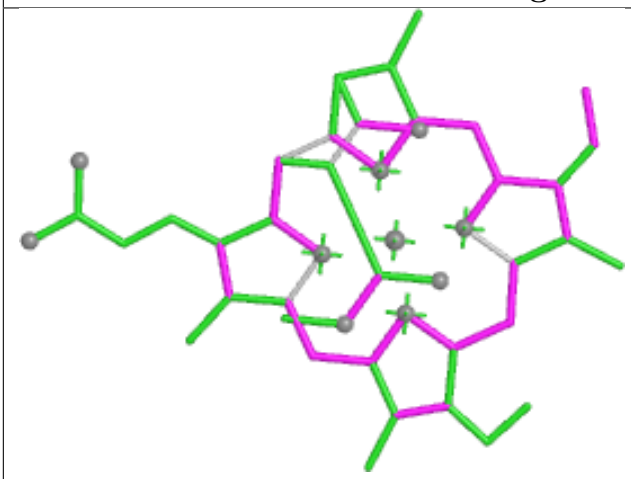


Rings

Ligand KC2 8 311



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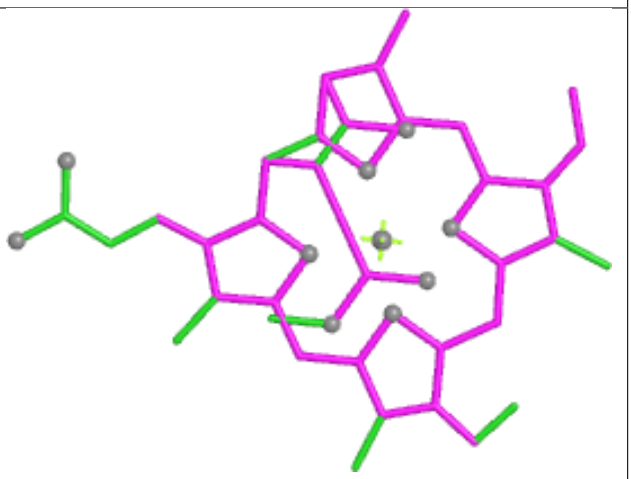
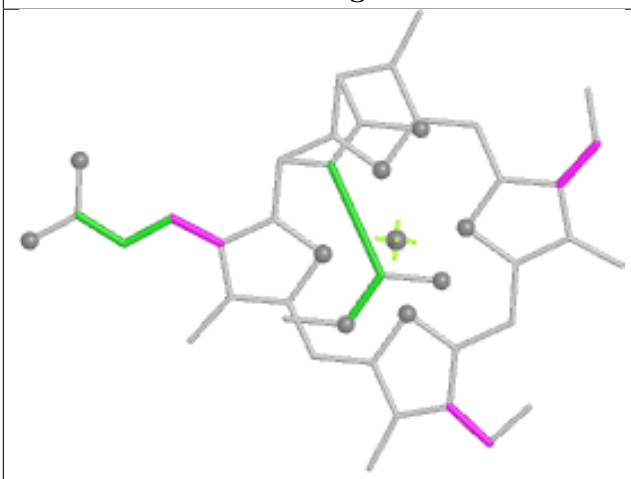


Bond angles



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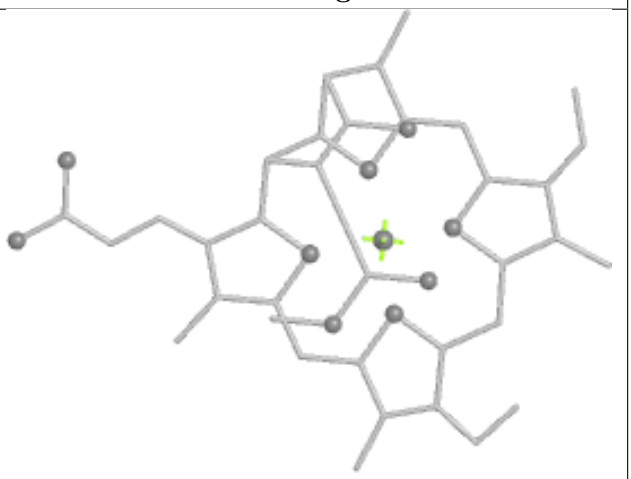
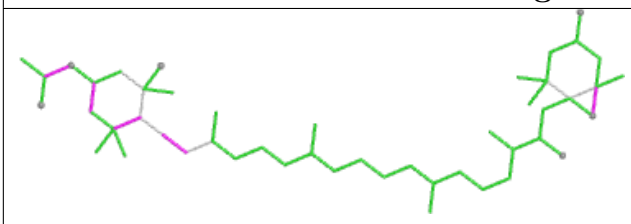
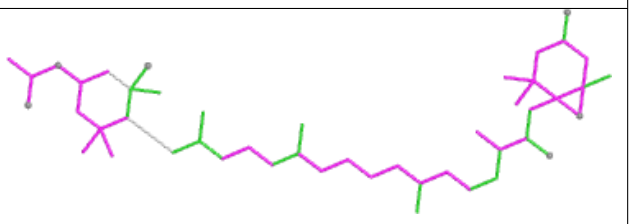


Rings

Ligand A86 7 305



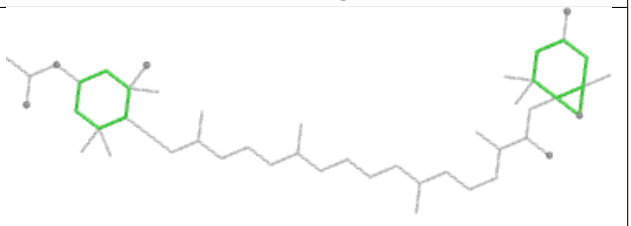
Bond lengths



Bond angles

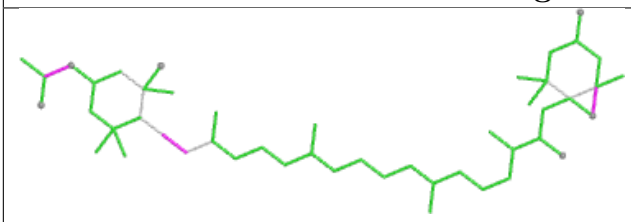


Torsions



Rings

Ligand A86 3 306



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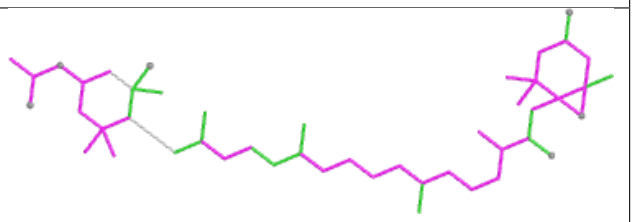

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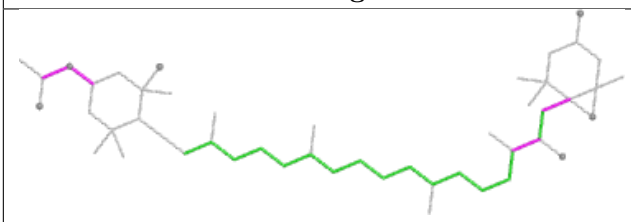

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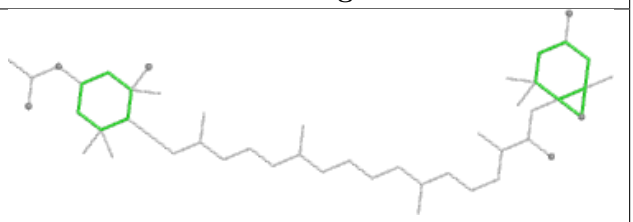

Rings

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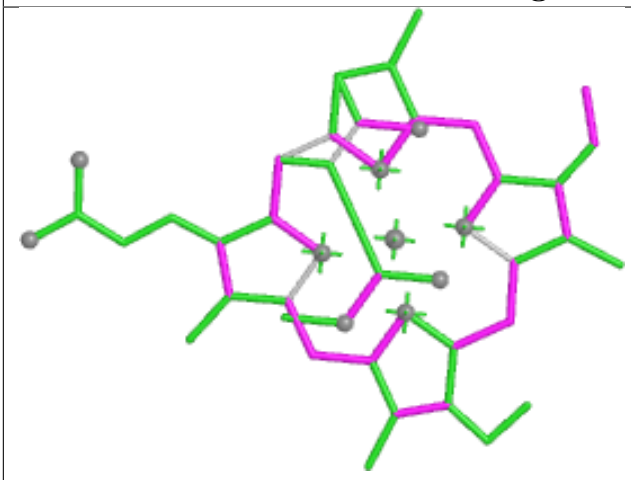

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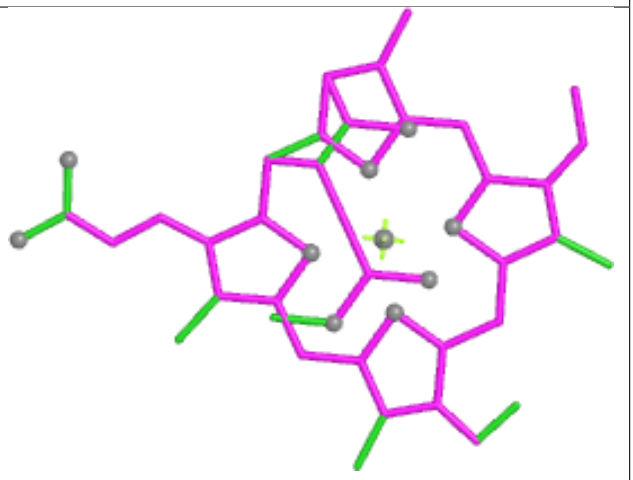

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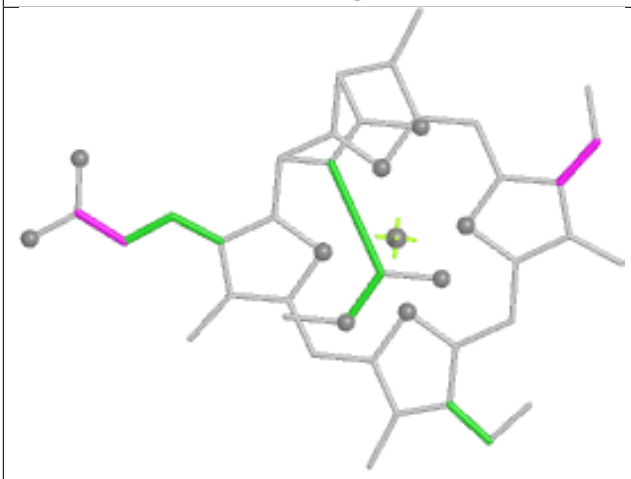

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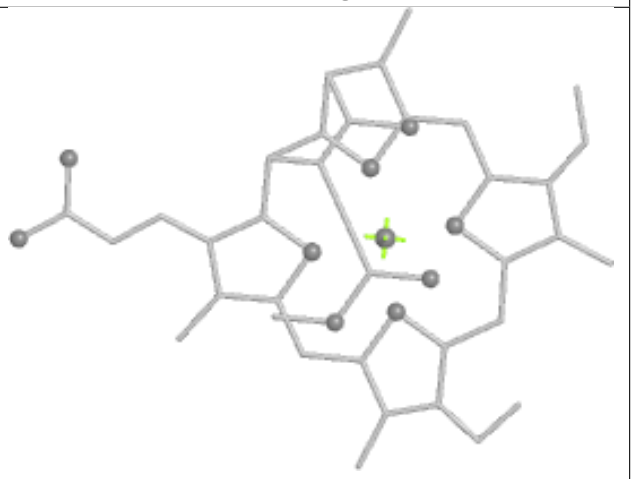
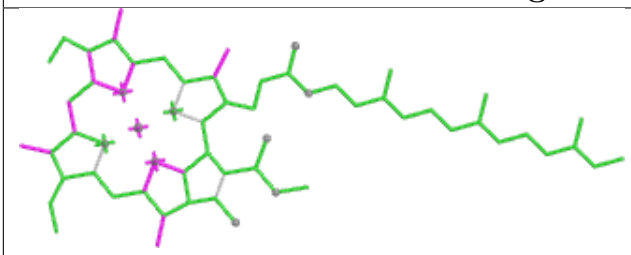


Rings

Ligand CLA 8 308



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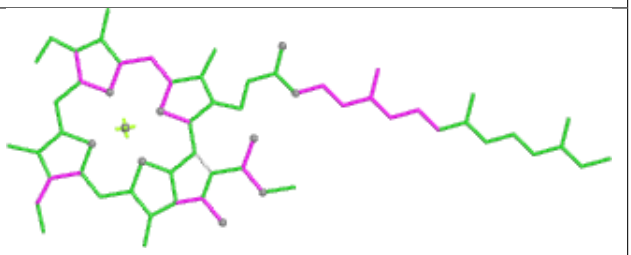

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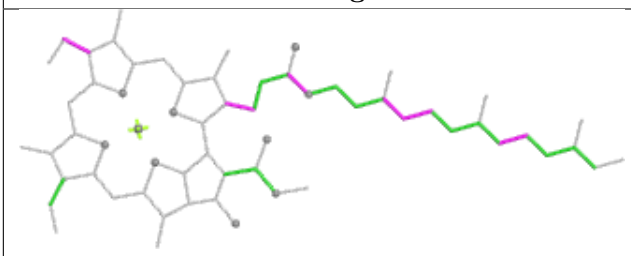

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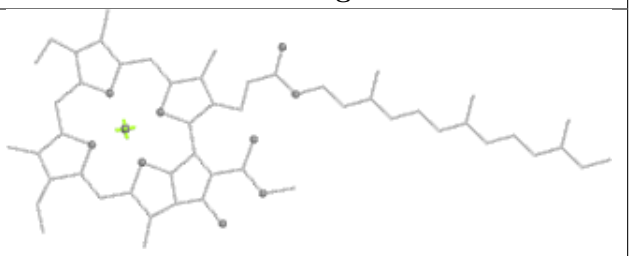
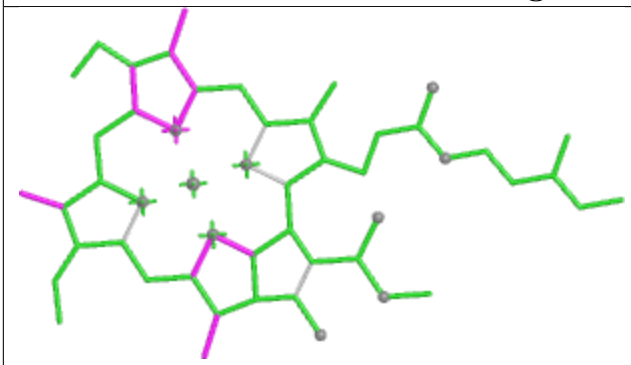


Rings

Ligand CLA p 608



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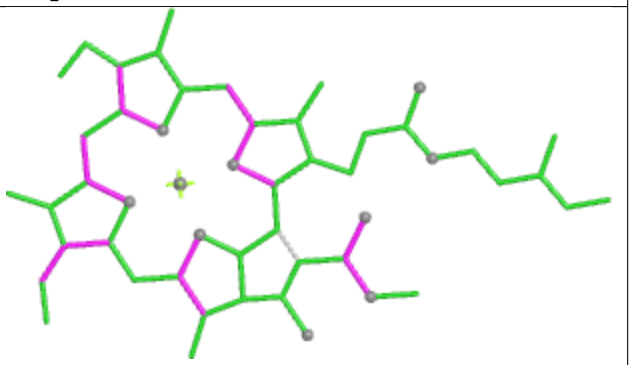

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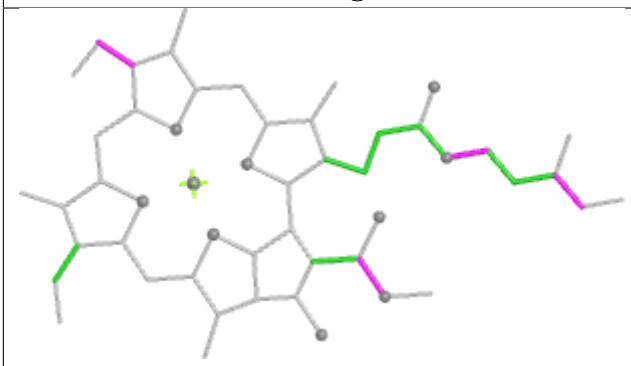

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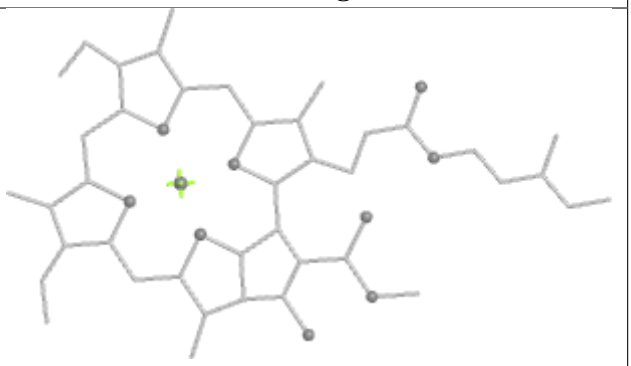

Rings

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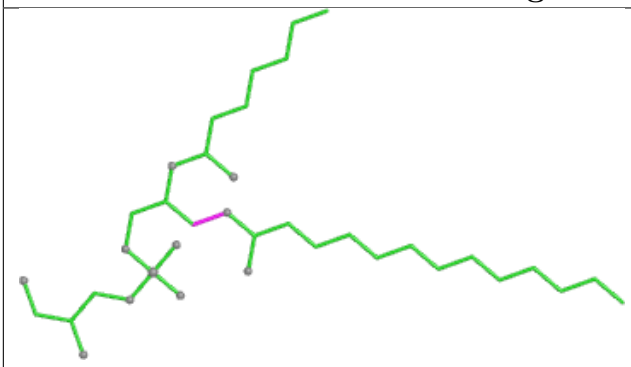

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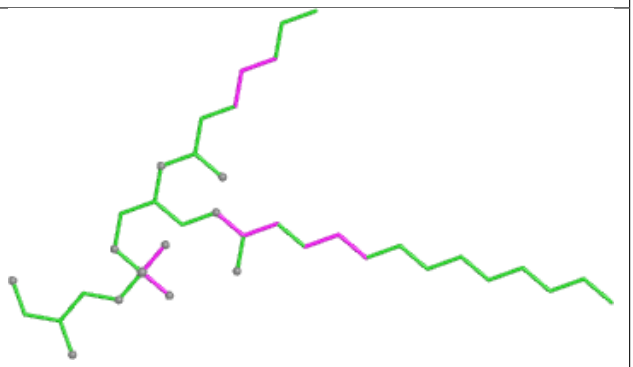

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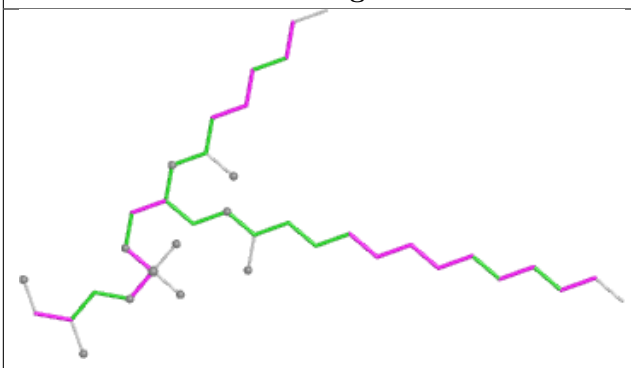

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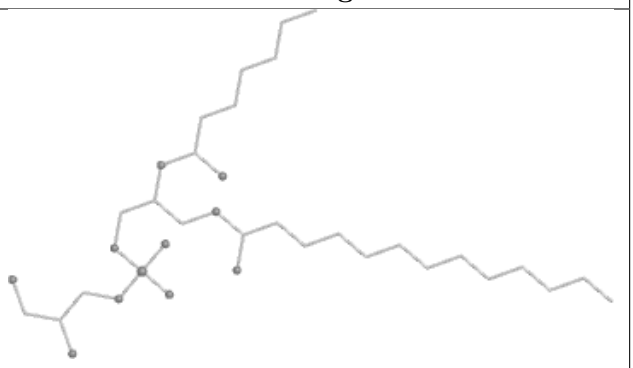
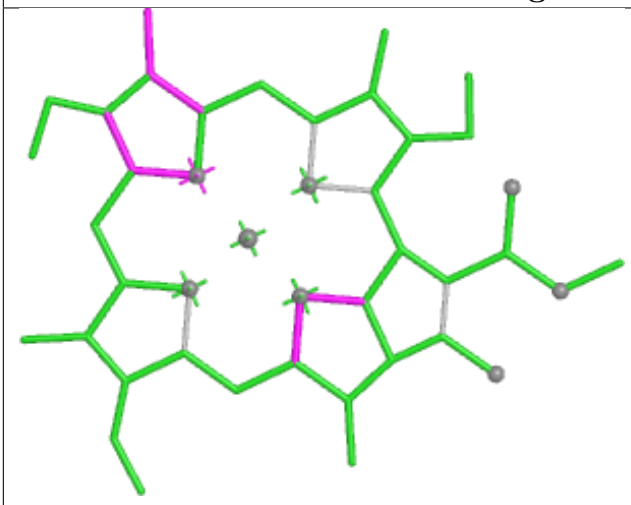


Rings

Ligand CLA 6 308



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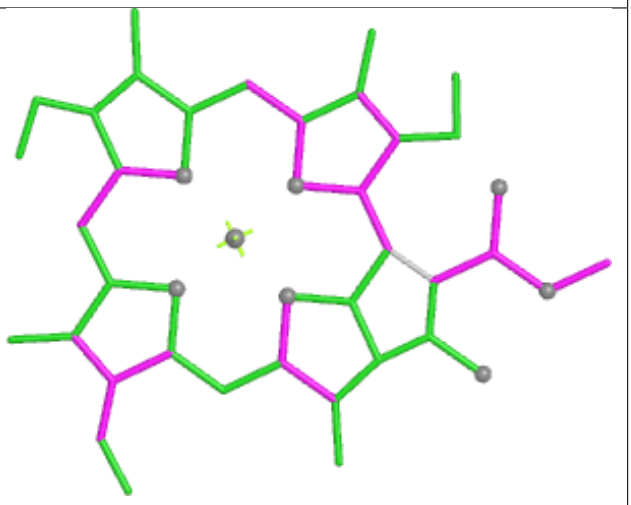

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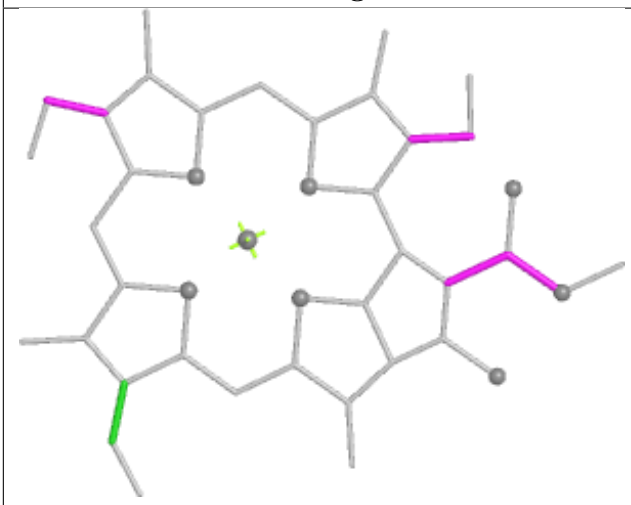
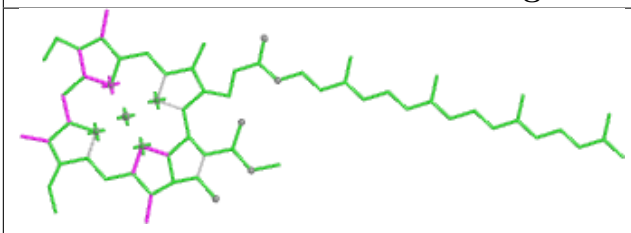


Torsions



Rings

Ligand CLA D 406



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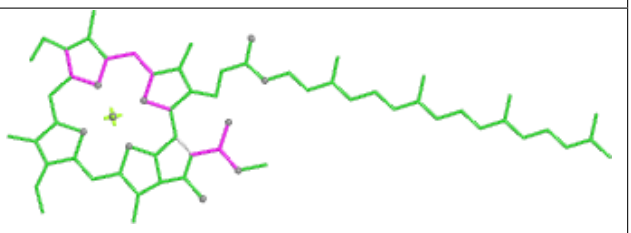

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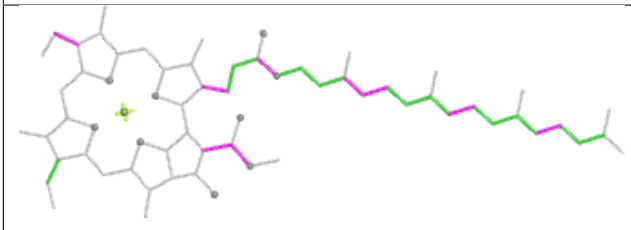

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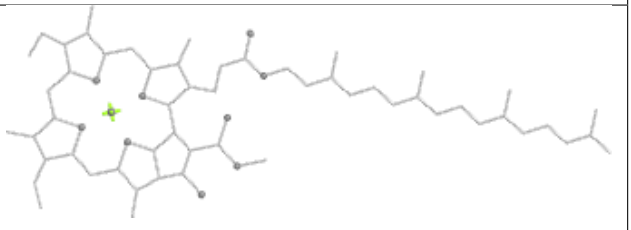

Rings

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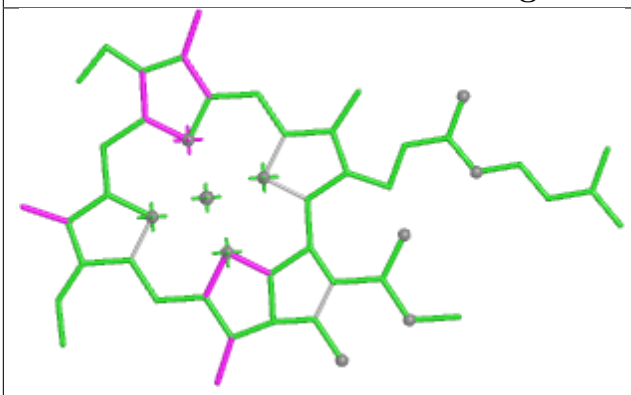

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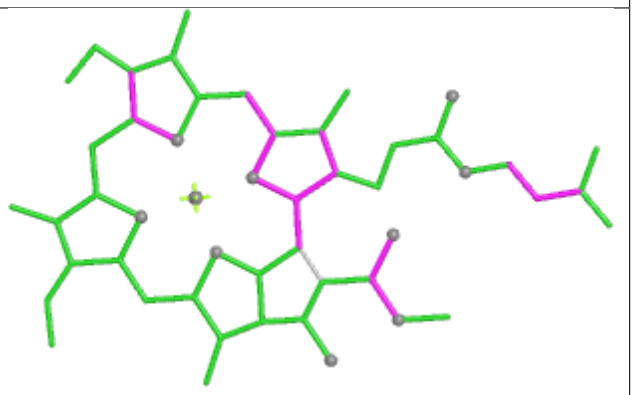

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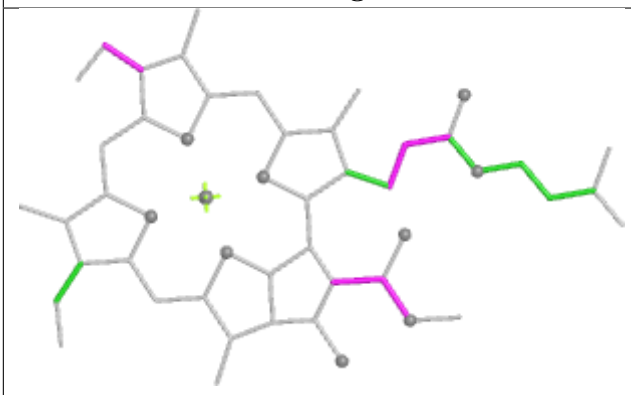

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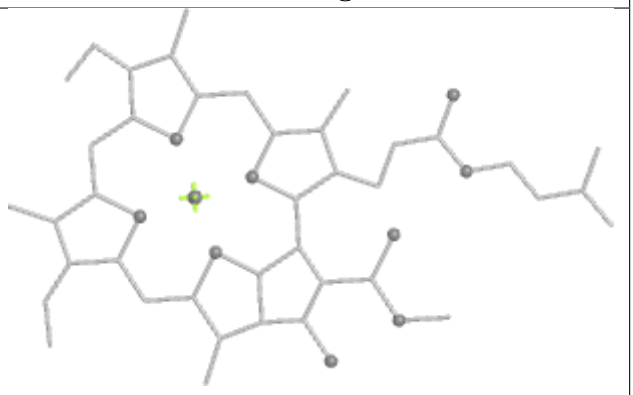

Rings

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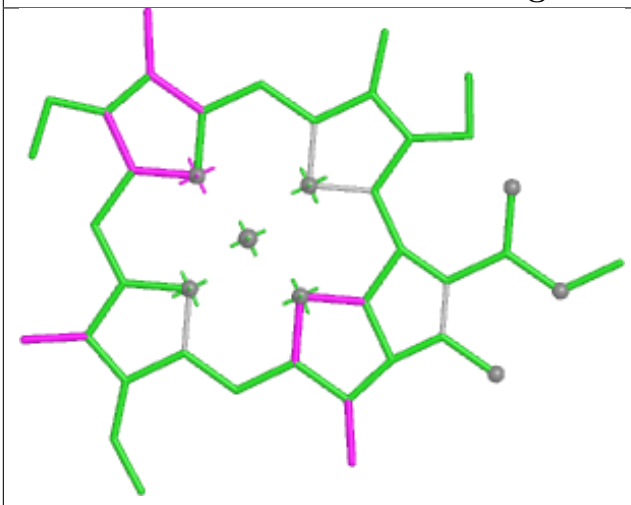

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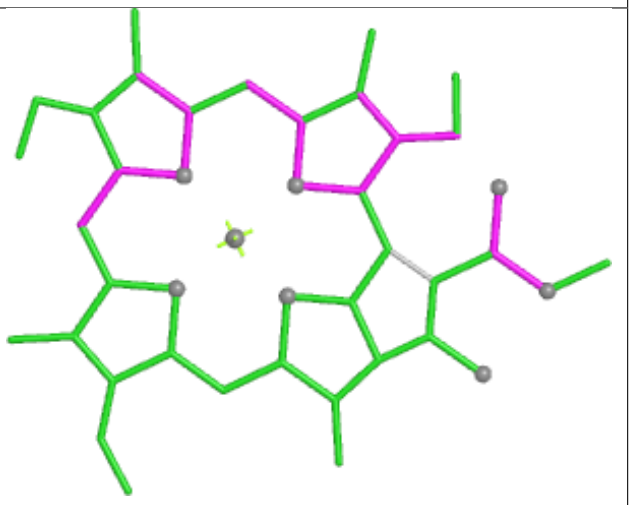

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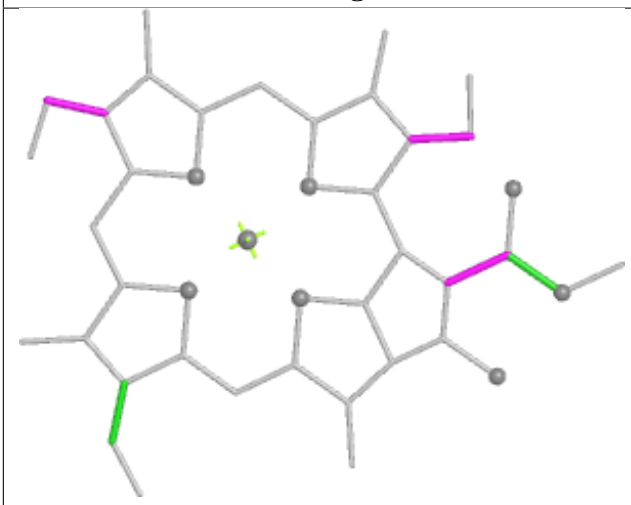


Torsions

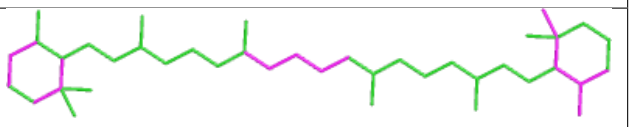


Rings

Ligand BCR h 101



Bond lengths



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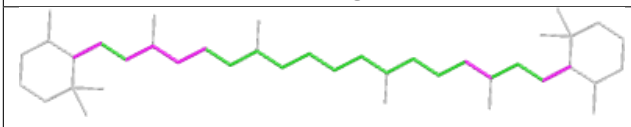

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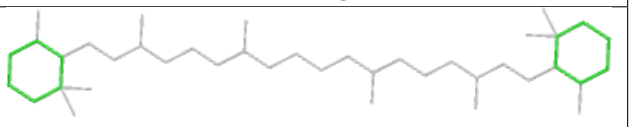
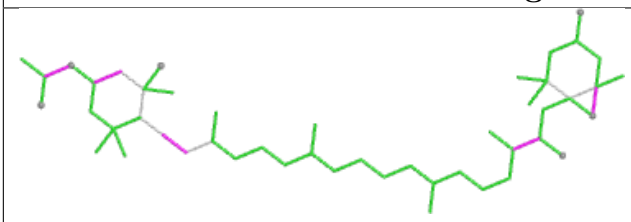


Rings

Ligand A86 19 303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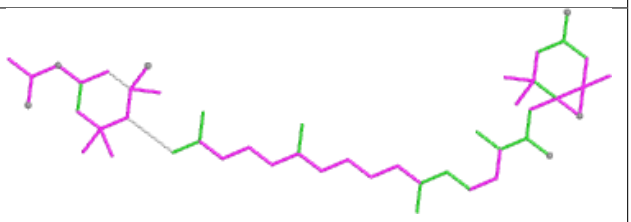
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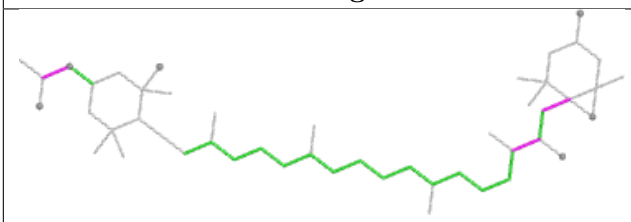
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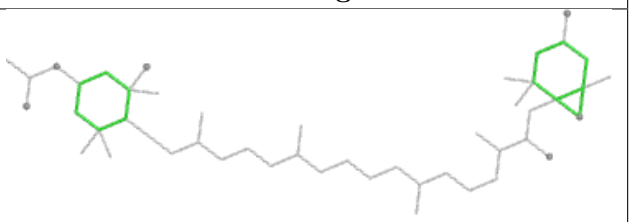
Rings

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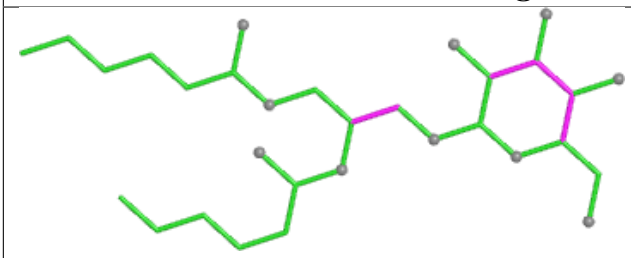
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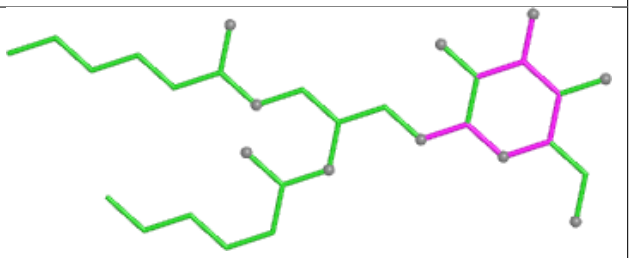
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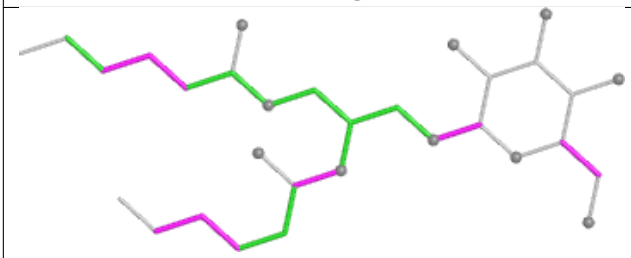
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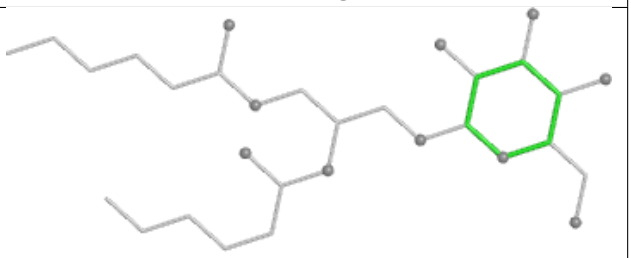
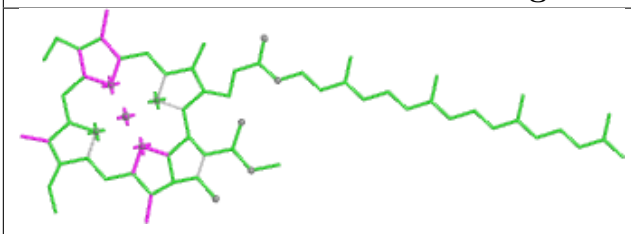

Rings

Ligand CLA c 504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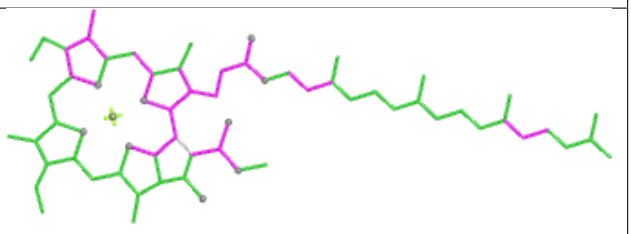
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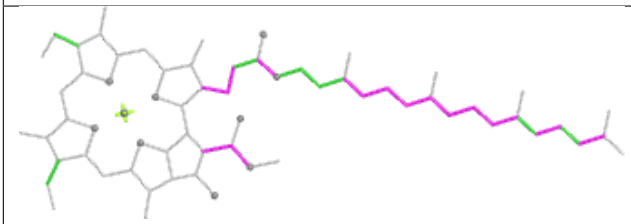
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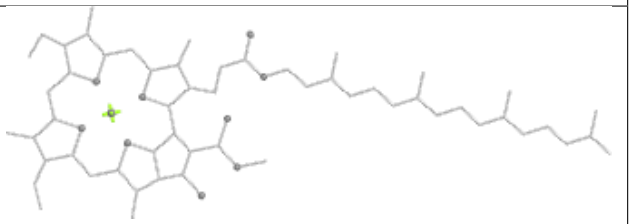
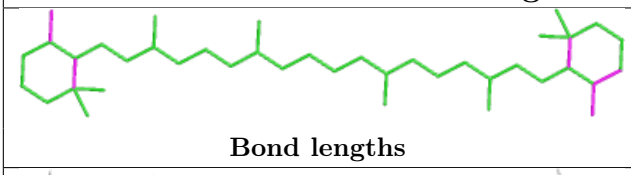

Rings

Ligand BCR C 516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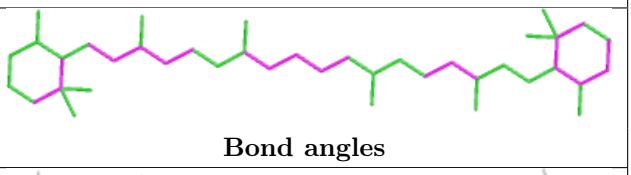
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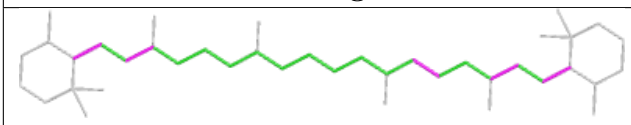
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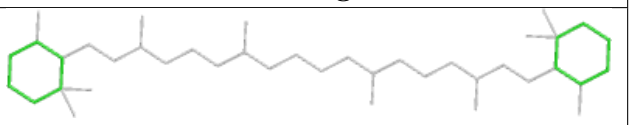
Rings

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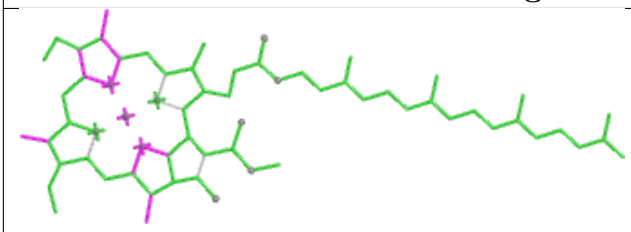
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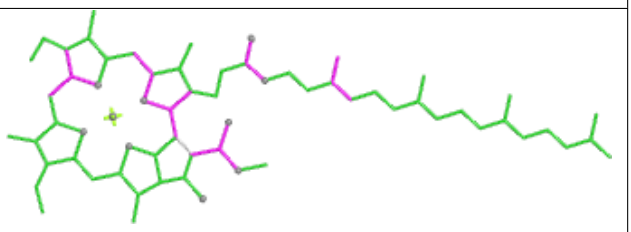
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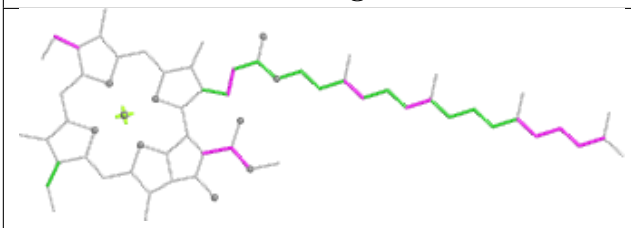
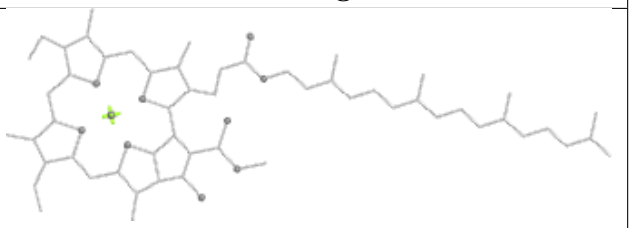

Torsions


Rings

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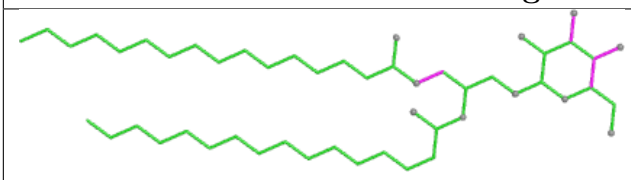
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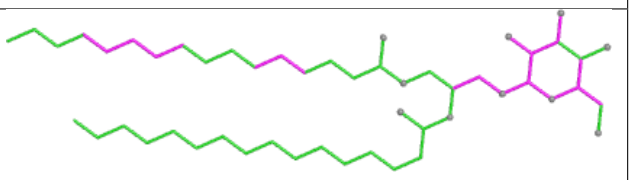
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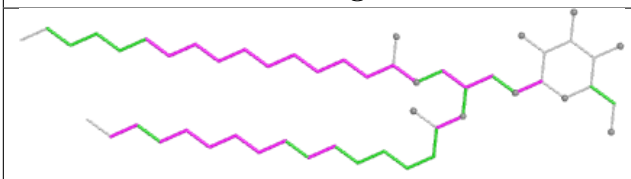
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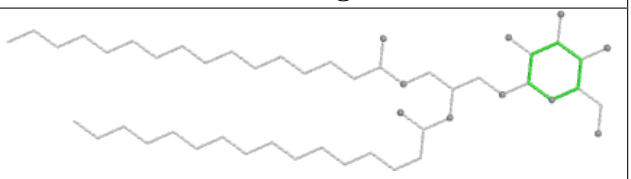
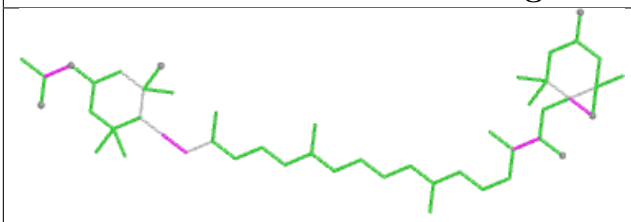

Rings

Ligand A86 10 304



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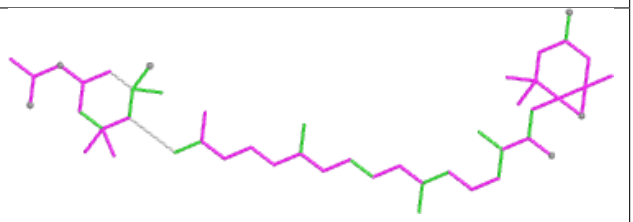

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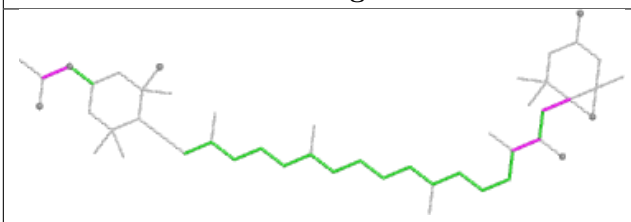

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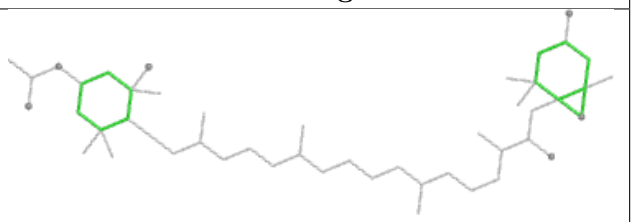
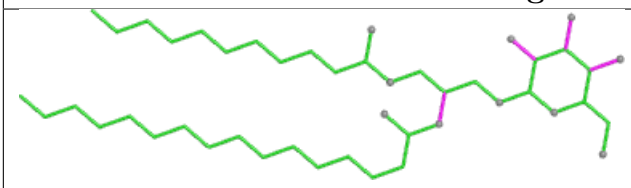


Rings

Ligand LMG f 102



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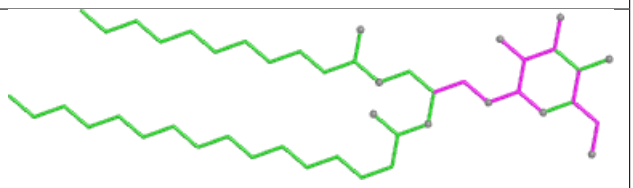

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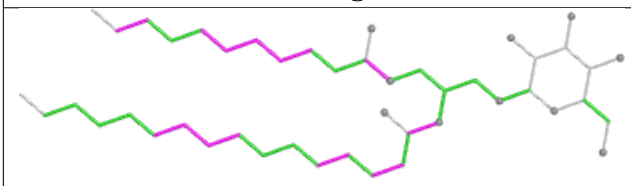

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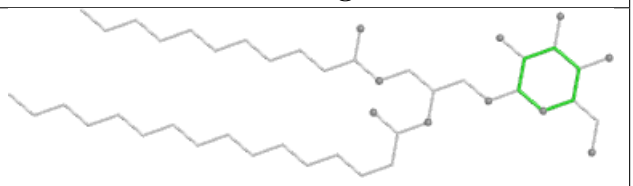
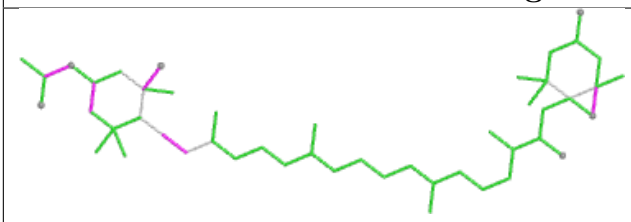


Rings

Ligand A86 16 306



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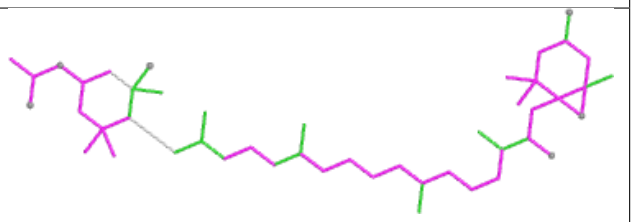

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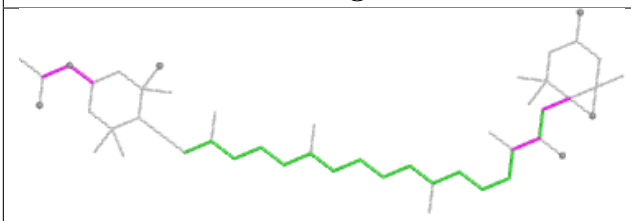

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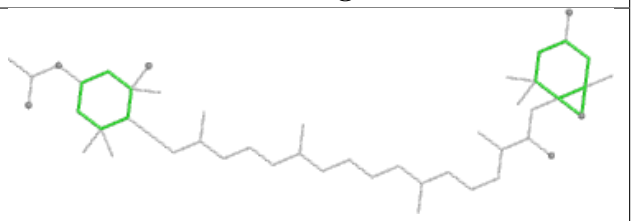

Rings

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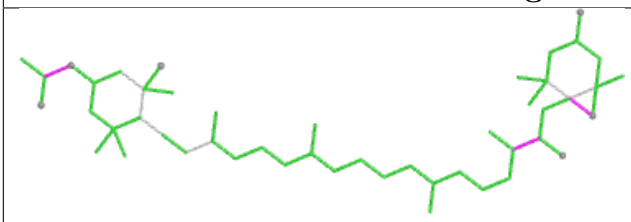

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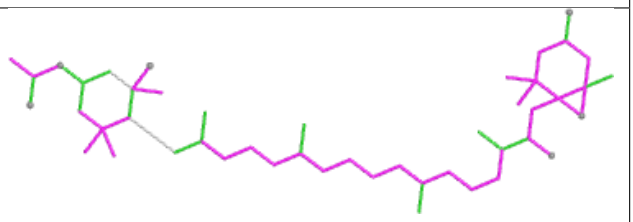

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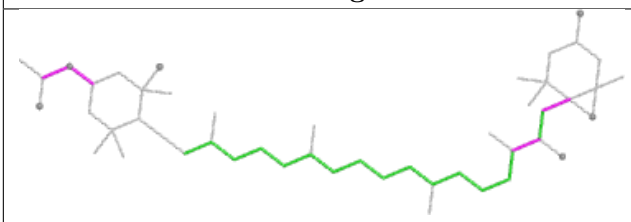

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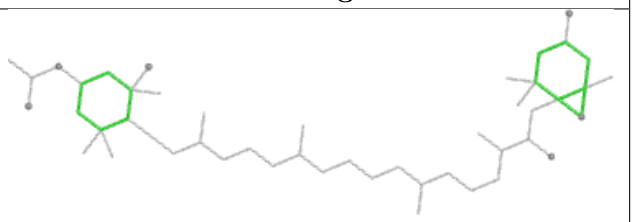
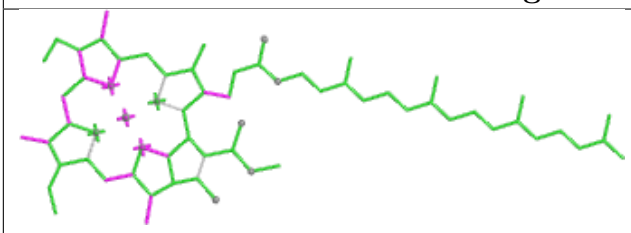


Rings

Ligand CLA D 405



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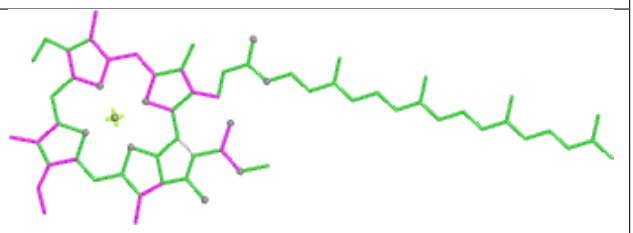

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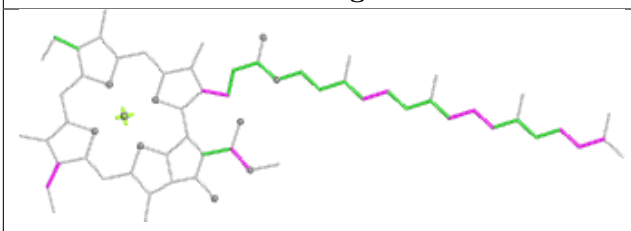

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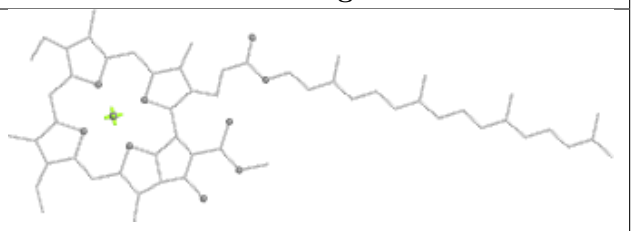
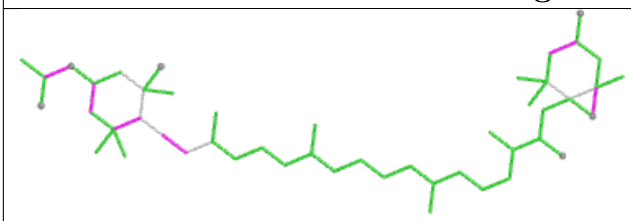


Rings

Ligand A86 8 306



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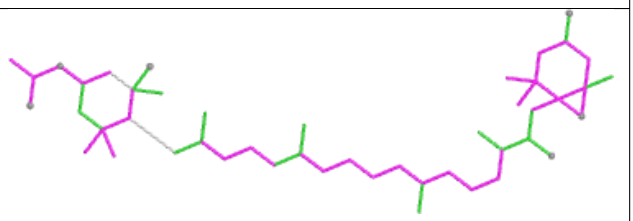

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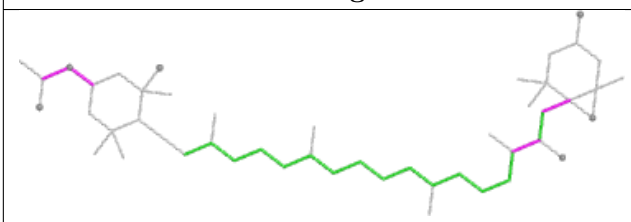

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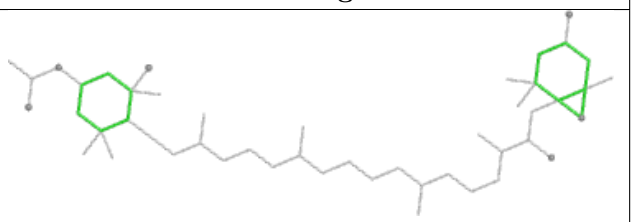

Rings

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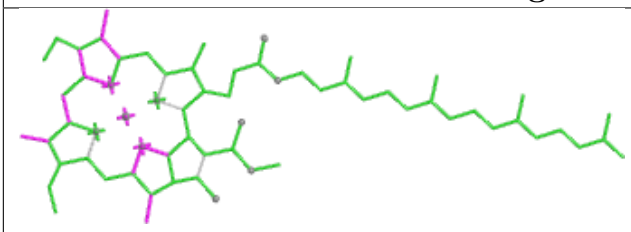

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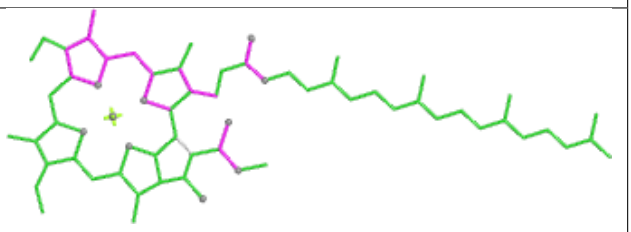

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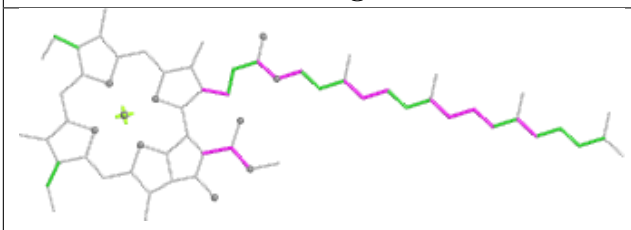

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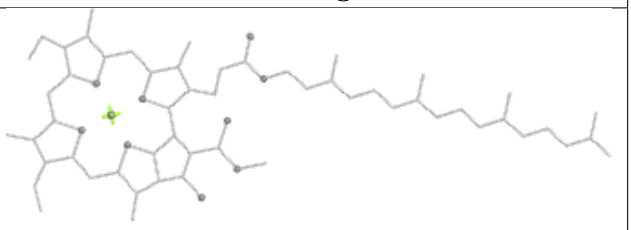
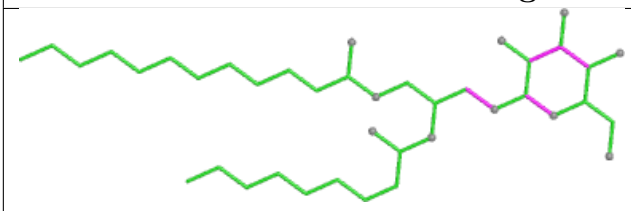


Rings

Ligand LMG D 404



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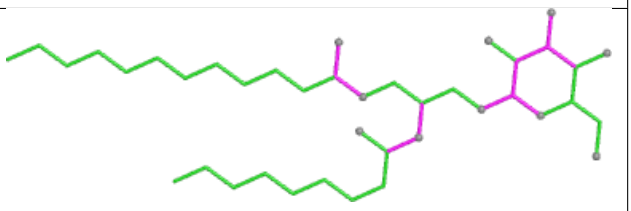

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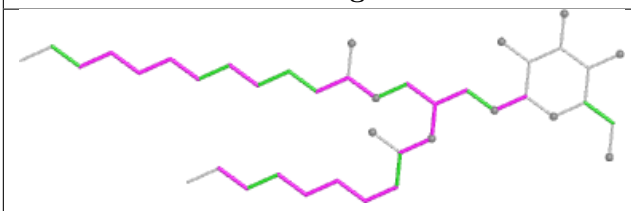

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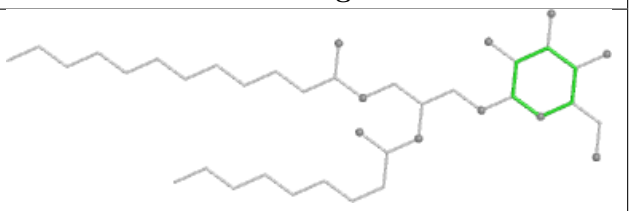
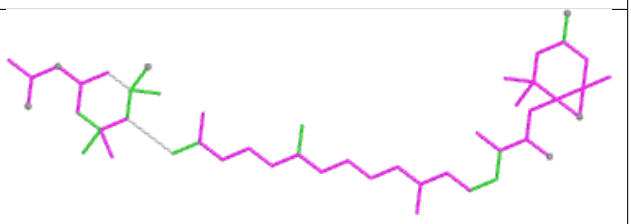


Rings

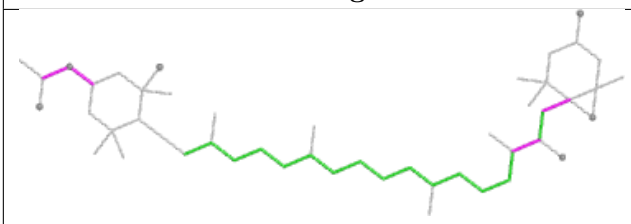
Ligand A86 12 301



Bond lengths



Bond angles



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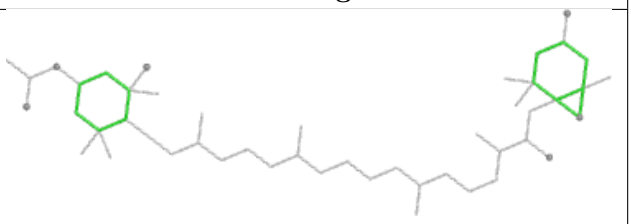
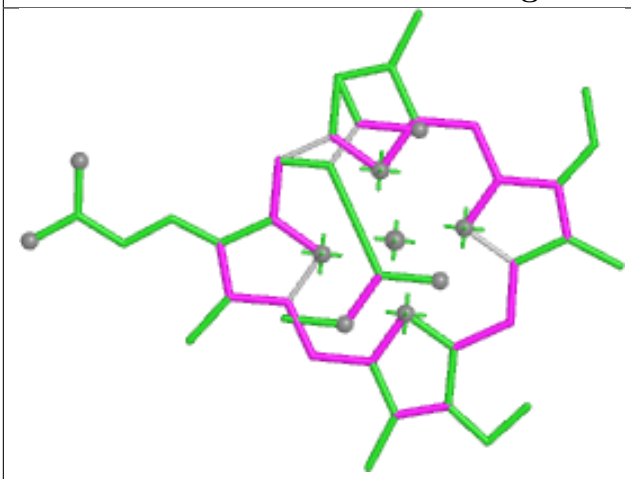


Rings

Ligand KC1 16 314



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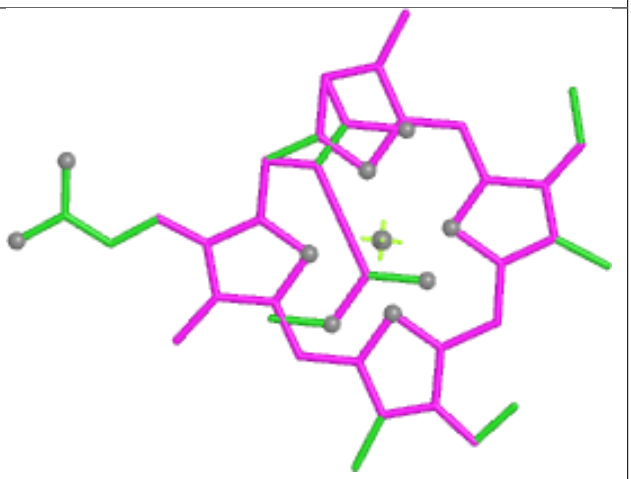

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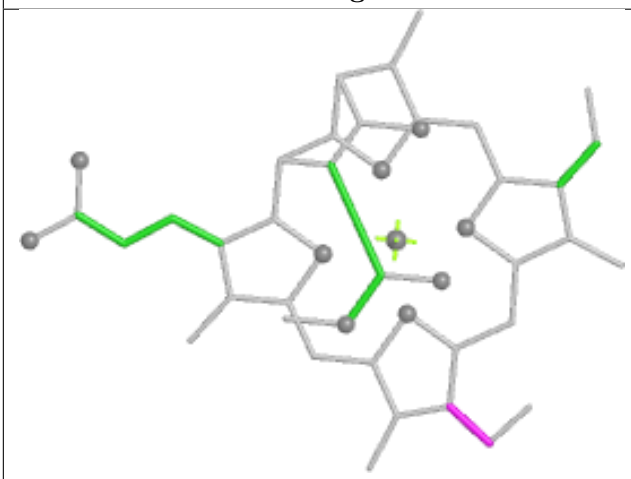

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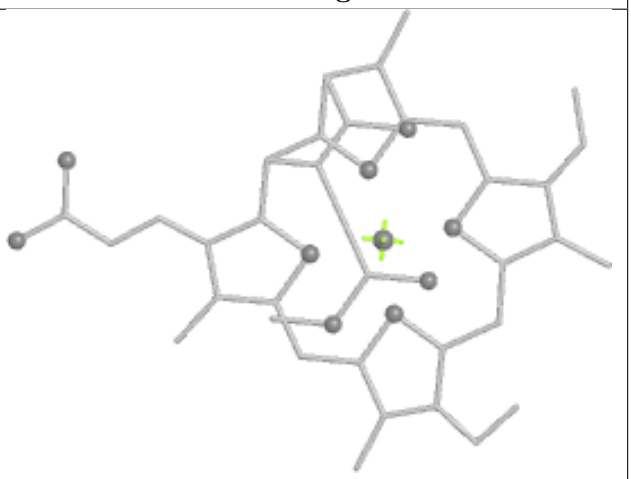
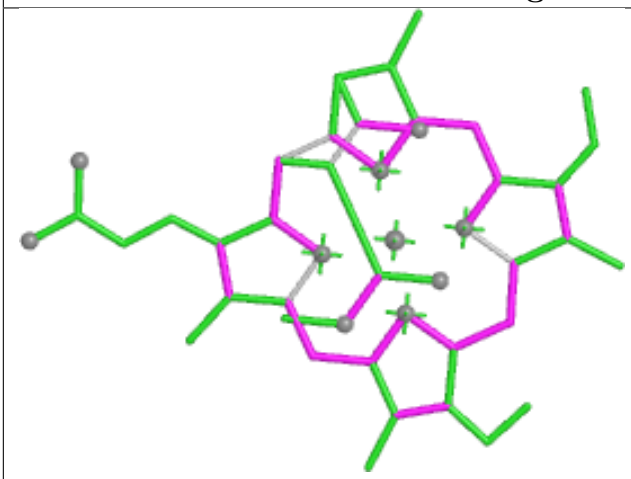


Rings

Ligand KC1 P 609



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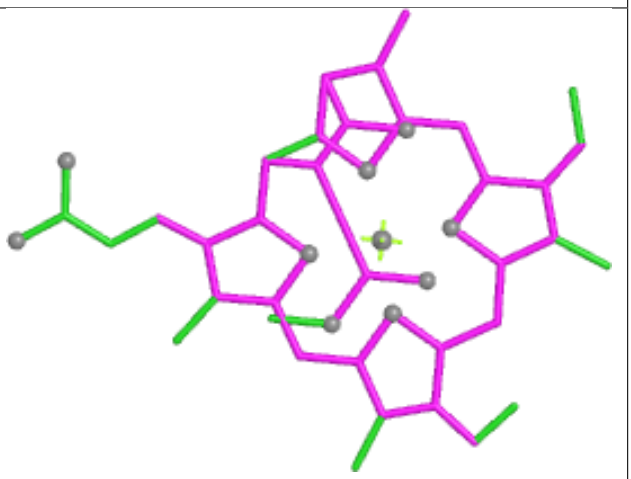
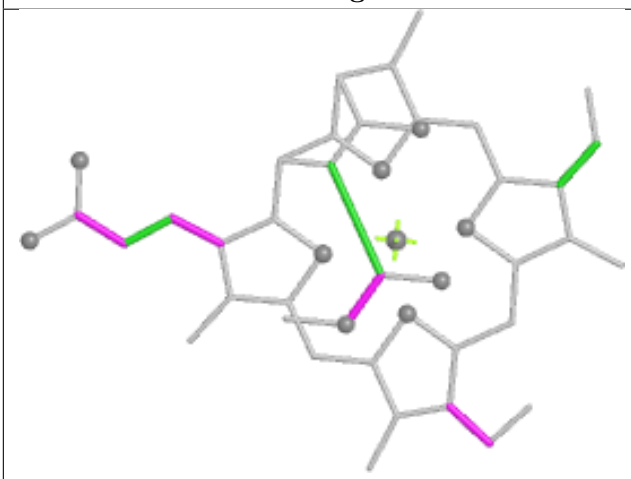


Bond angles



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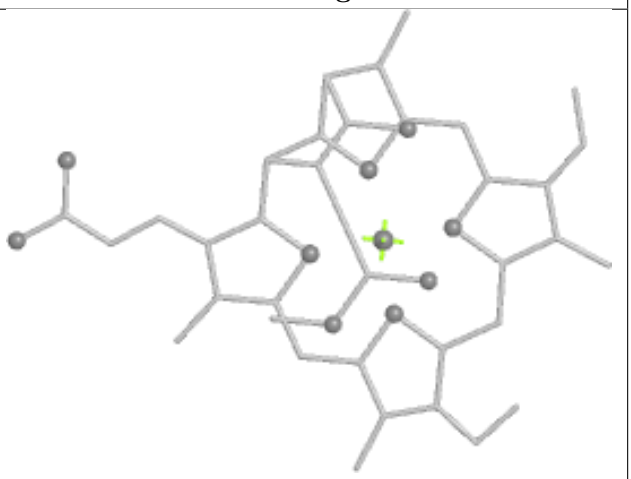
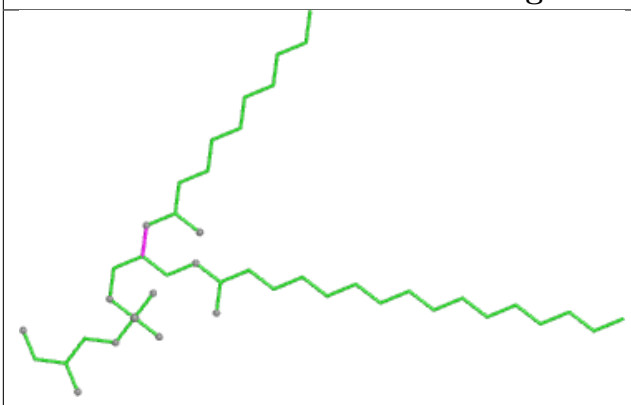


Rings

Ligand LHG b 623



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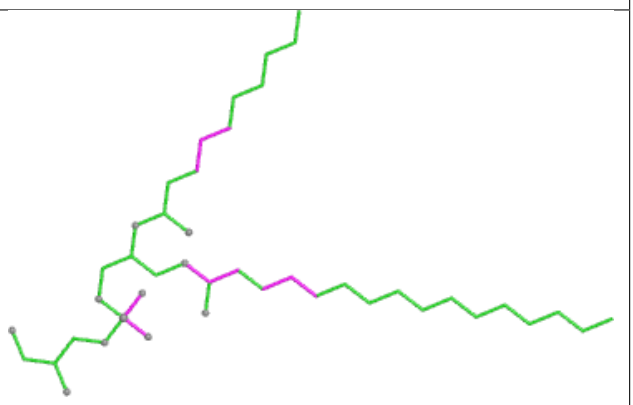
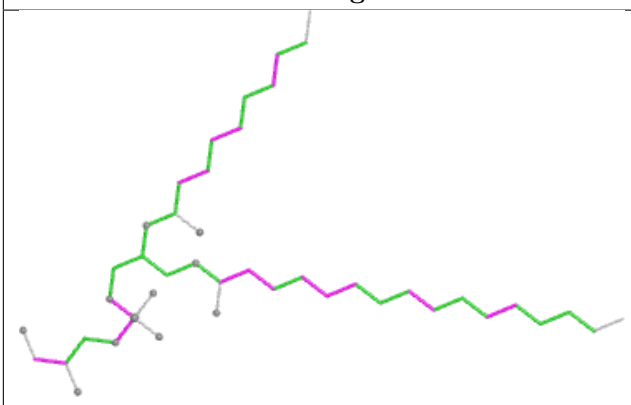


Bond angles



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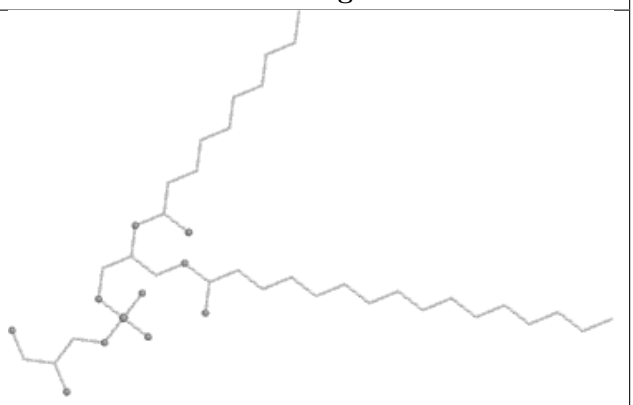
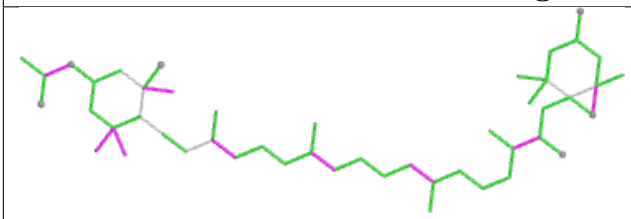


Rings

Ligand A86 4 305



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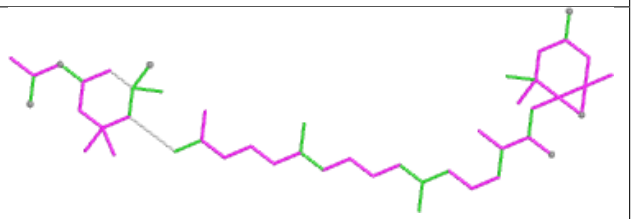
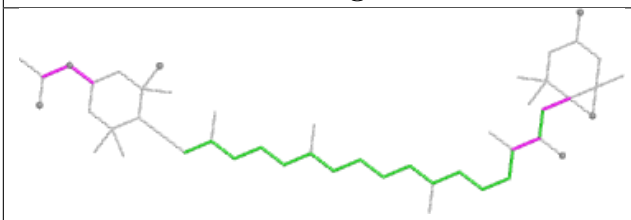


Bond angles



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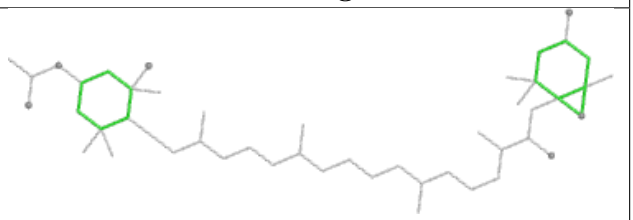
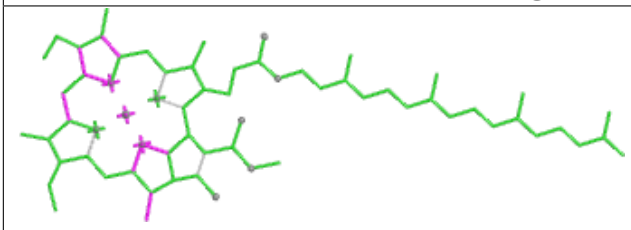


Rings

Ligand CLA 9 312



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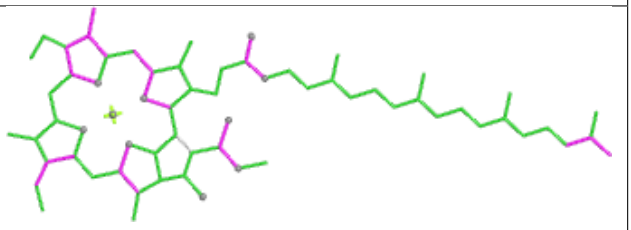
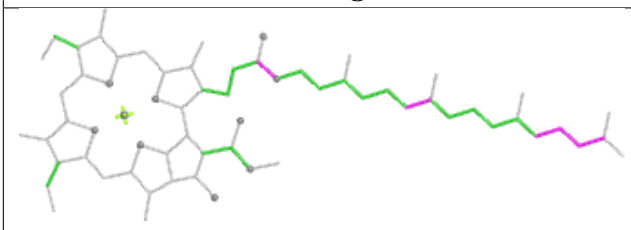
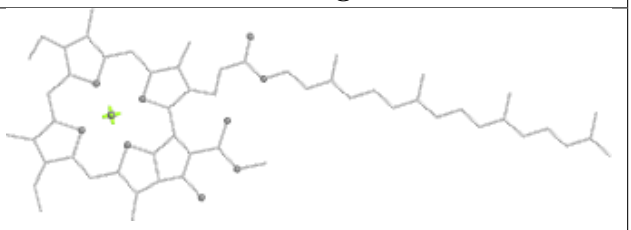


Bond angles

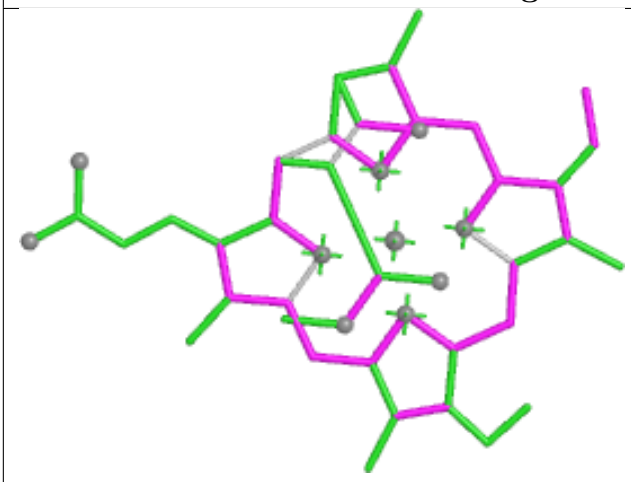


Torsions



Rings

Ligand KC2 15 308



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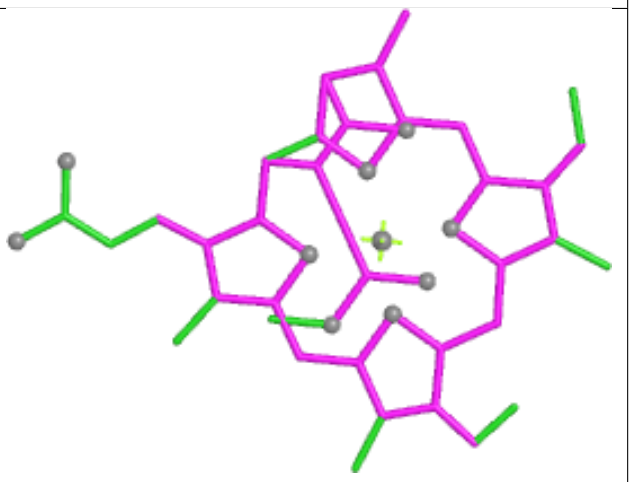

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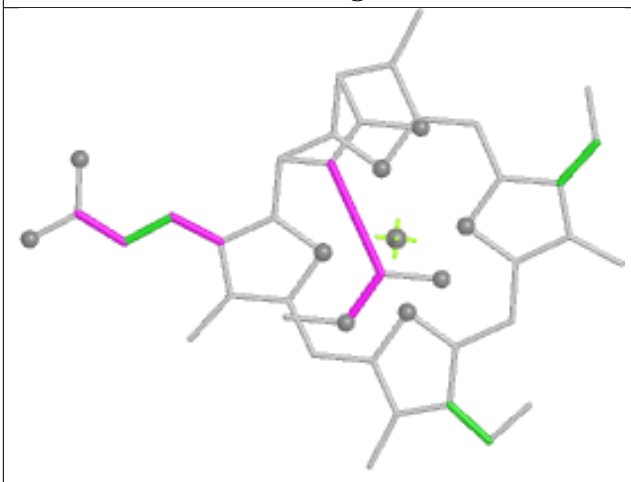

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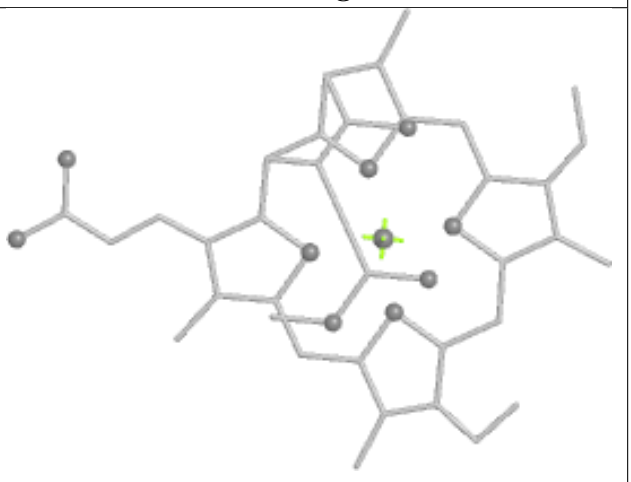
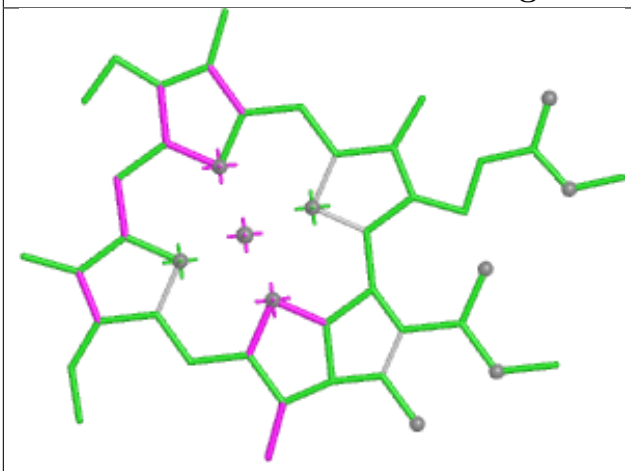


Rings

Ligand CLA 14 311



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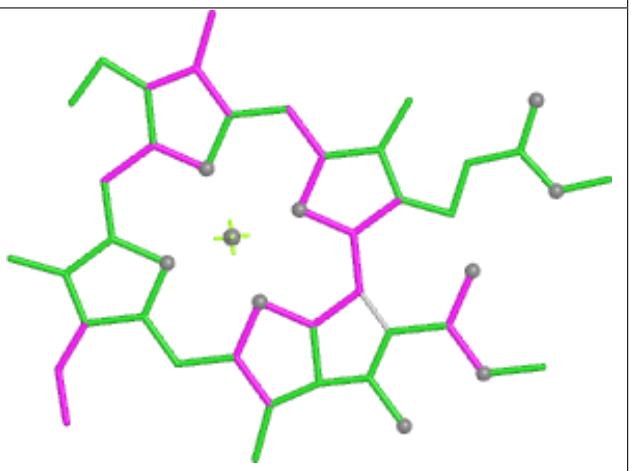

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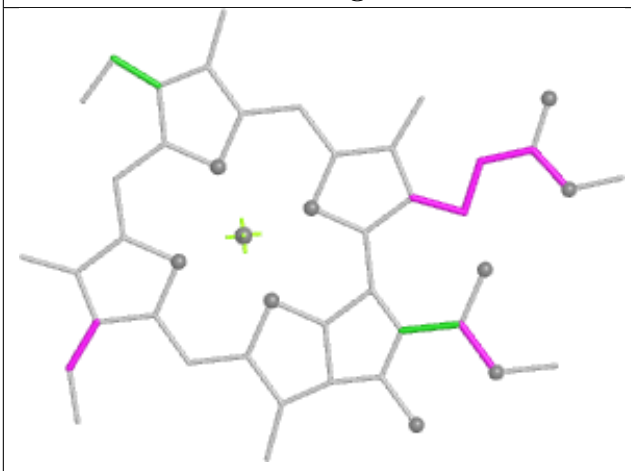

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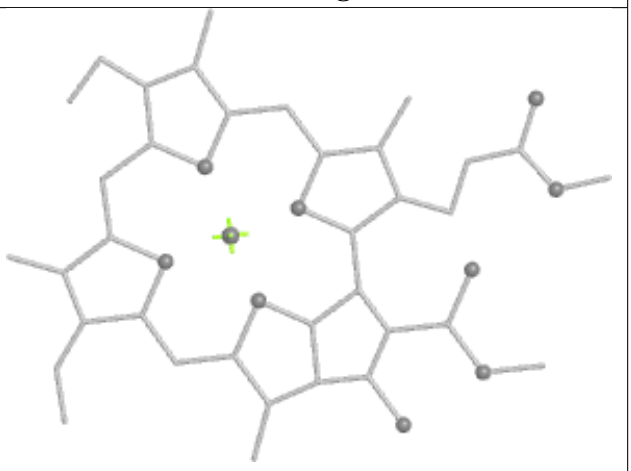

Rings

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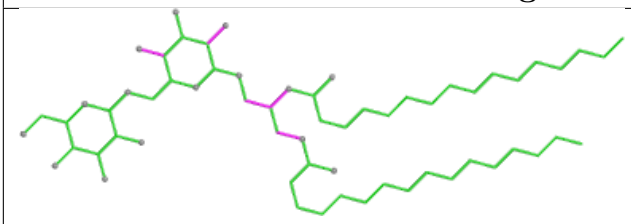

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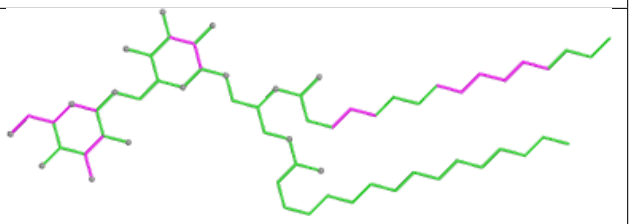

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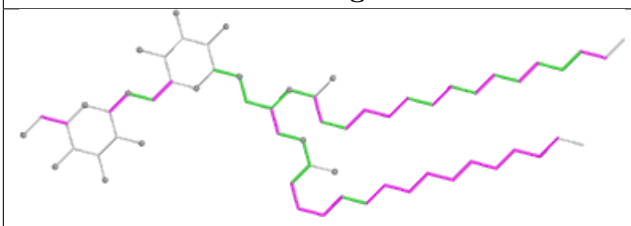

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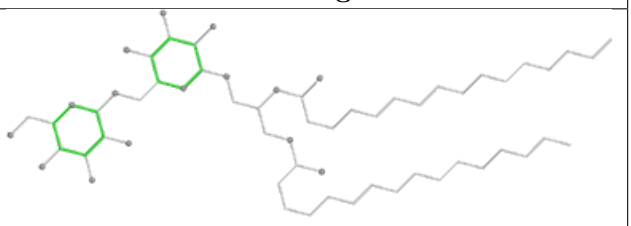
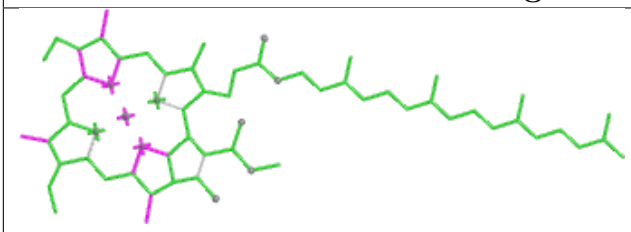


Rings

Ligand CLA B 608



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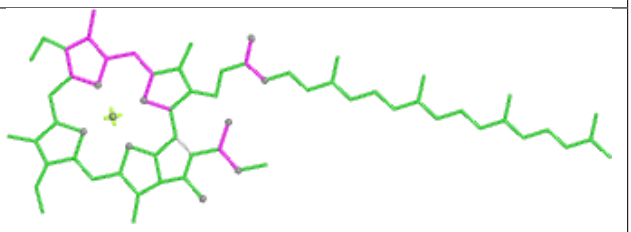

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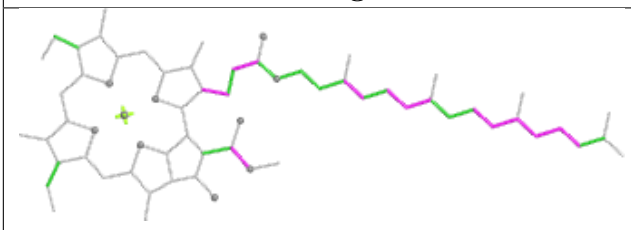

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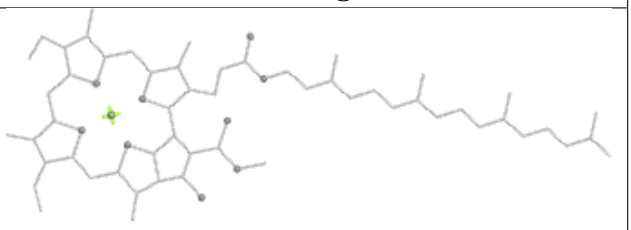

Rings

Ligand BCR y 101



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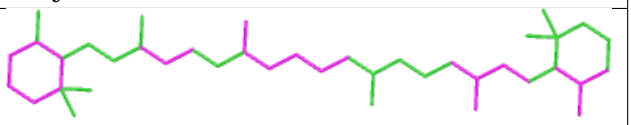

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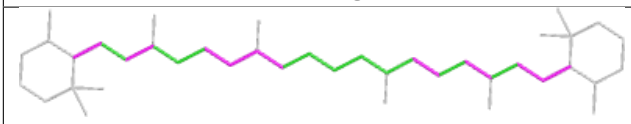

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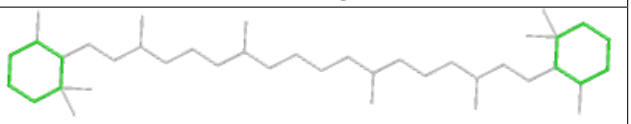
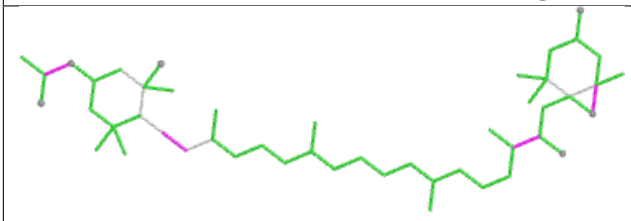


Rings

Ligand A86 6 301



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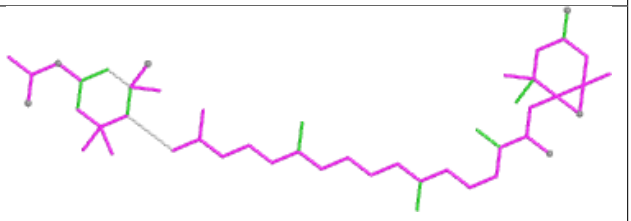

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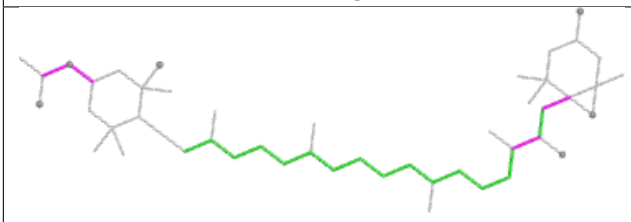

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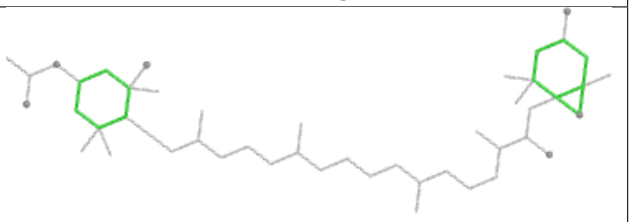
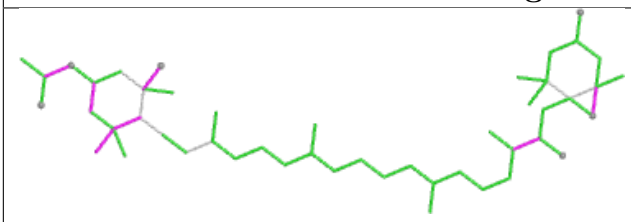


Rings

Ligand A86 15 301



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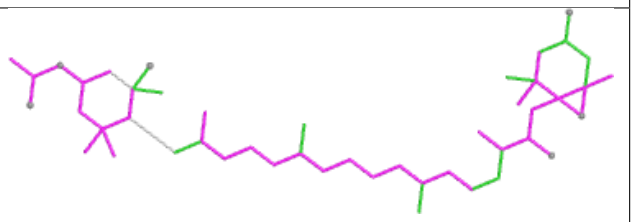

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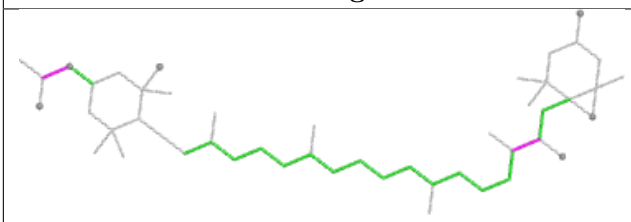

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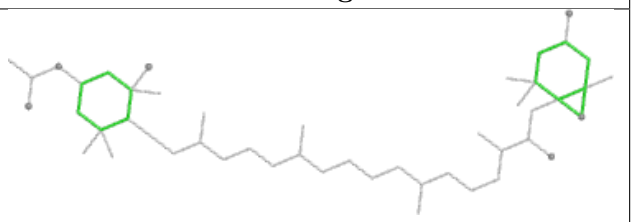

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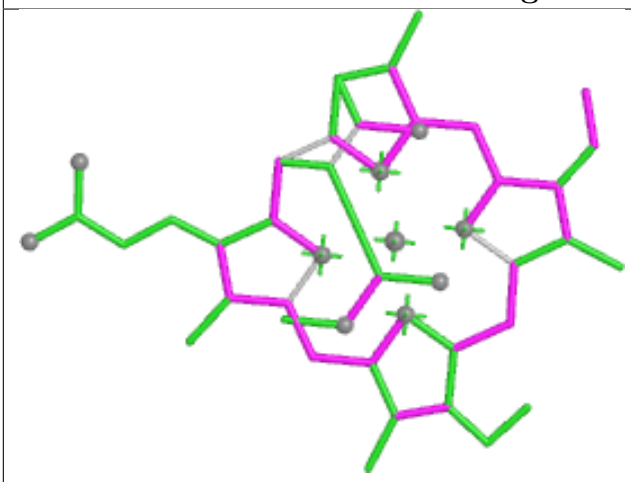

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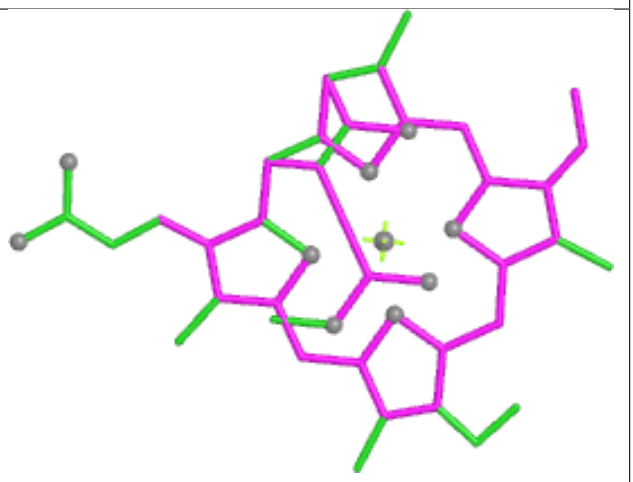

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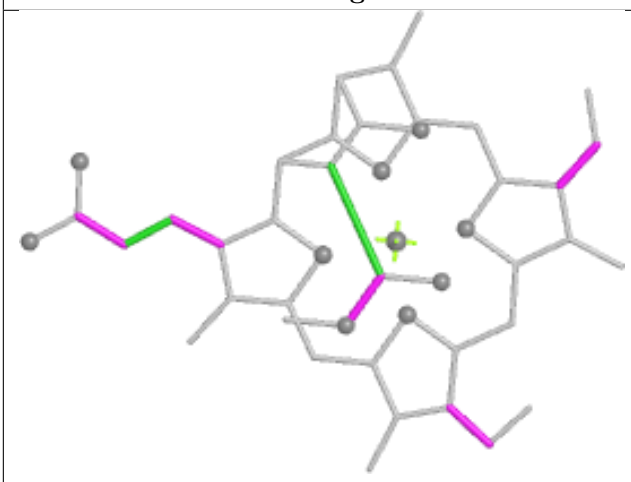

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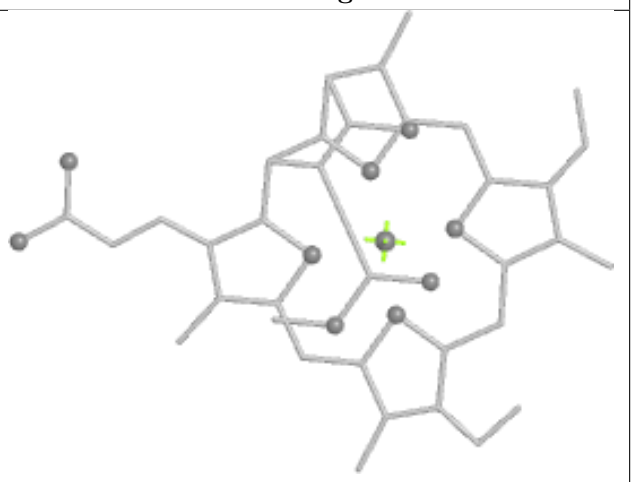
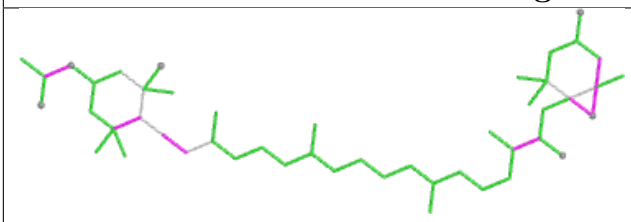


Rings

Ligand A86 1 306



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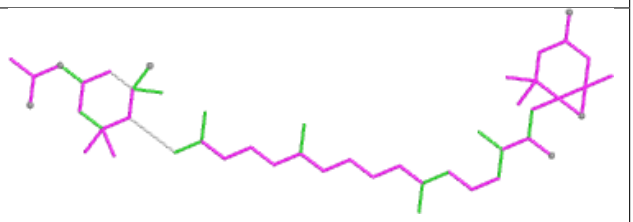

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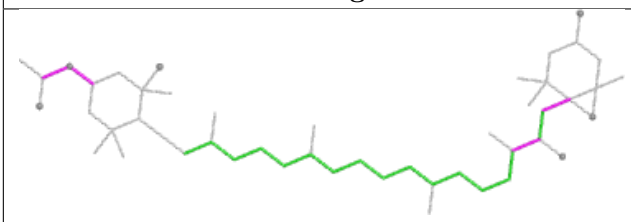

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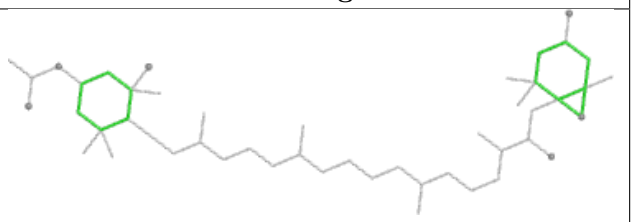
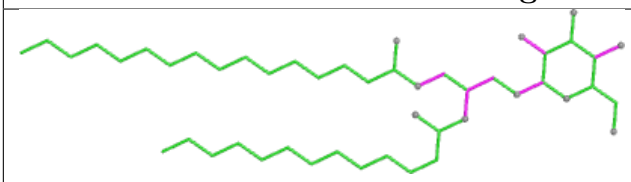


Rings

Ligand LMG w 201



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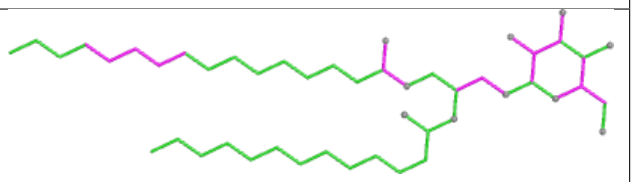

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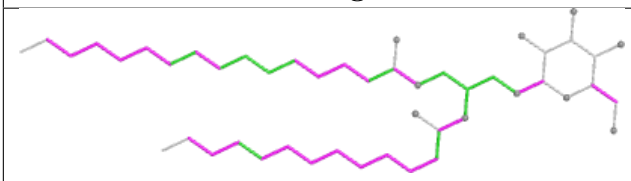

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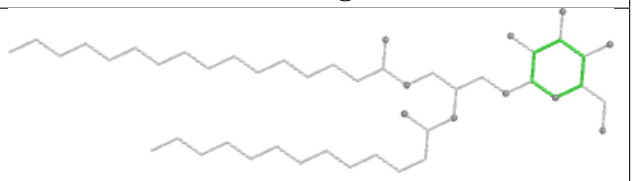
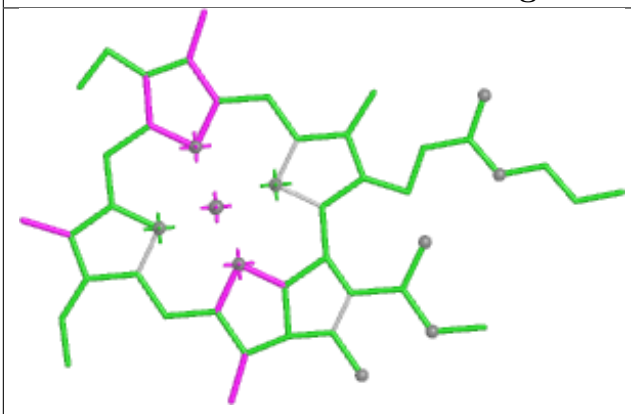


Rings

Ligand CLA 10 317



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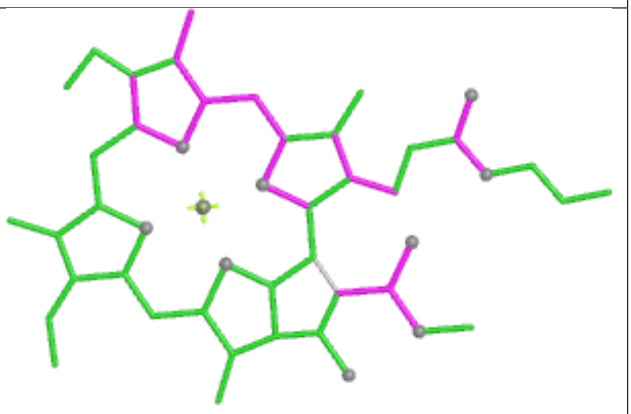

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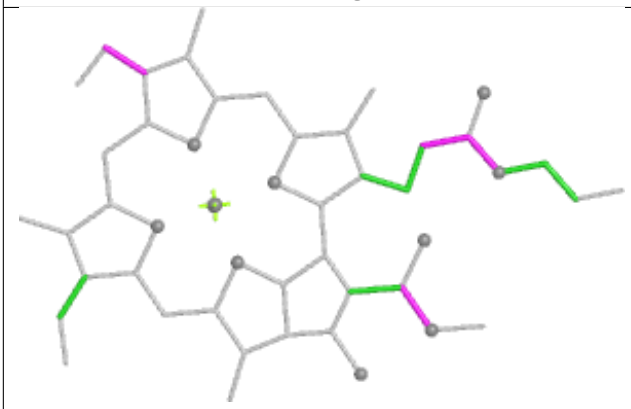

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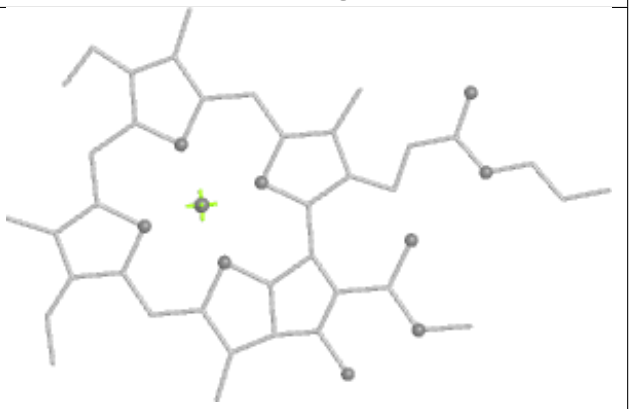
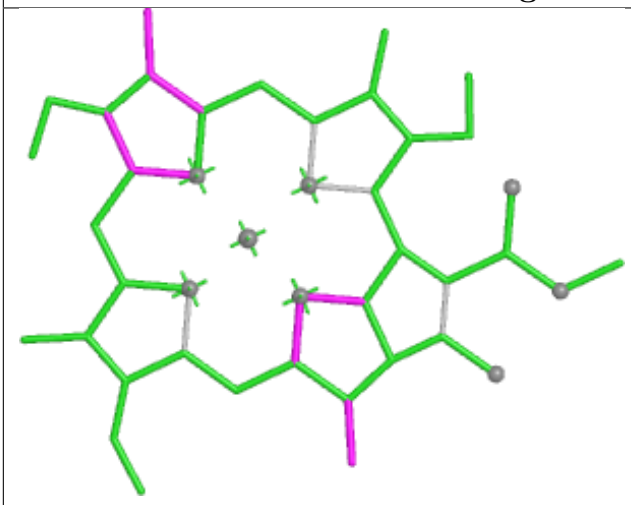


Rings

Ligand CLA 15 306



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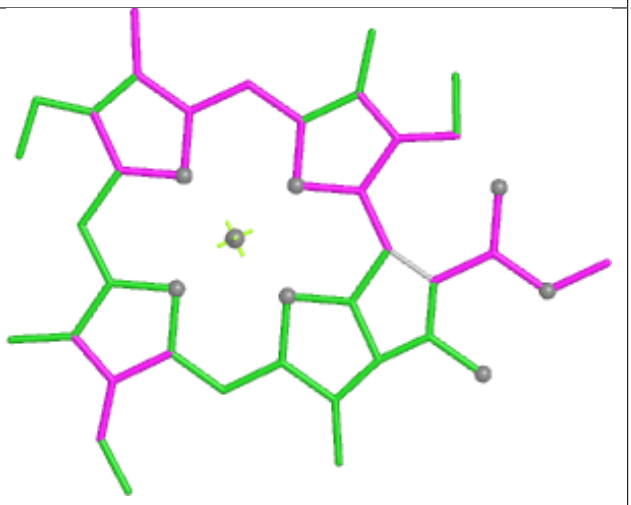
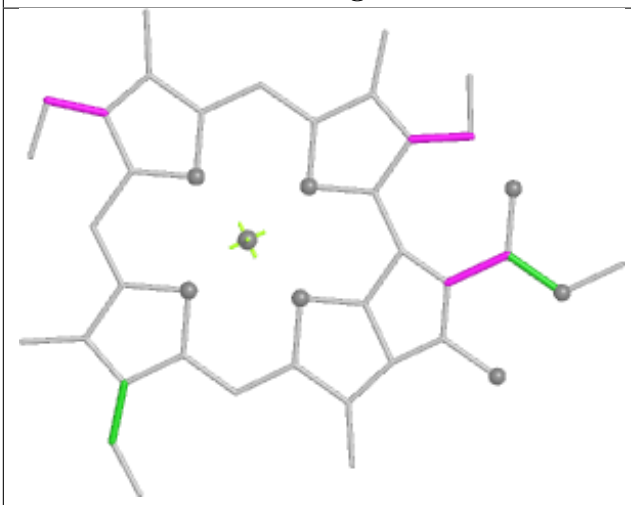


Bond angles



Torsions



Rings

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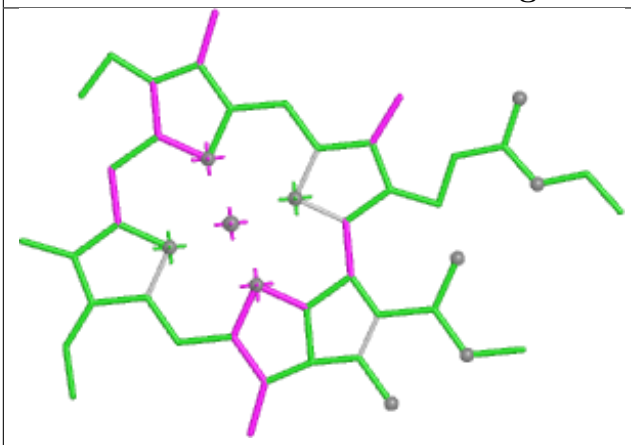

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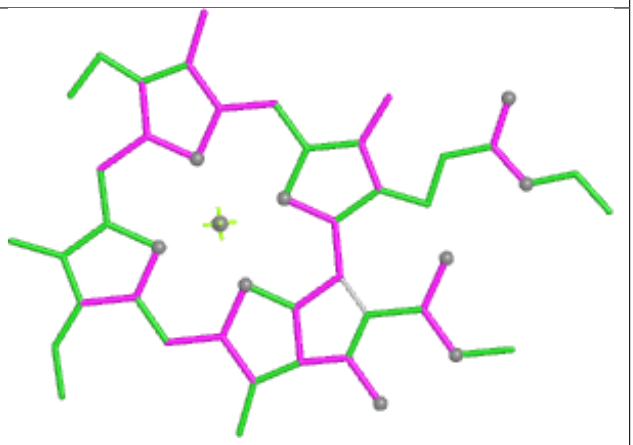

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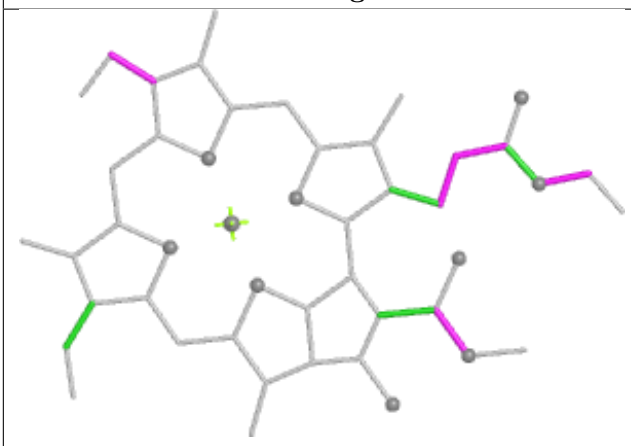

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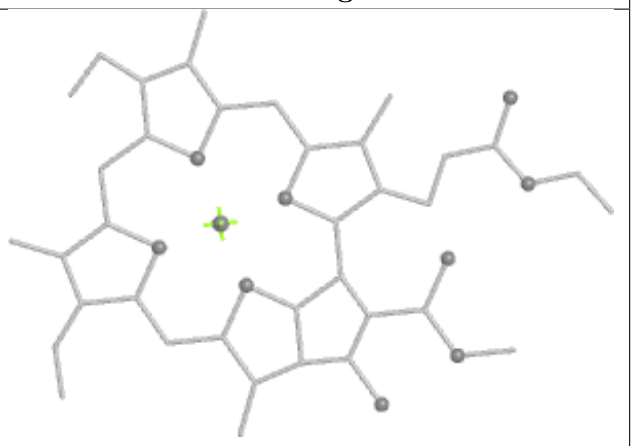
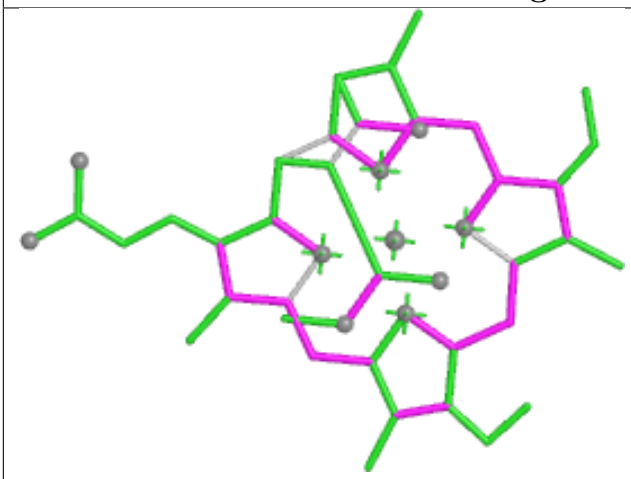


Rings

Ligand KC1 1 314



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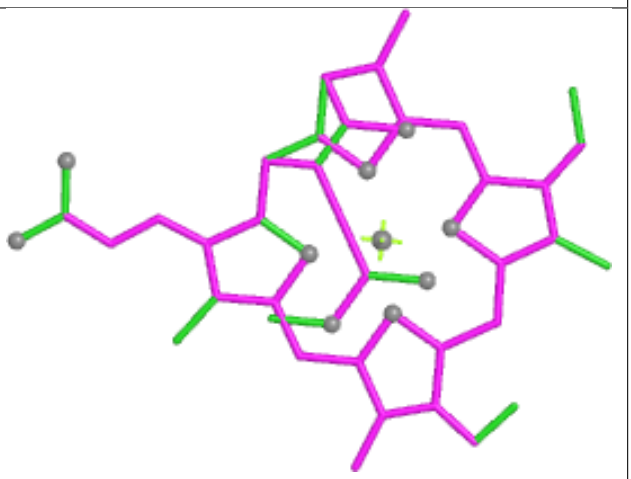
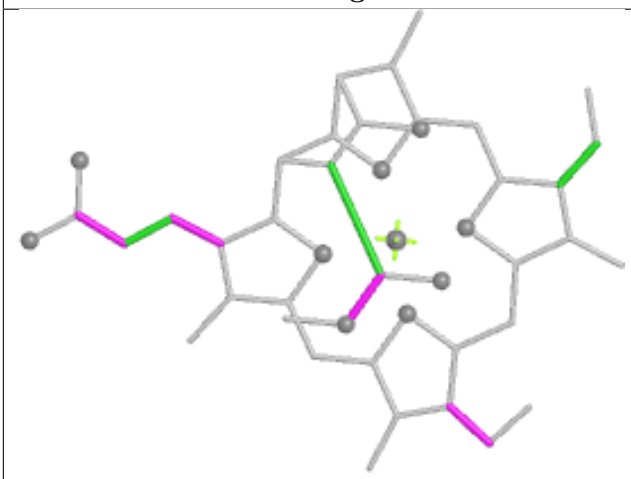


Bond angles



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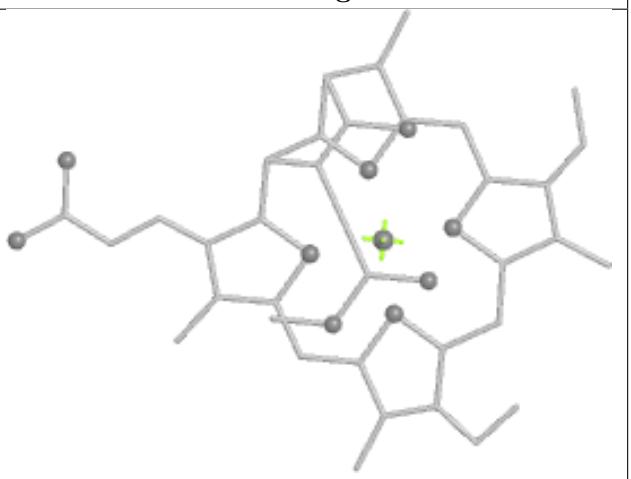
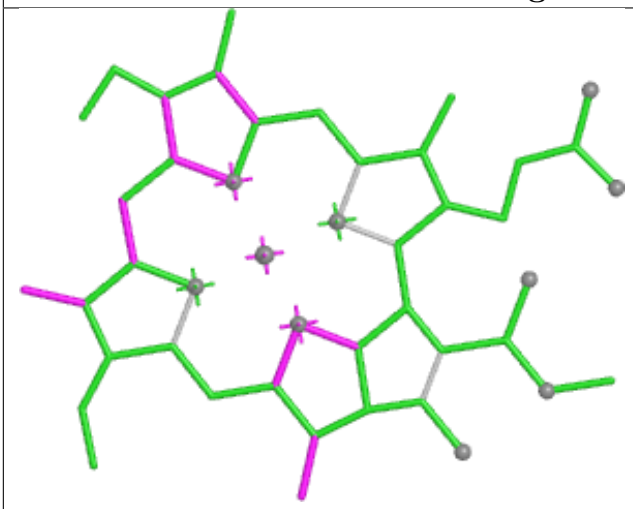


Rings

Ligand CLA 2 311



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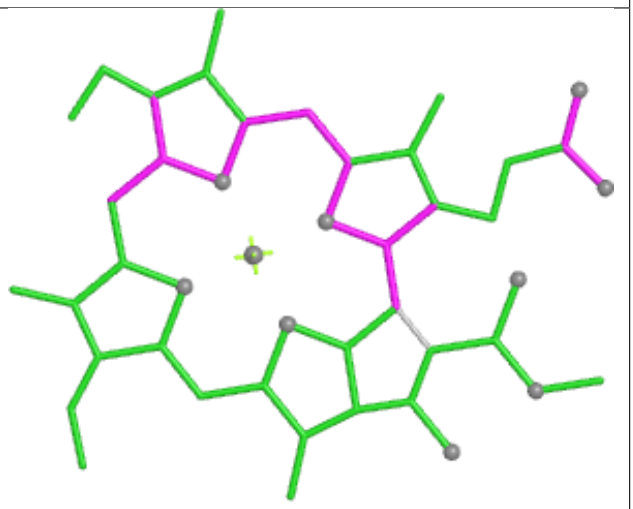
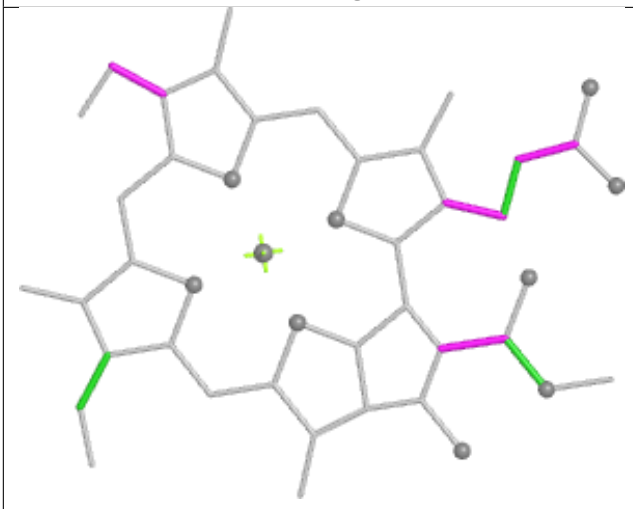


Bond angles

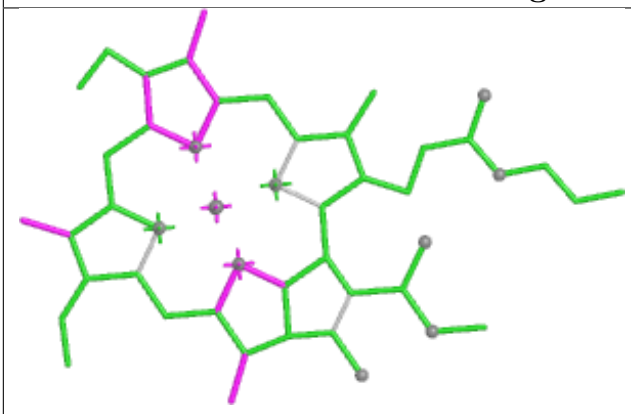


Torsions



Rings

Ligand CLA z 103



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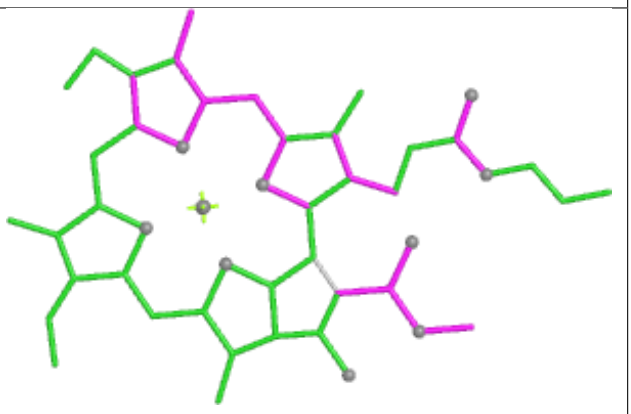

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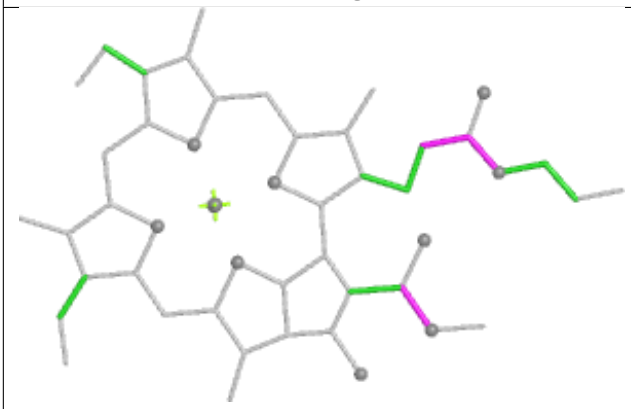

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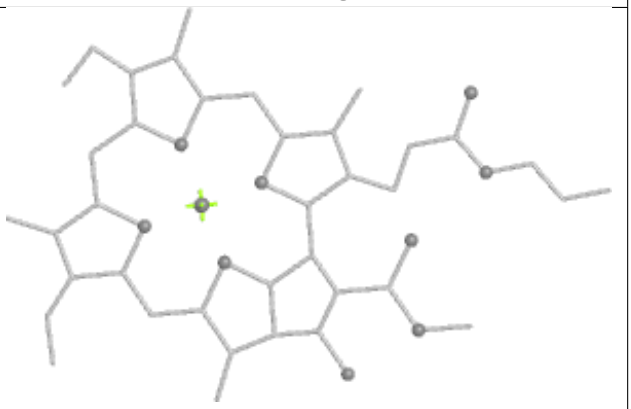
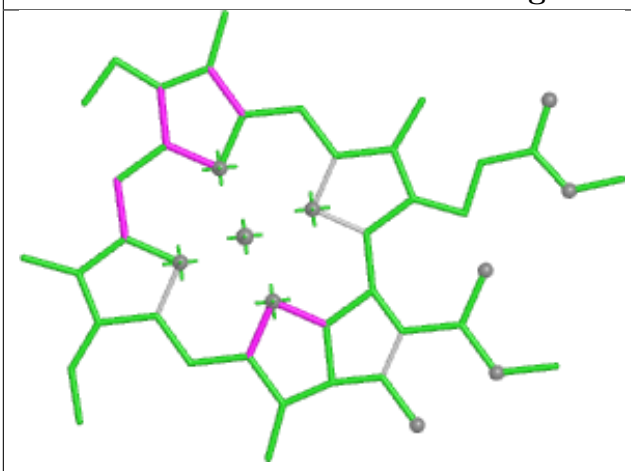


Rings

Ligand CLA 9 311



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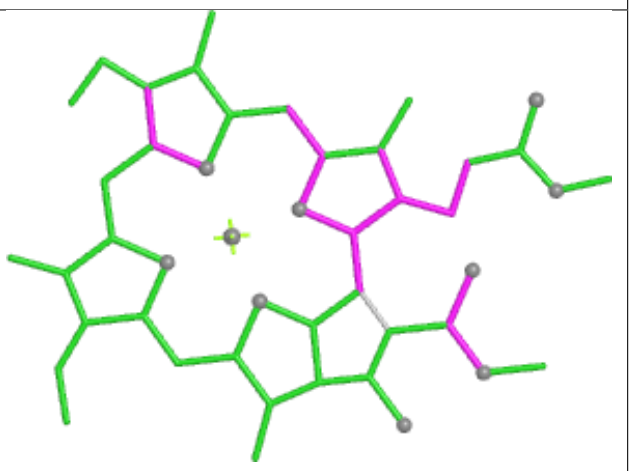

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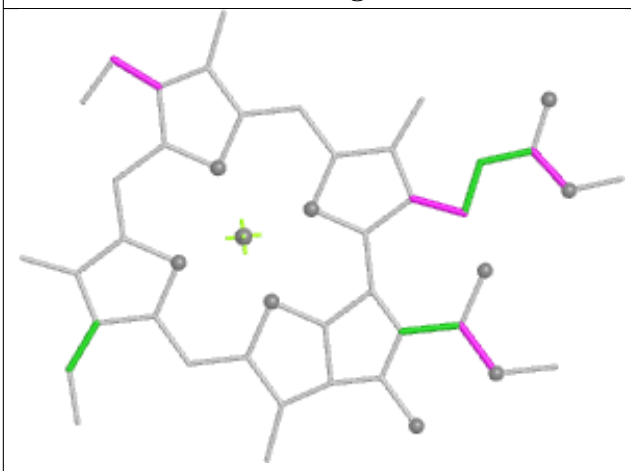

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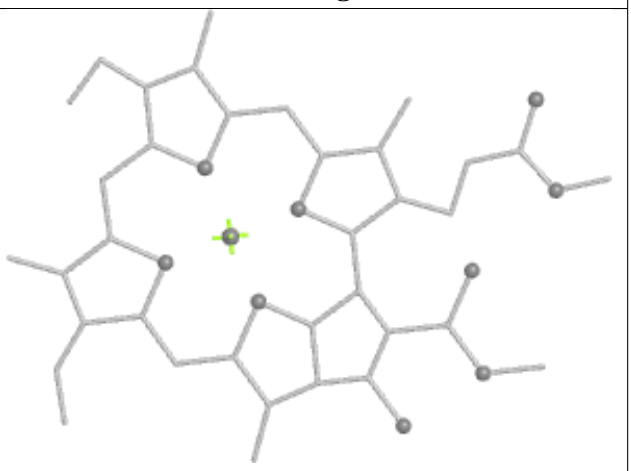
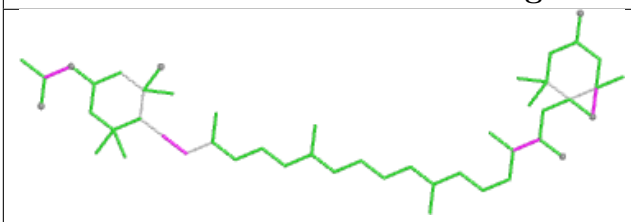


Rings

Ligand A86 11 319



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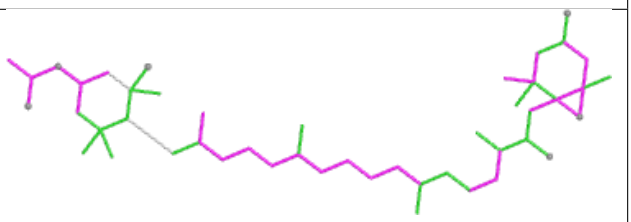

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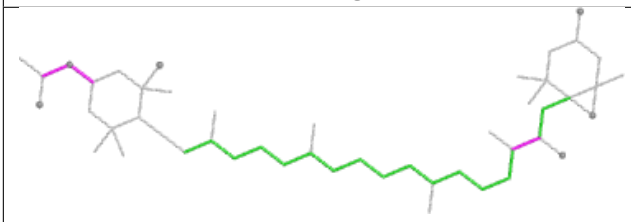

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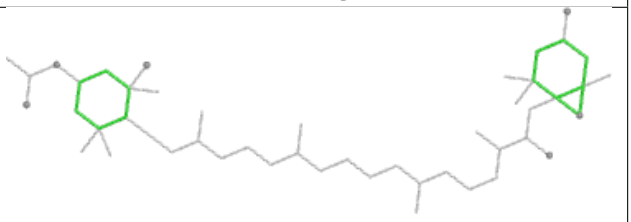
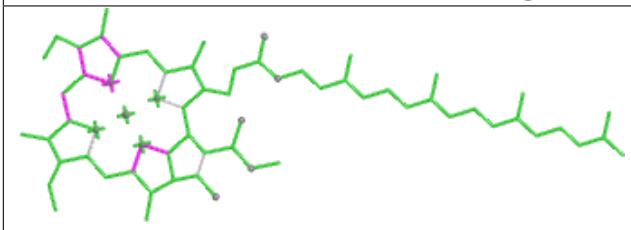


Rings

Ligand CLA 19 310



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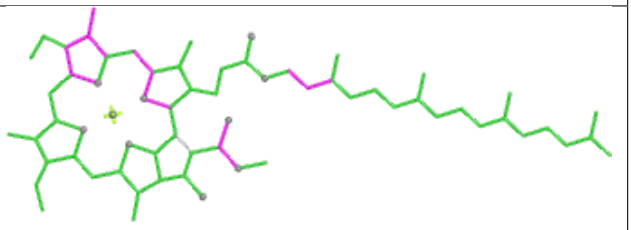

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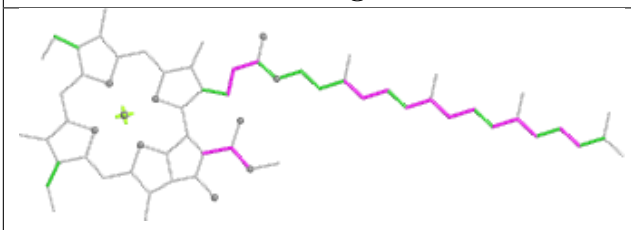

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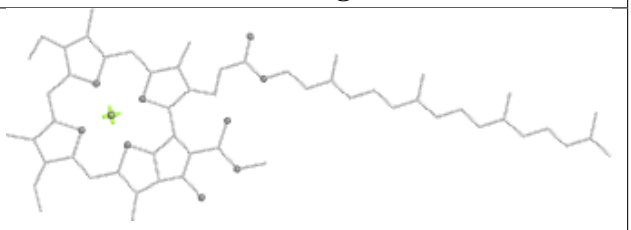
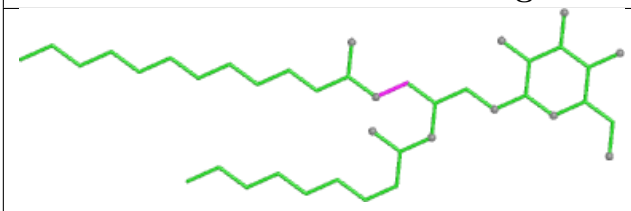


Rings

Ligand LMG M 101



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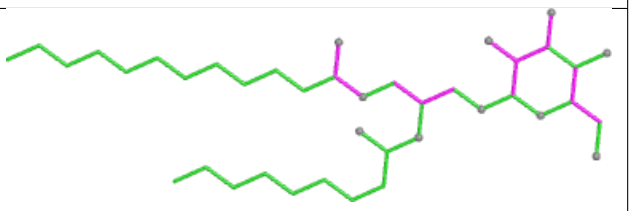

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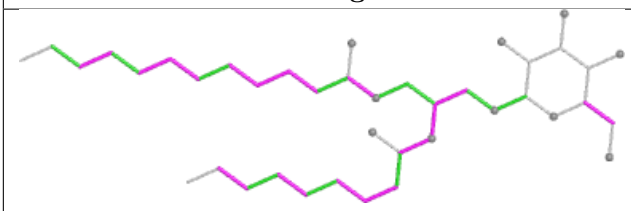

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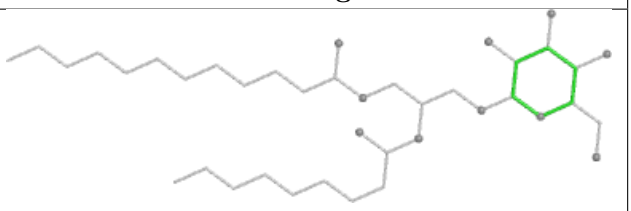
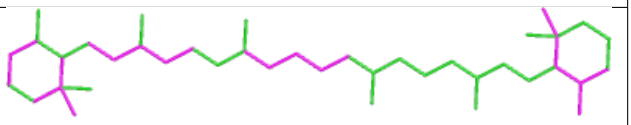


Rings

Ligand BCR b 619



Bond lengths



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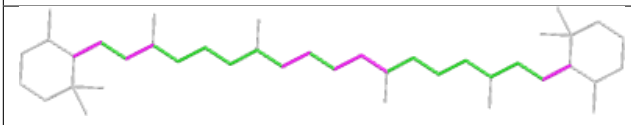

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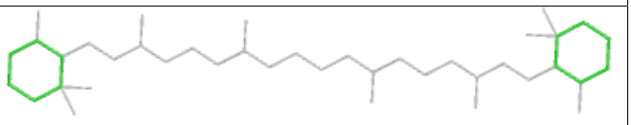
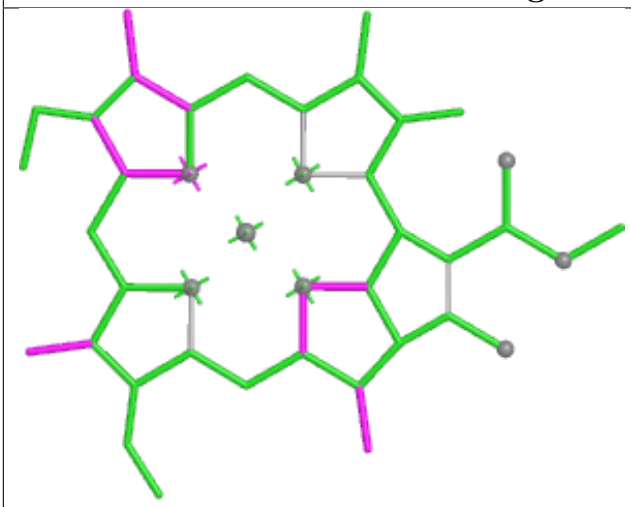


Rings

Ligand CLA p 605



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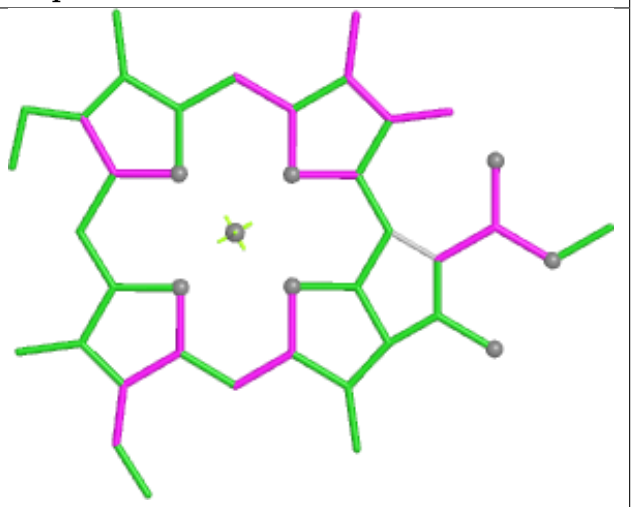

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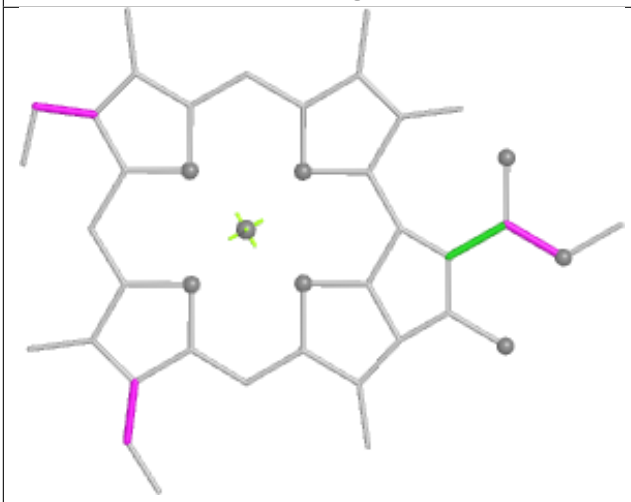

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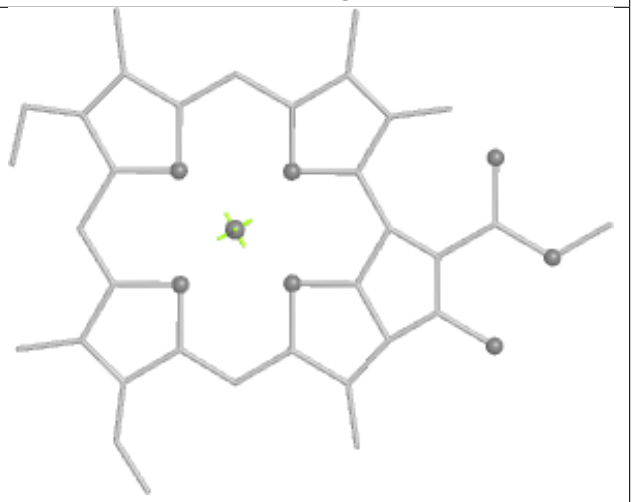
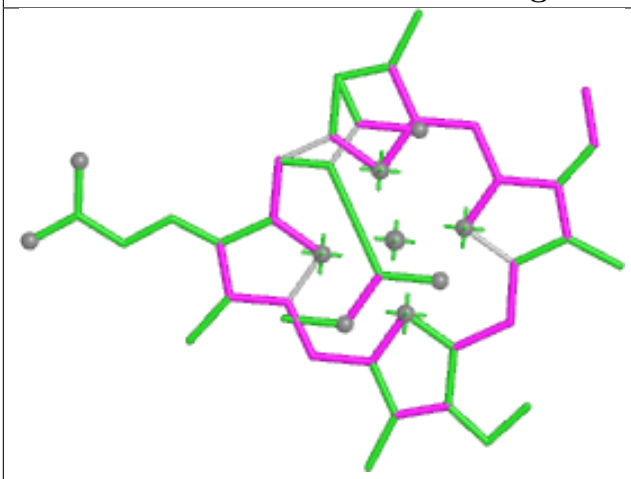


Rings

Ligand KC2 2 308



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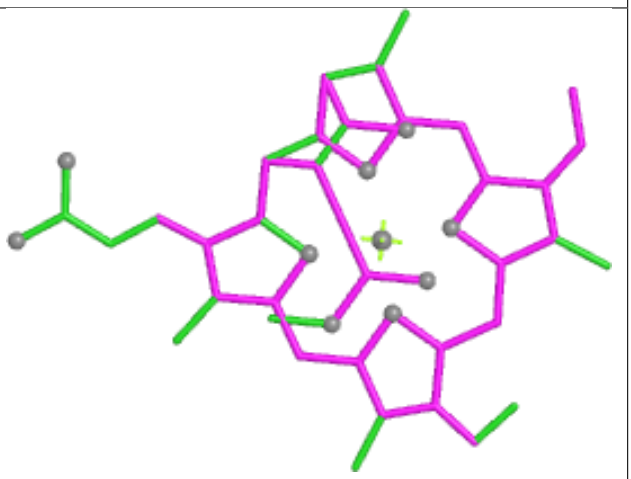

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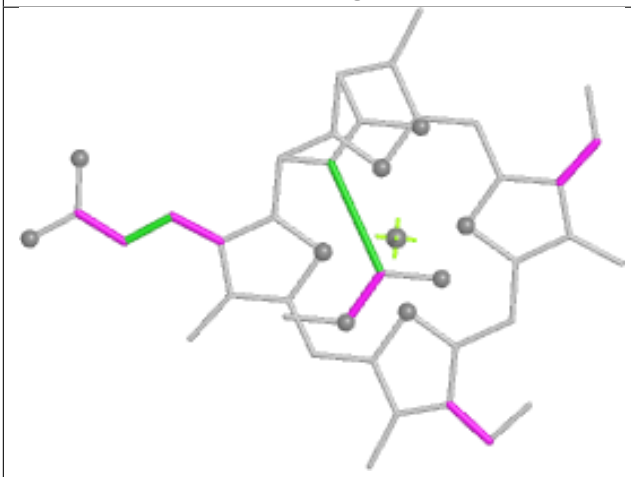

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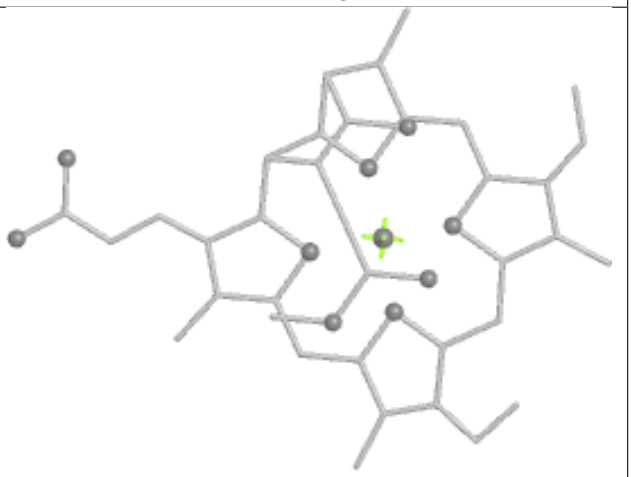
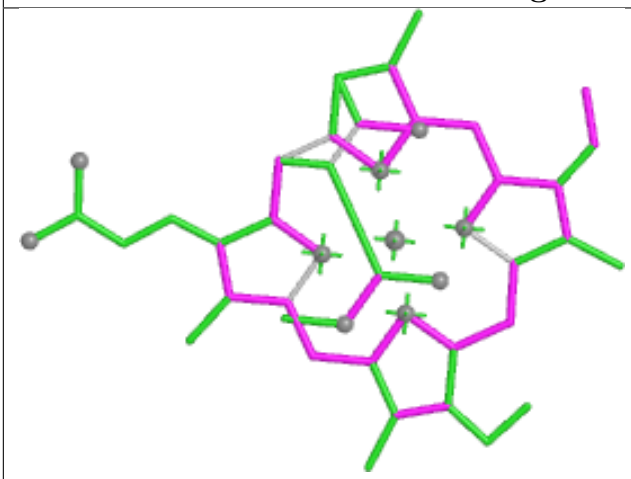


Rings

Ligand KC2 6 310



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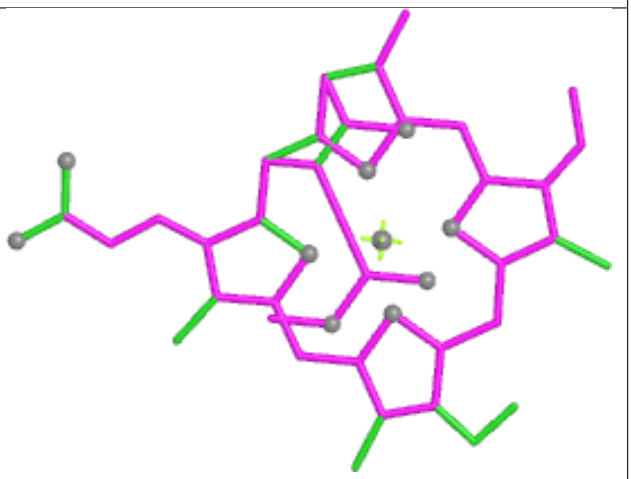
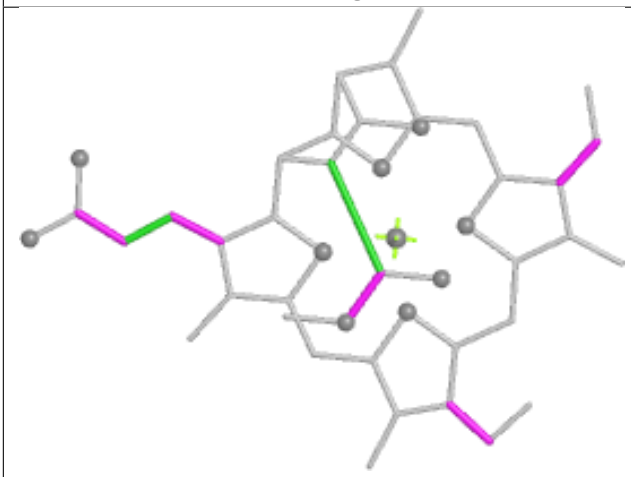


Bond angles



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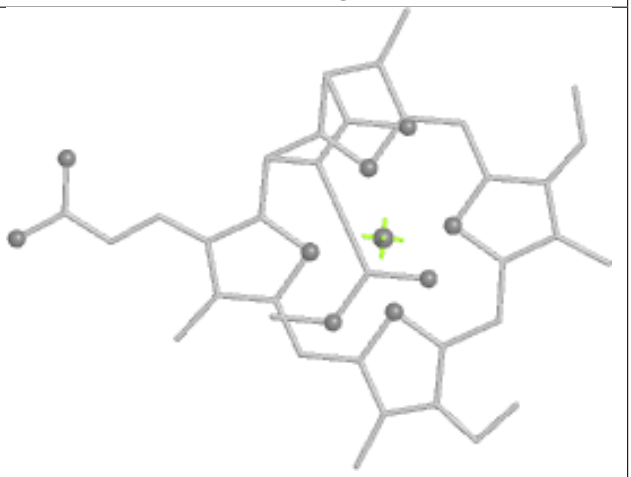
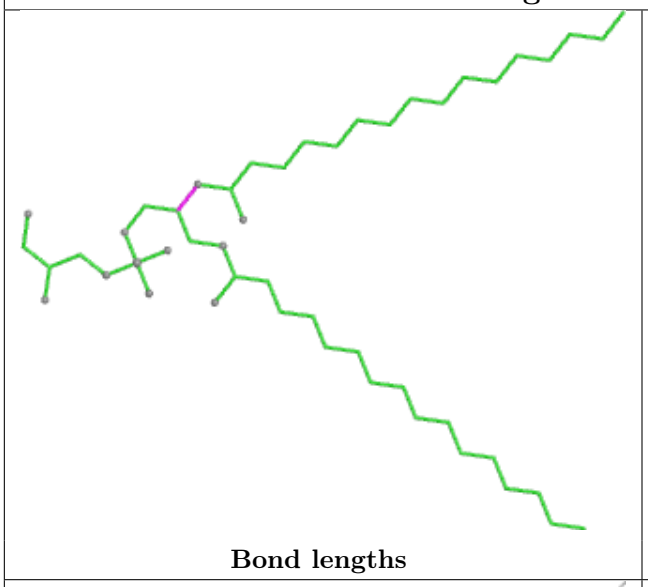


Rings

Ligand LHG D 408



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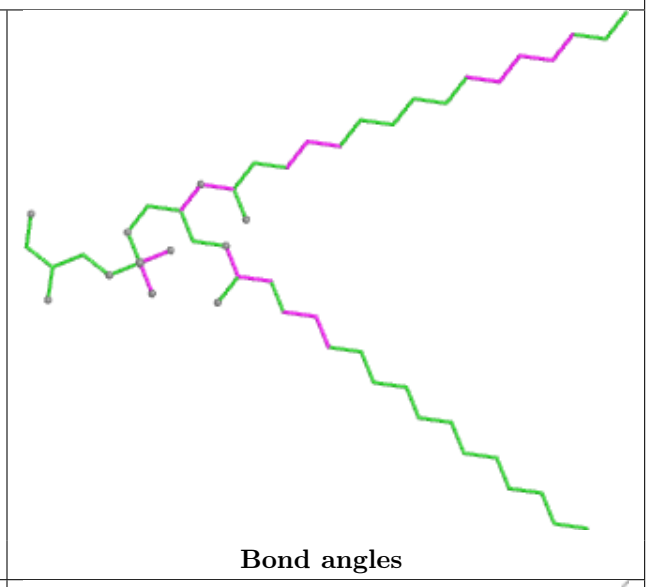
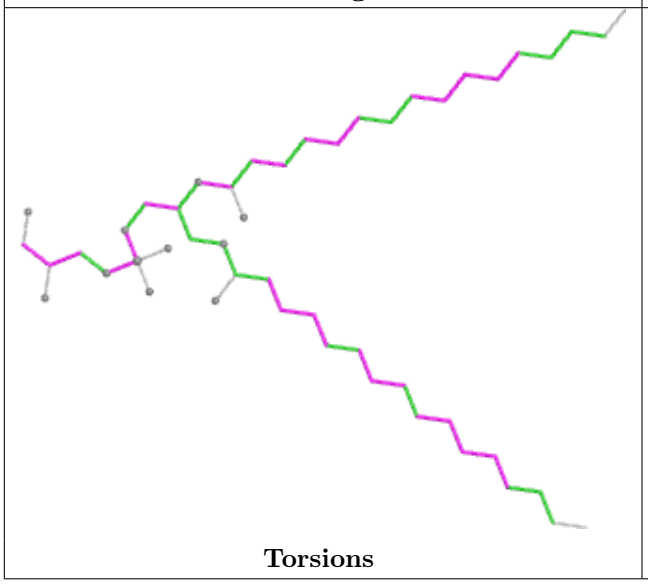


Bond angles



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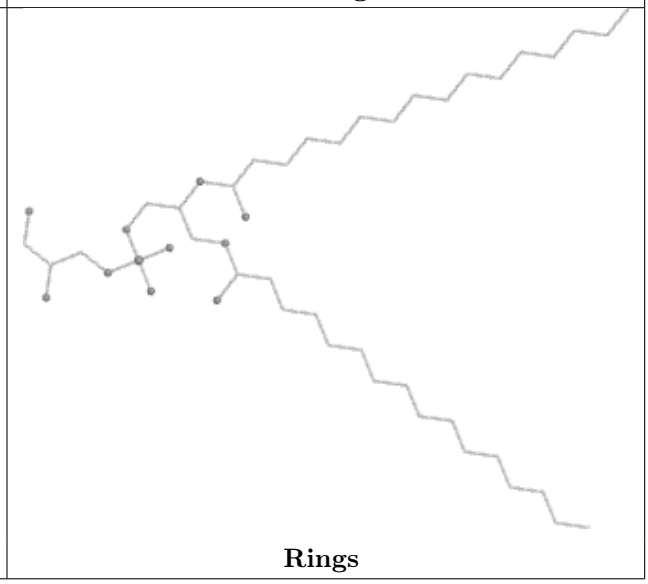
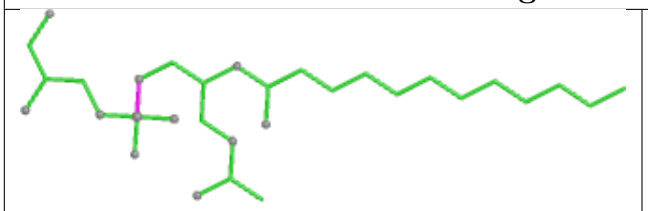


Rings

Ligand LHG 18 316



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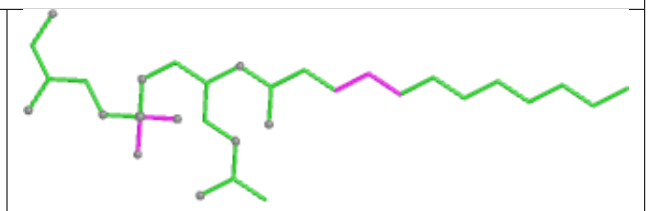

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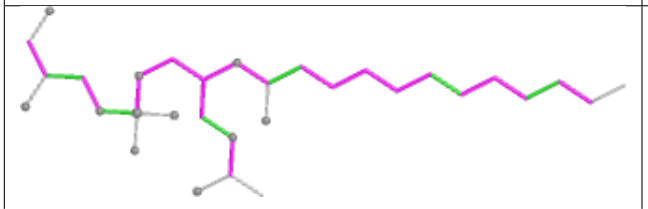

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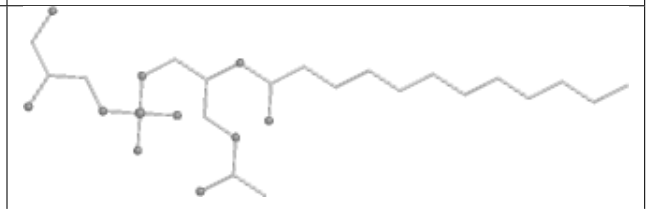
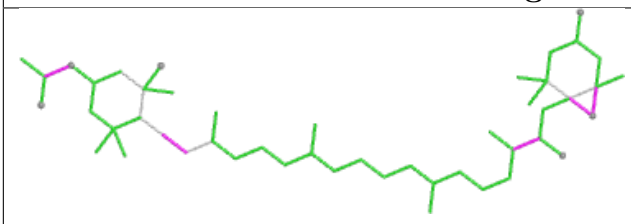


Rings

Ligand A86 18 301



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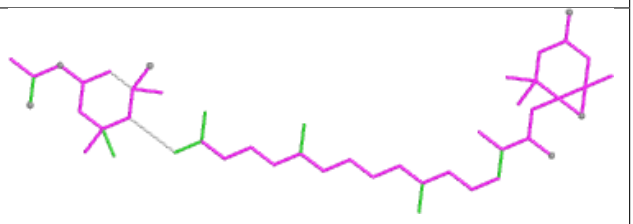
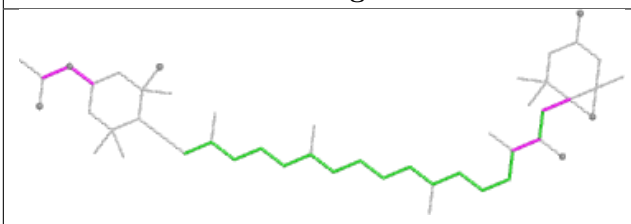


Bond angles



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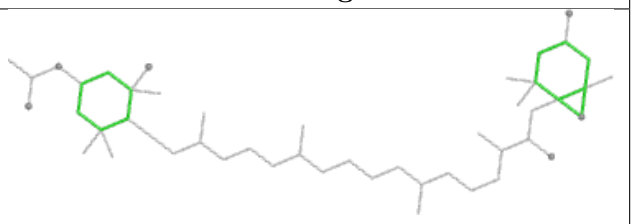
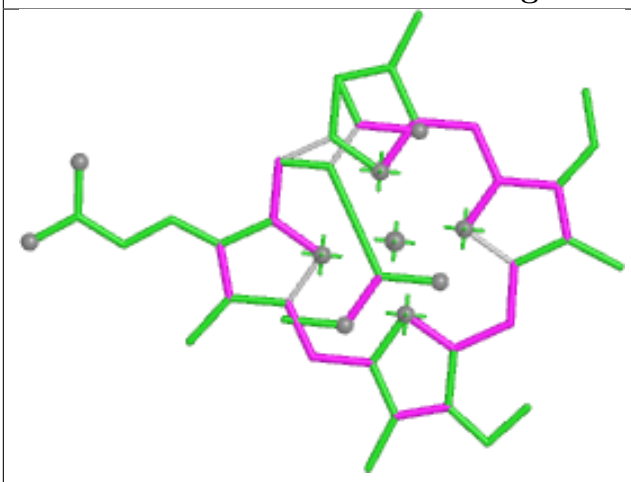


Rings

Ligand KC1 12 314



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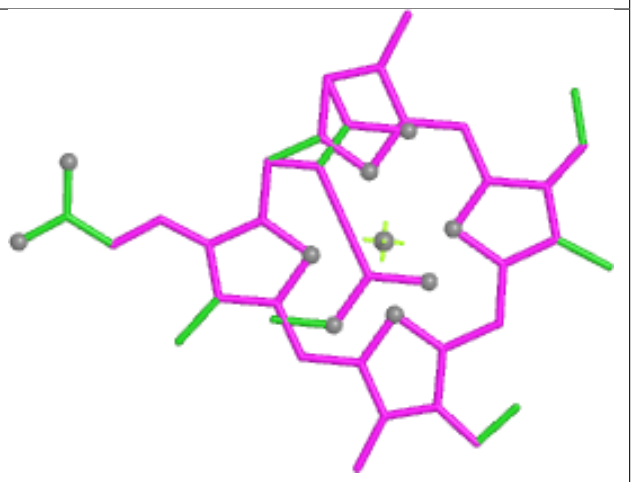
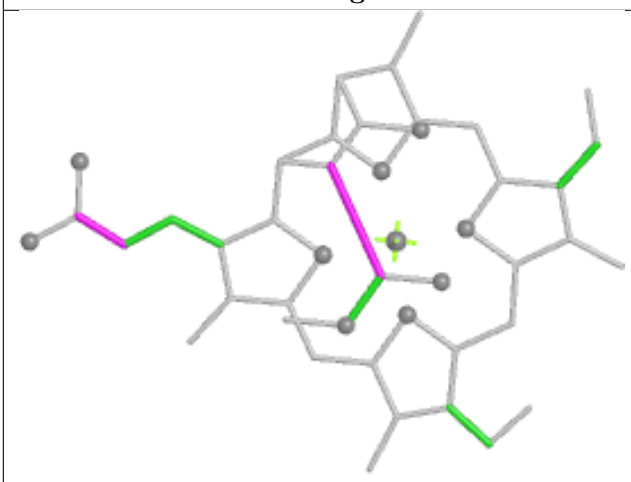


Bond angles



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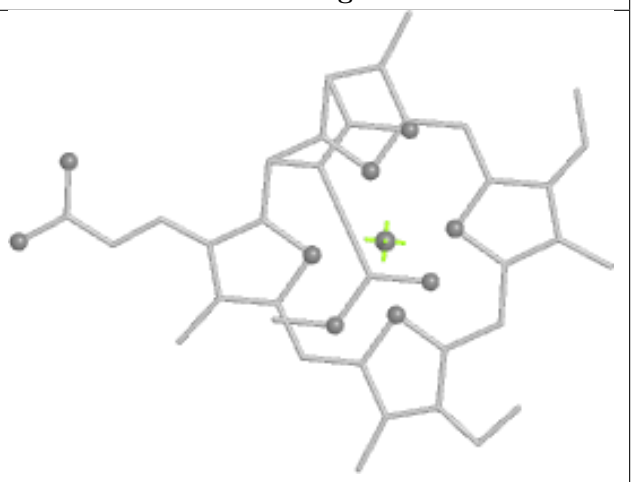
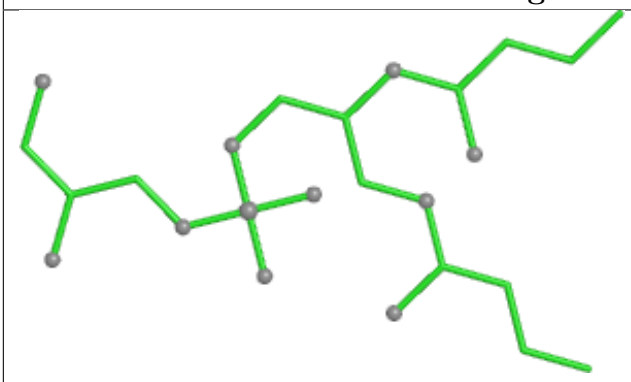


Rings

Ligand LHG z 102



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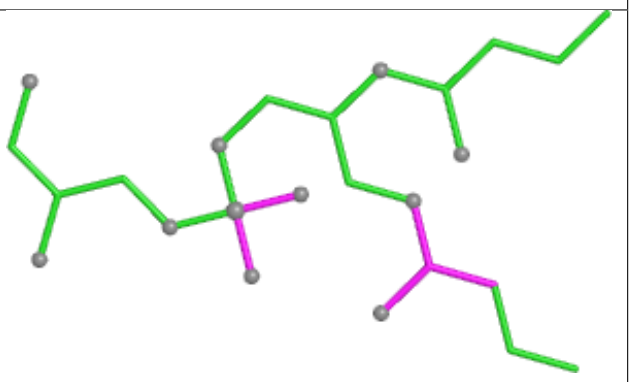
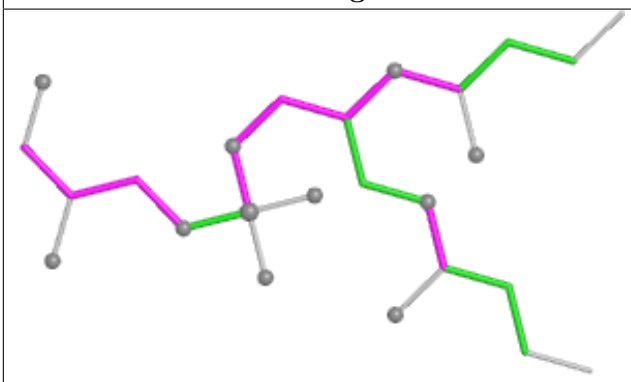


Bond angles



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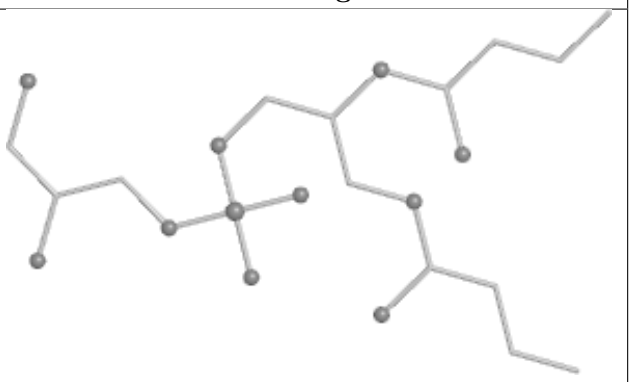
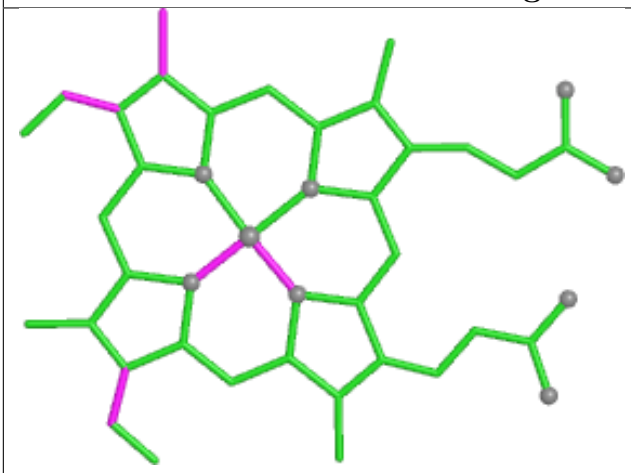


Rings

Ligand HEM e 101



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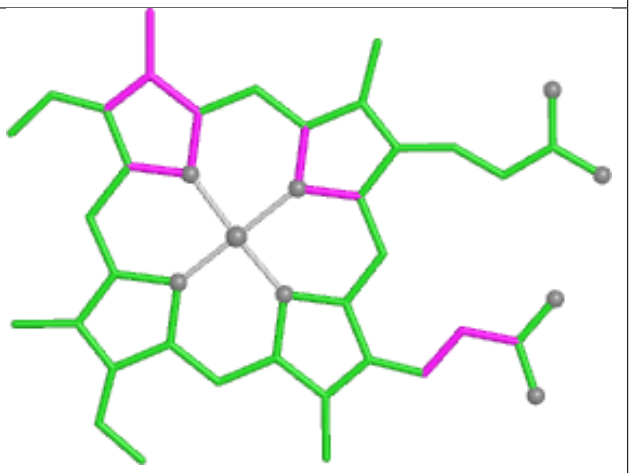
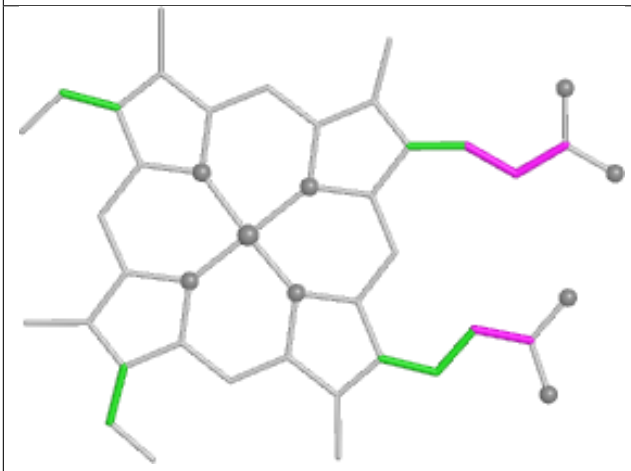


Bond angles



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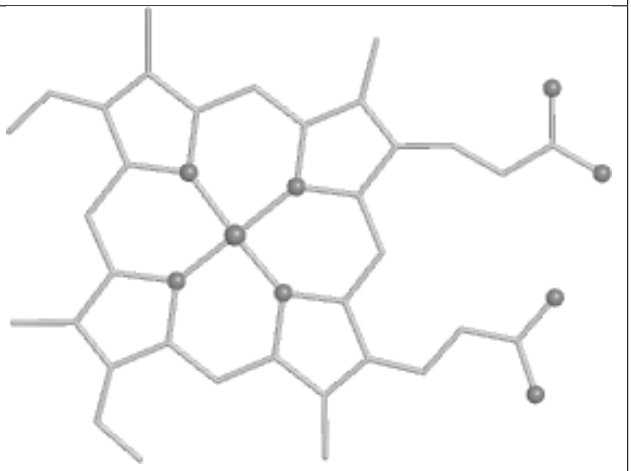
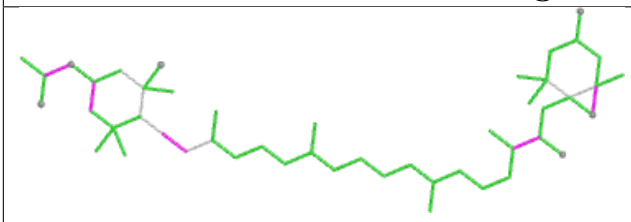


Rings

Ligand A86 5 301



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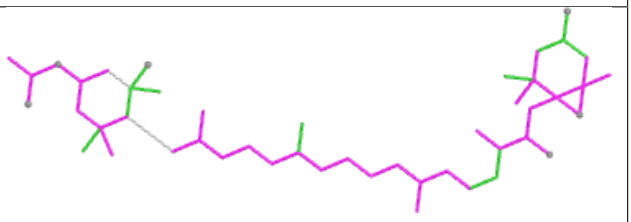

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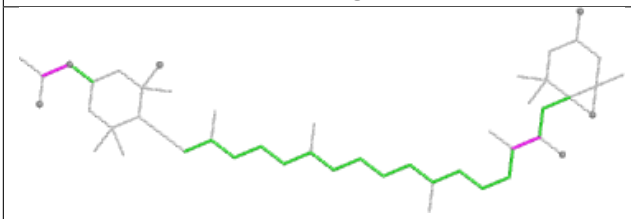

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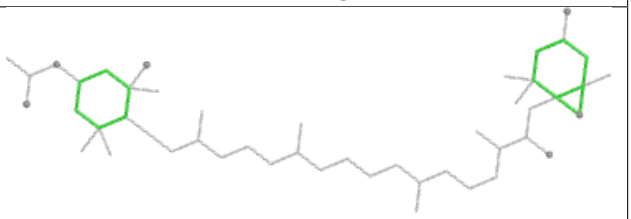

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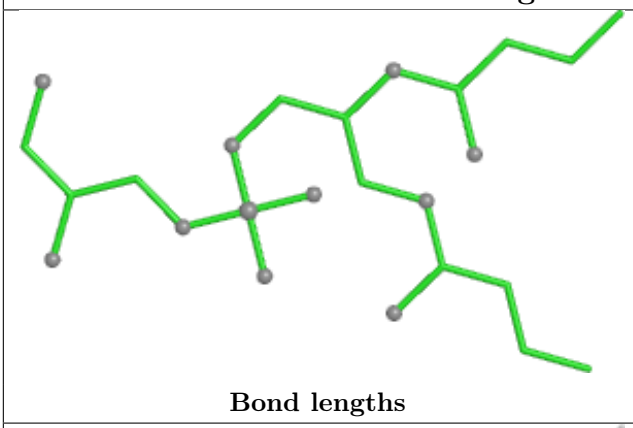

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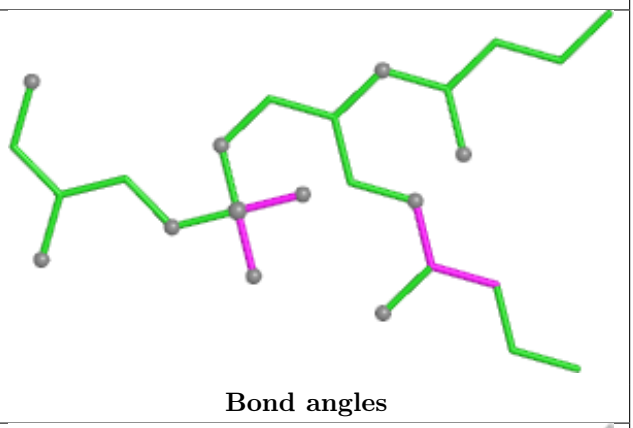

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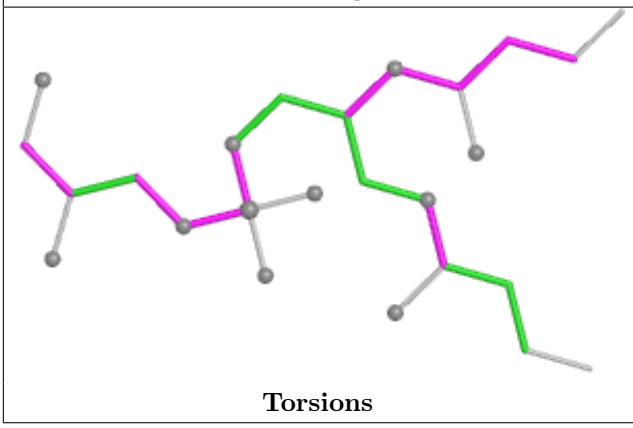

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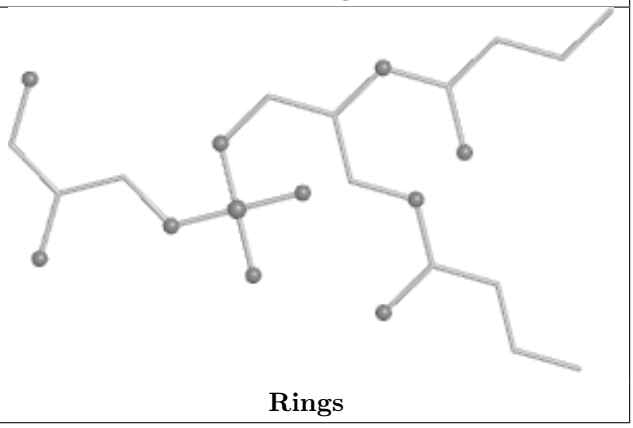

Rings

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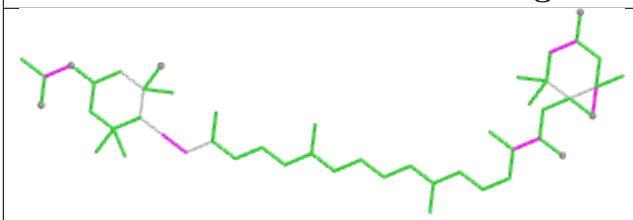

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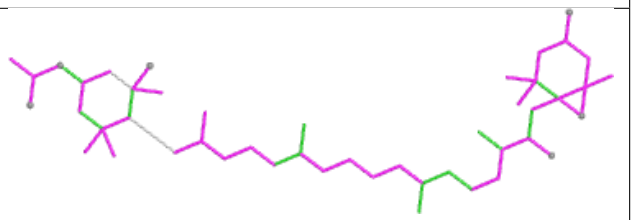

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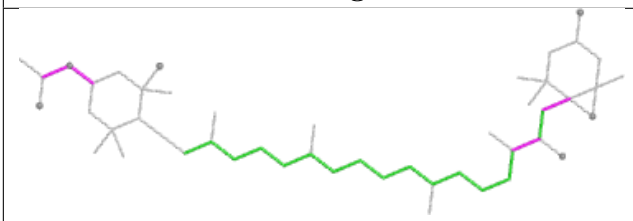

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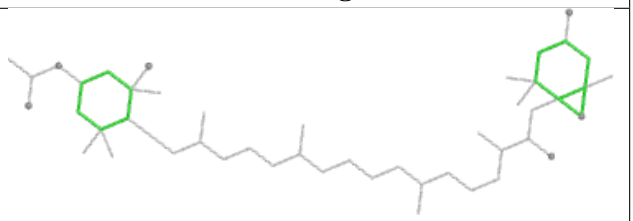

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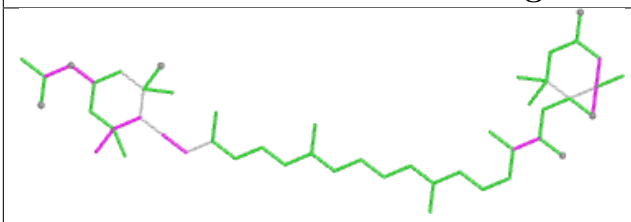

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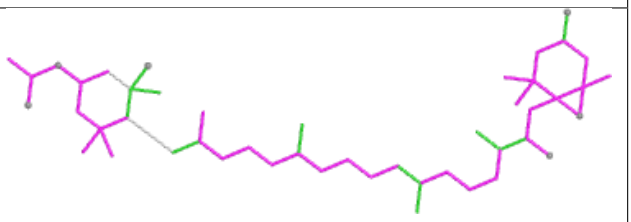

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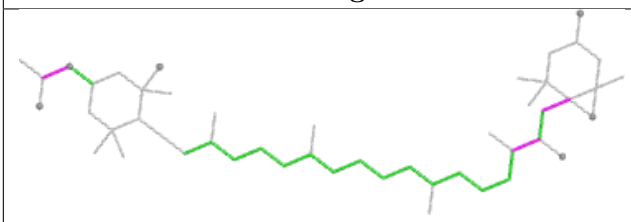

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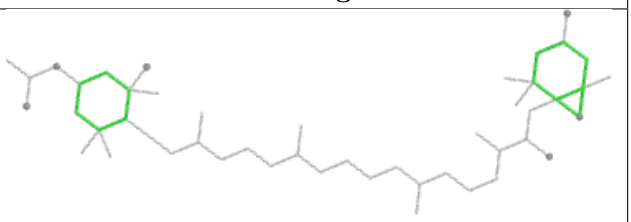

Rings

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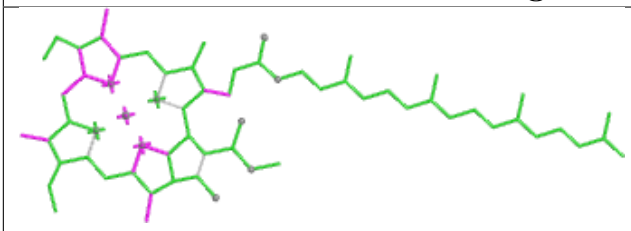

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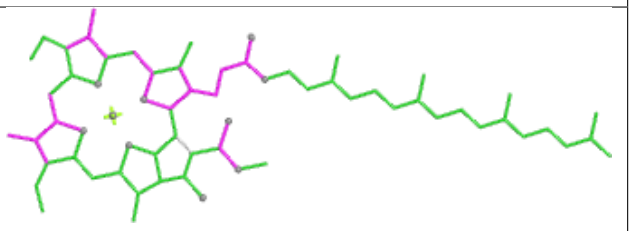

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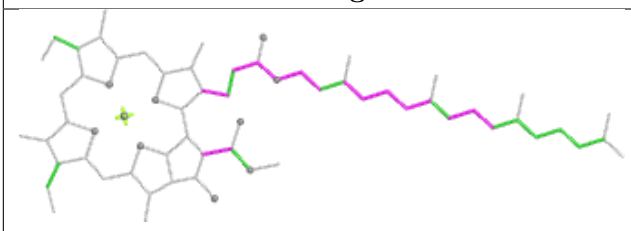

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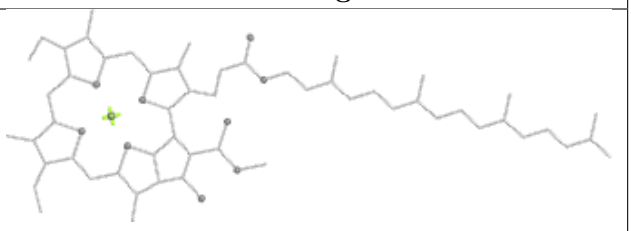

Rings

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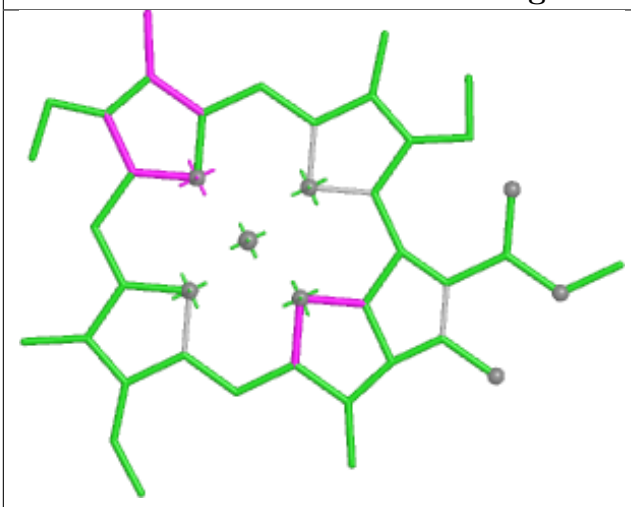

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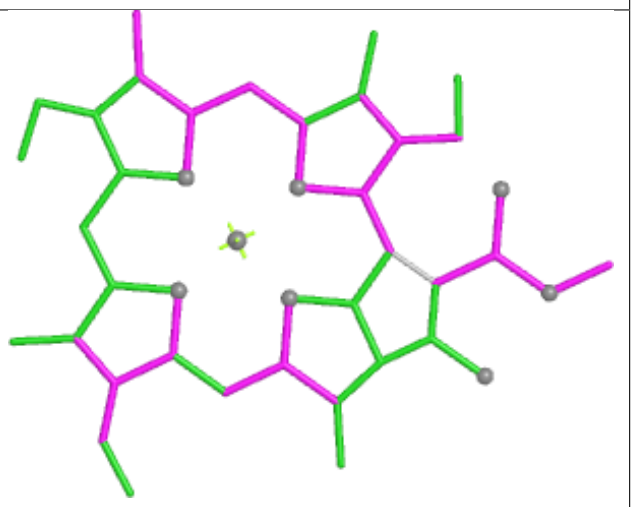

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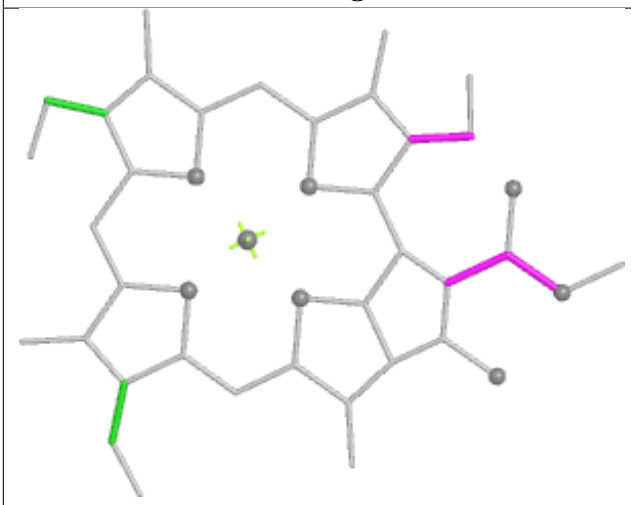
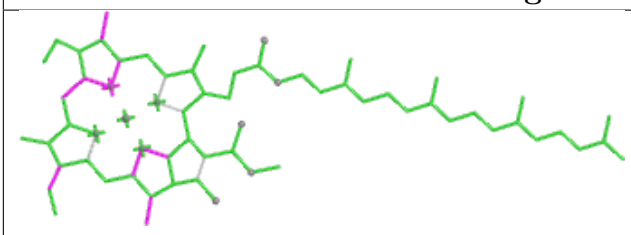


Torsions



Rings

Ligand CLA B 603



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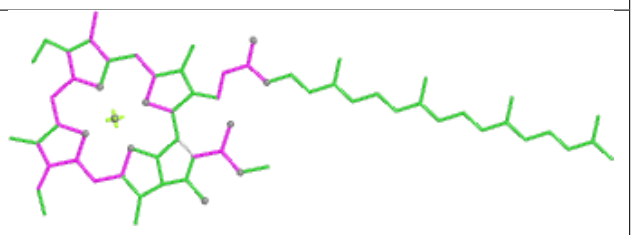

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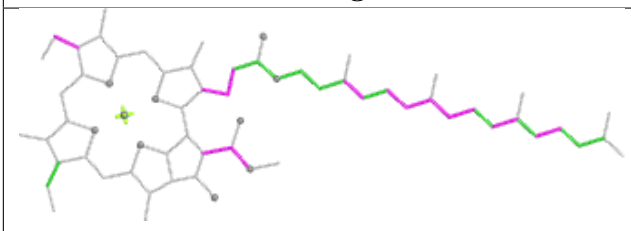

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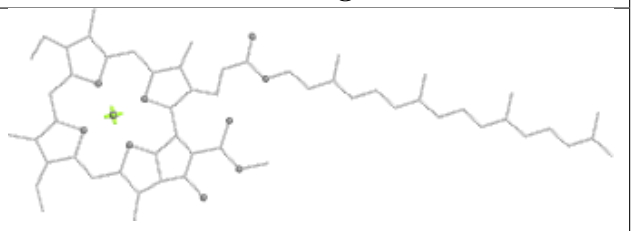

Rings

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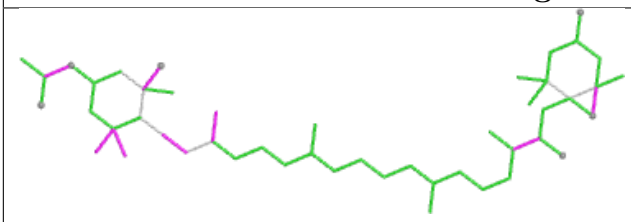

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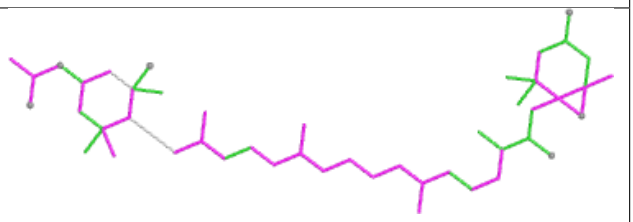

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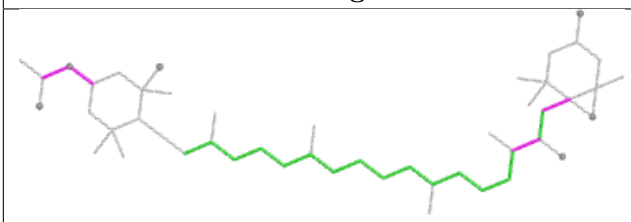

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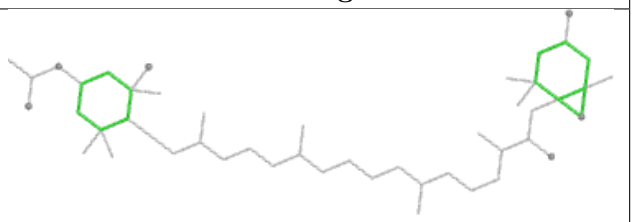

Rings

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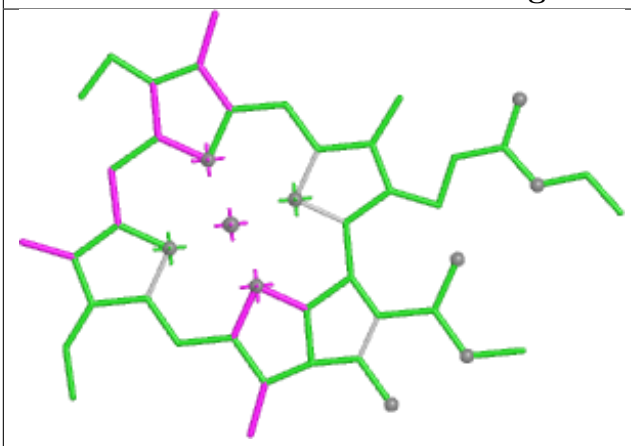

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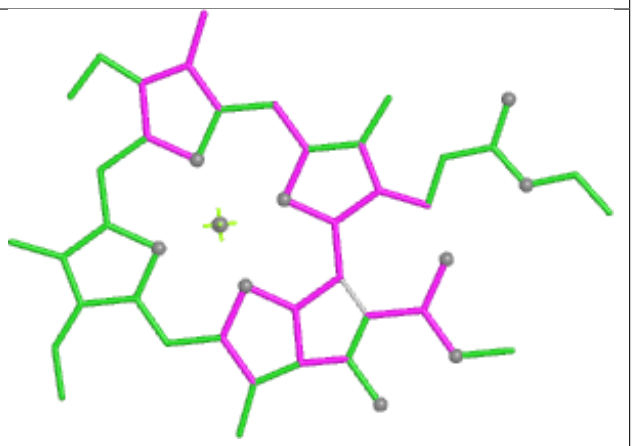

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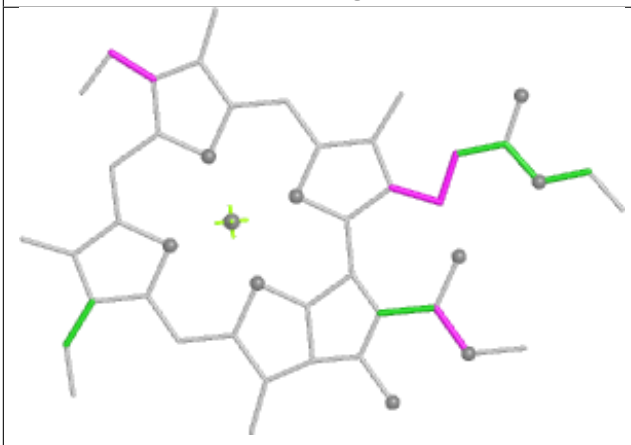

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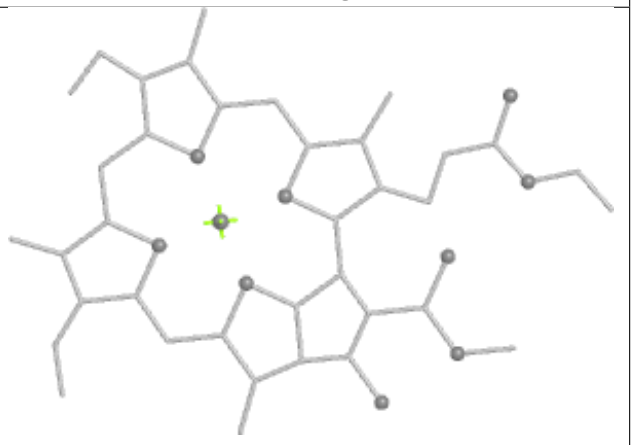

Rings

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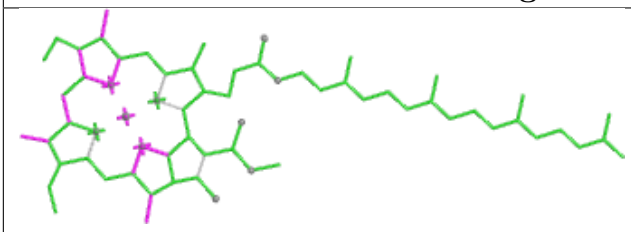

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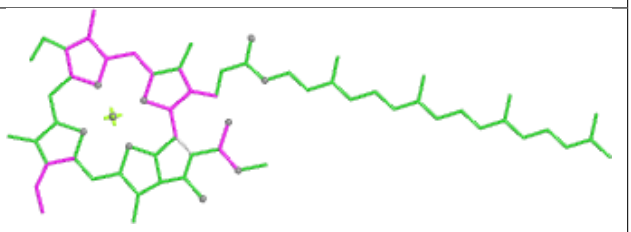

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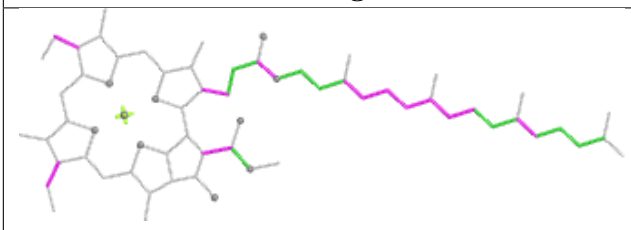

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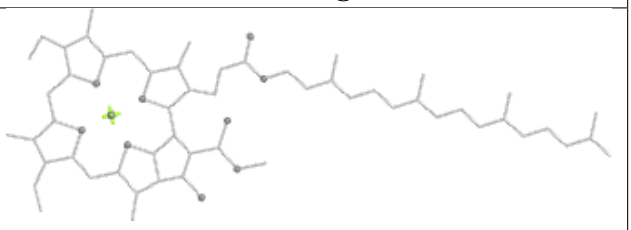

Rings

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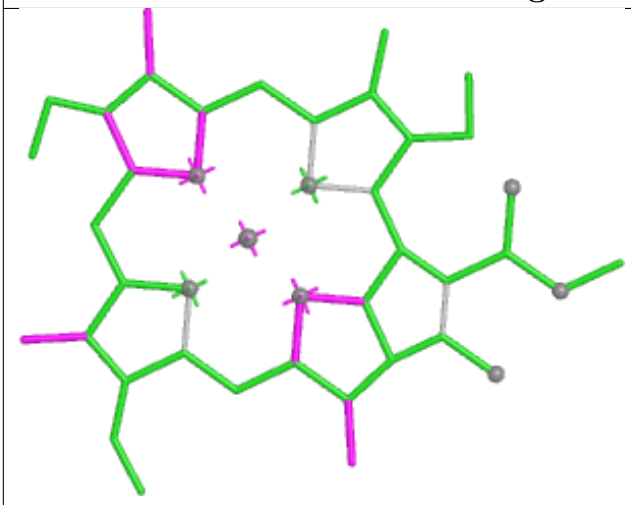

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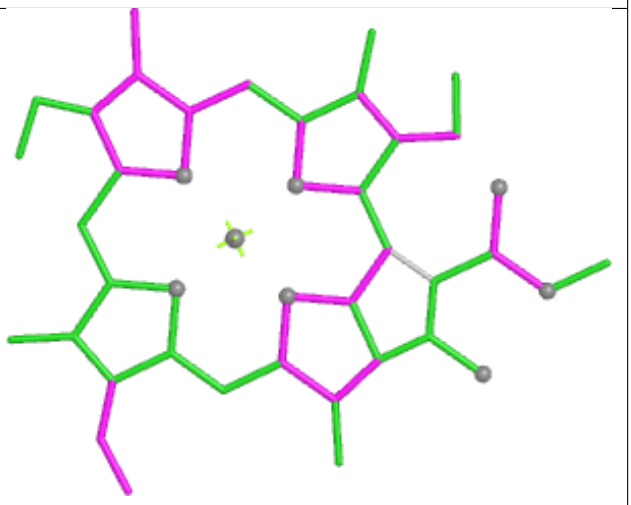

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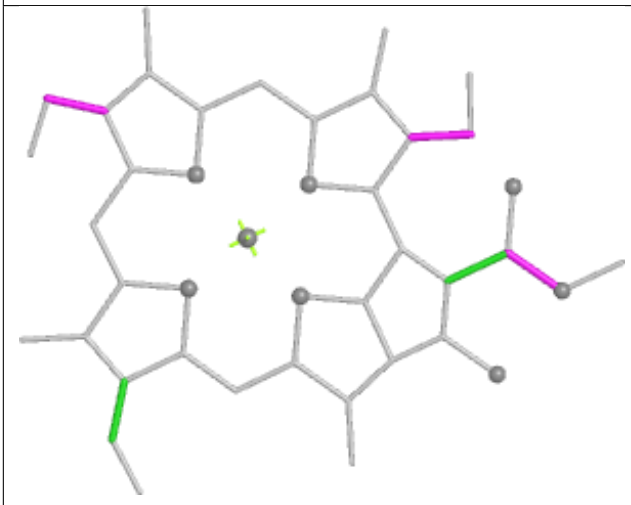

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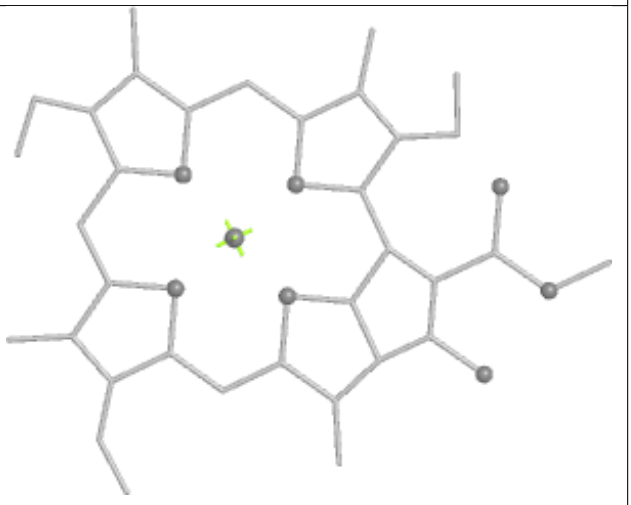
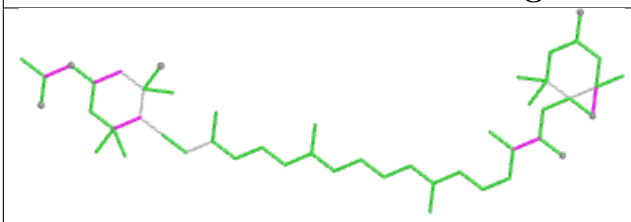


Rings

Ligand A86 14 304



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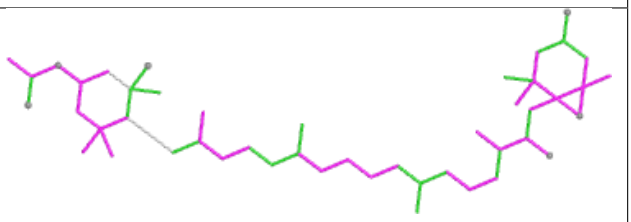

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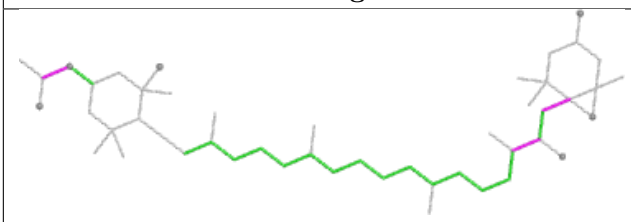

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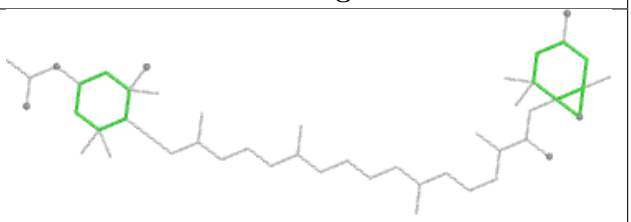

Rings

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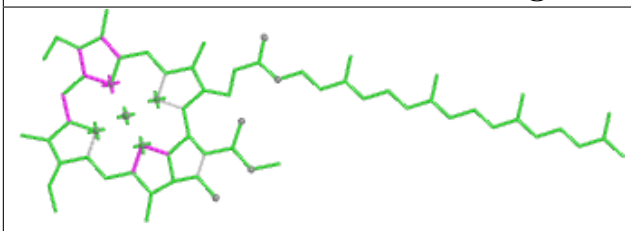

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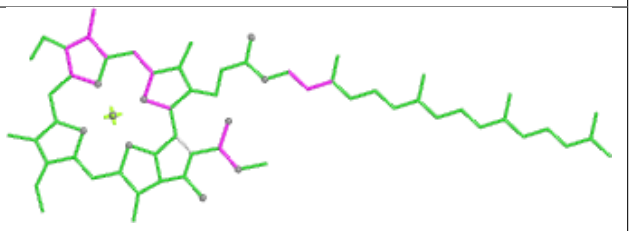
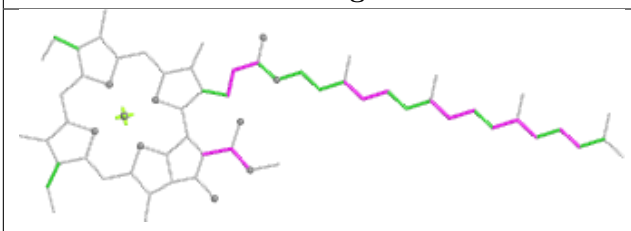


Bond angles



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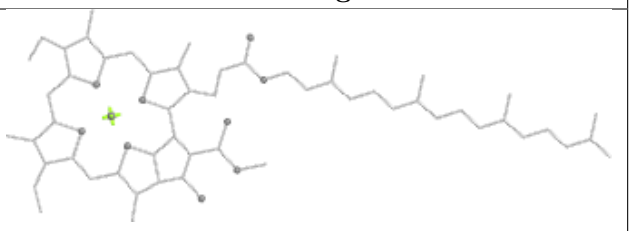
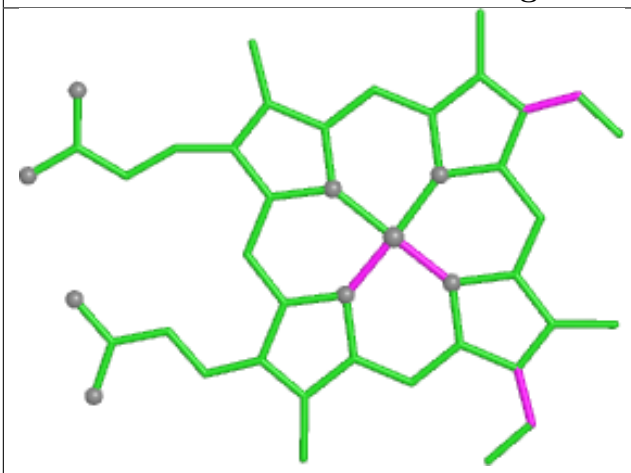


Rings

Ligand HEM E 101



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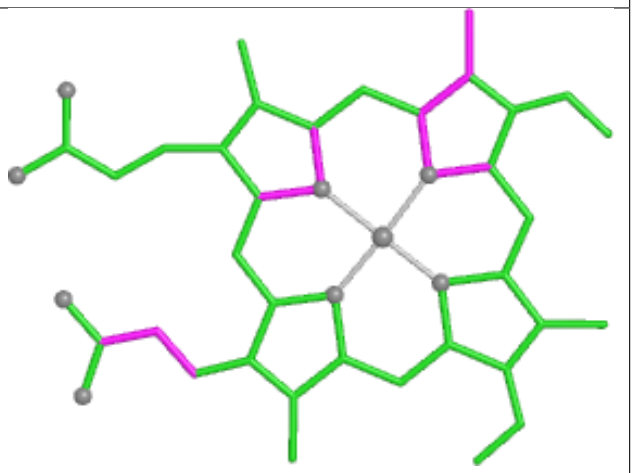
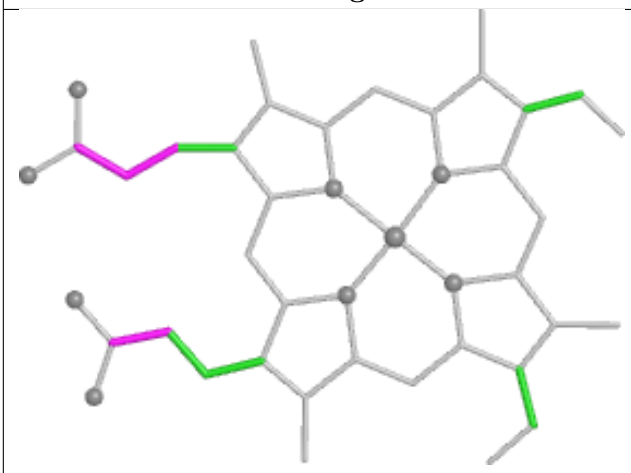


Bond angles



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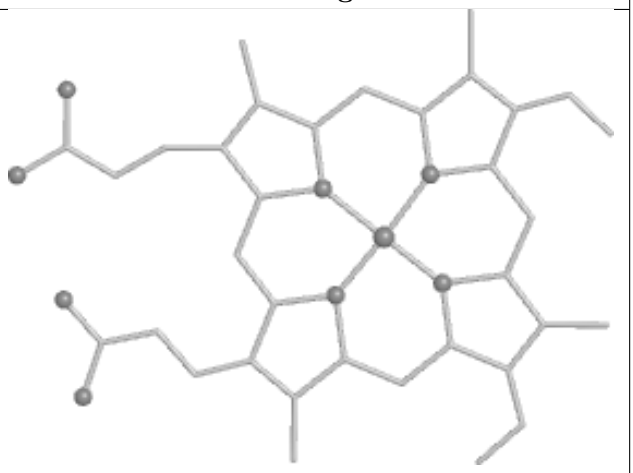
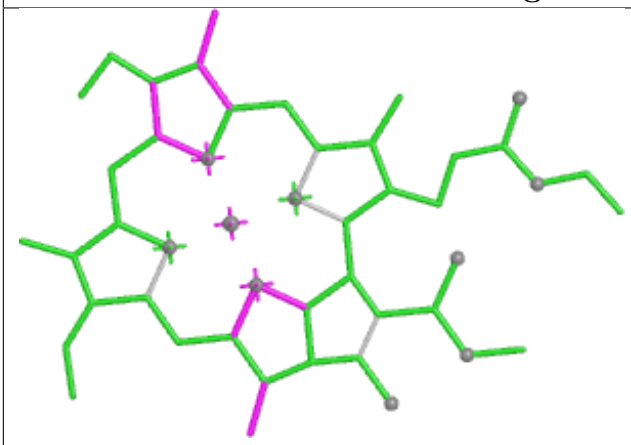


Rings

Ligand CLA R 101



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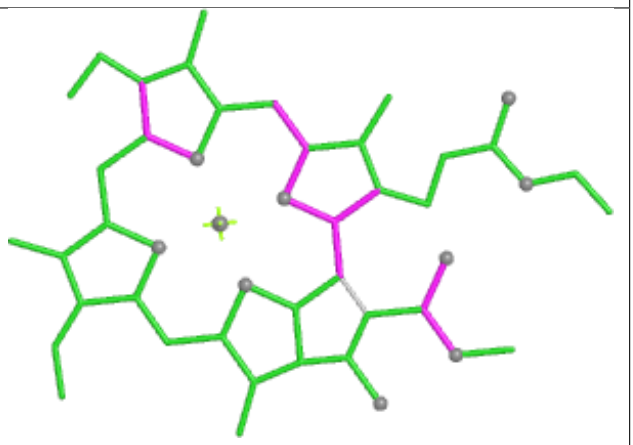
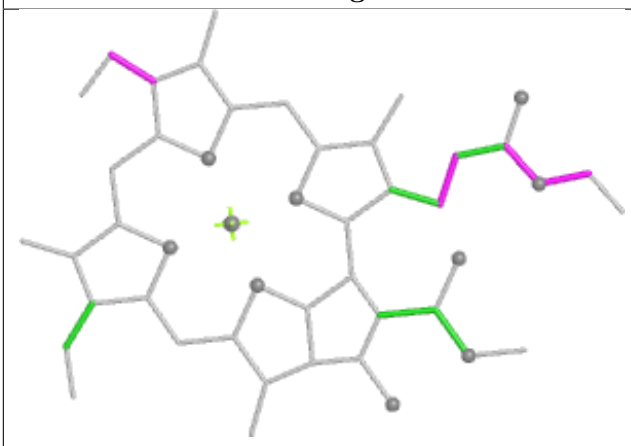
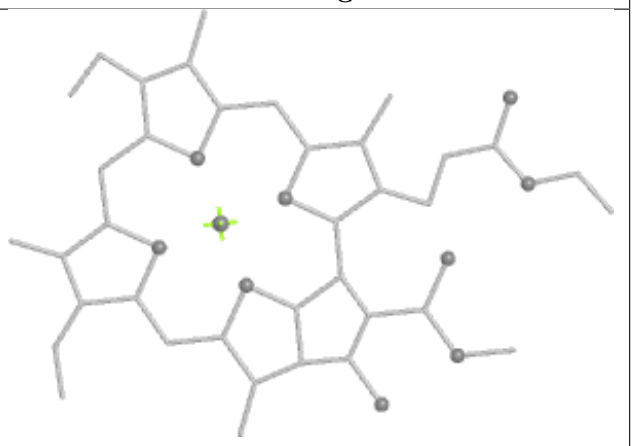


Bond angles



Torsions

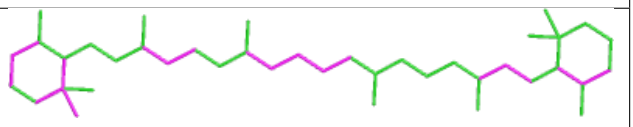


Rings

Ligand BCR C 515



Bond lengths



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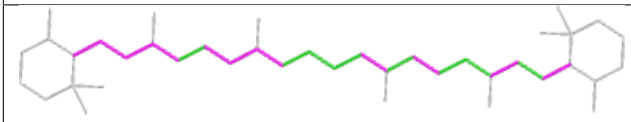

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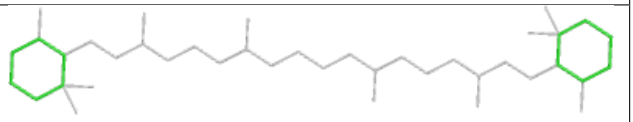
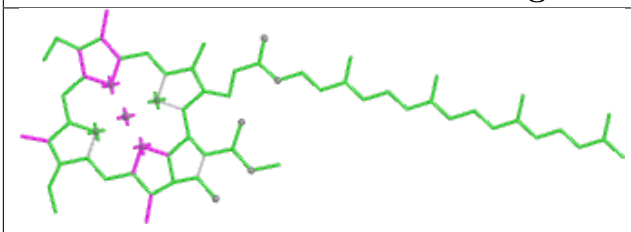


Rings

Ligand CLA 5 307



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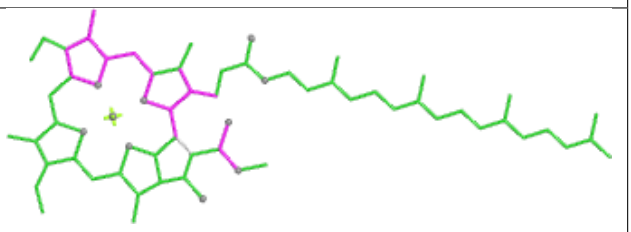

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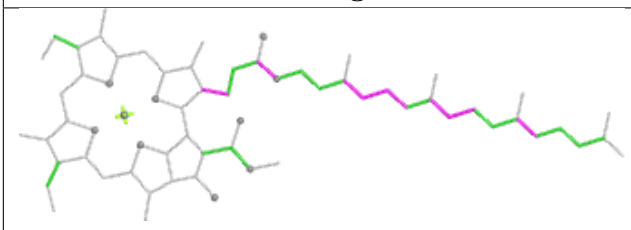

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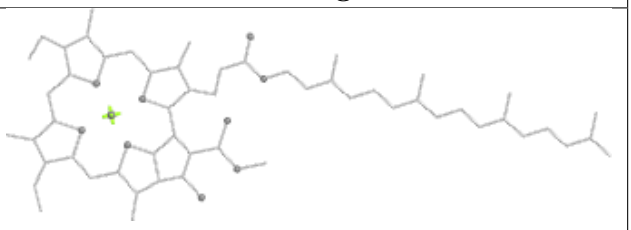
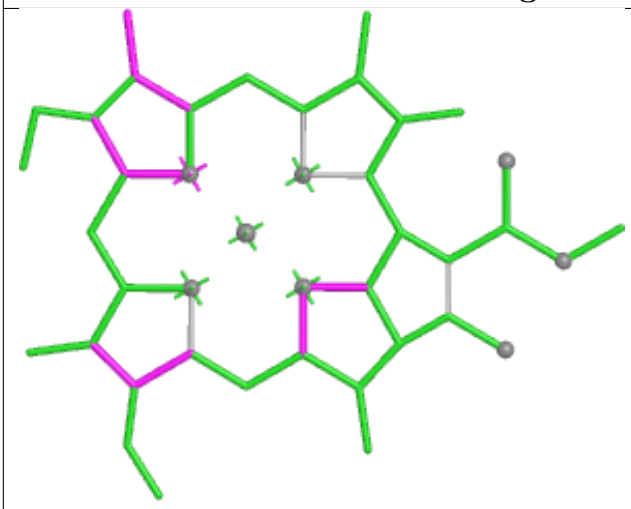


Rings

Ligand CLA 11 315



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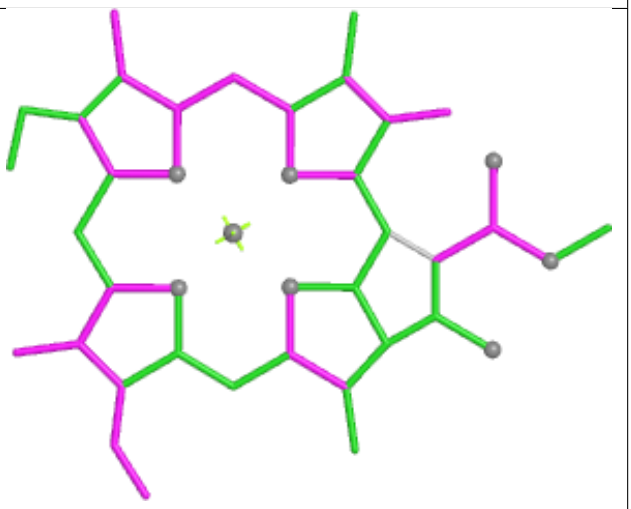

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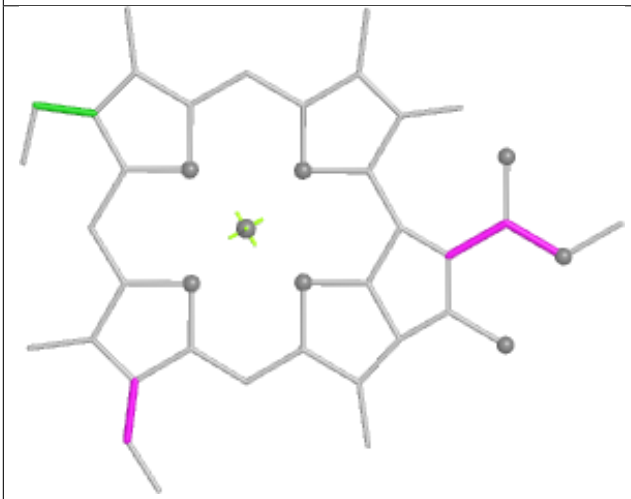

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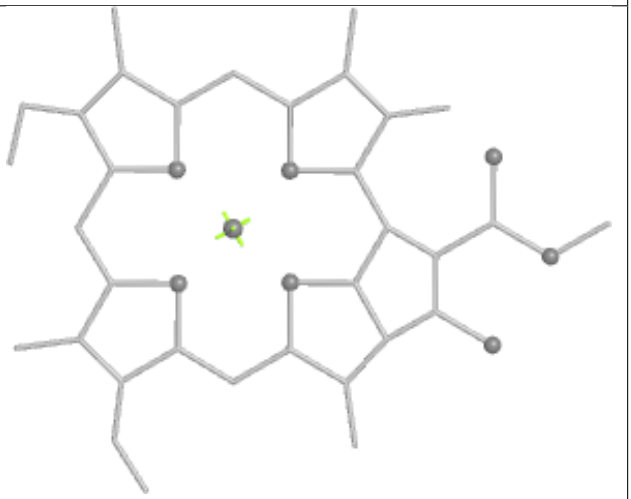
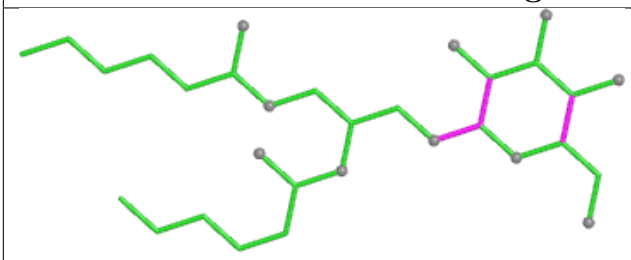


Rings

Ligand LMG c 522



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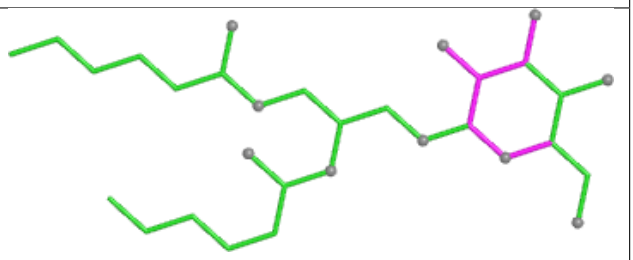

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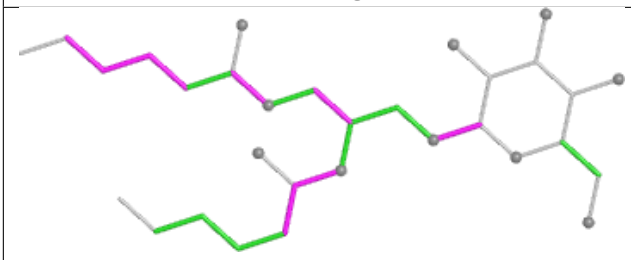

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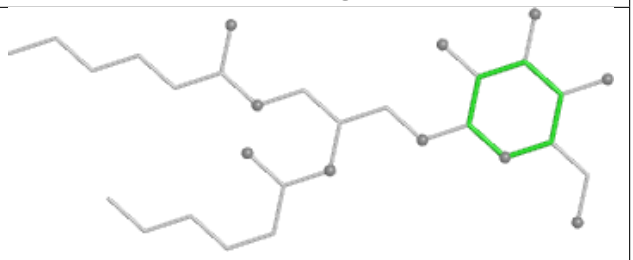
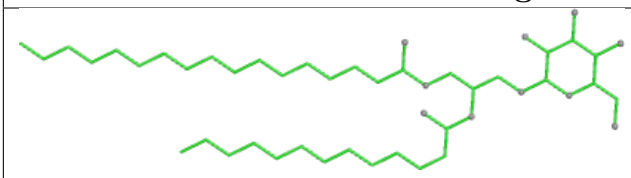


Rings

Ligand LMG 14 316



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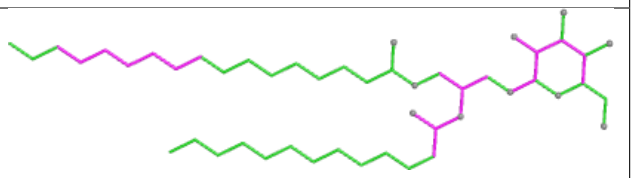

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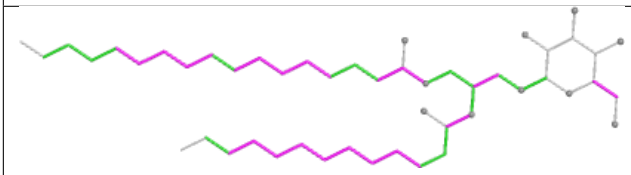

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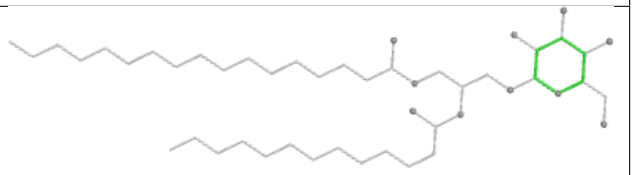
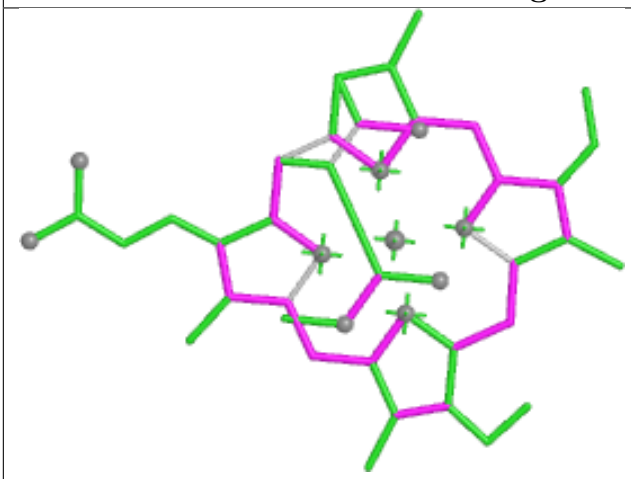


Rings

Ligand KC1 2 313



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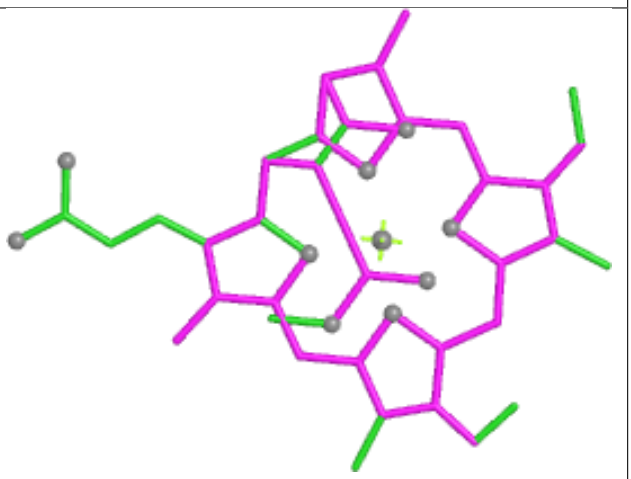
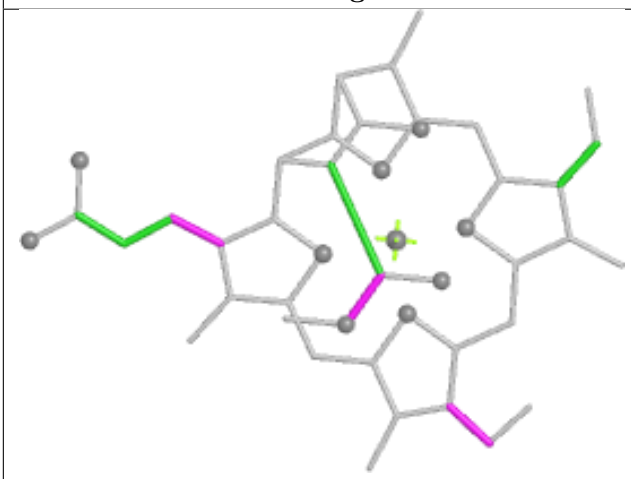


Bond angles



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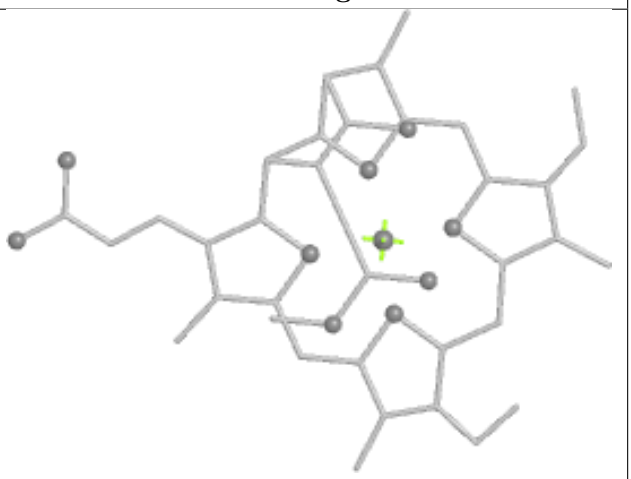
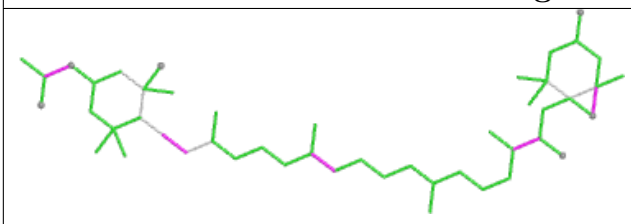


Rings

Ligand A86 2 301



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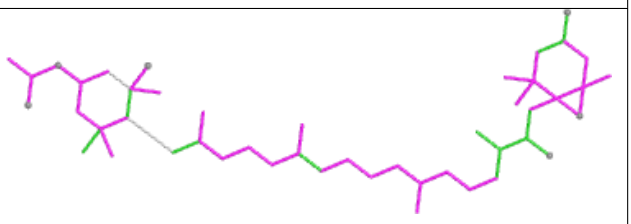

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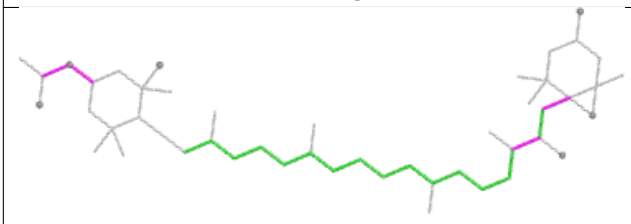

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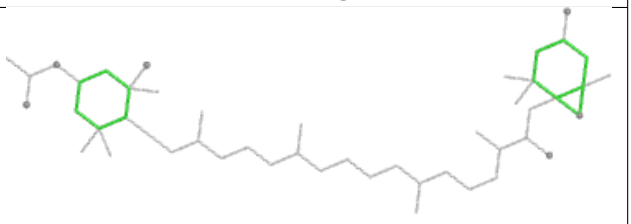
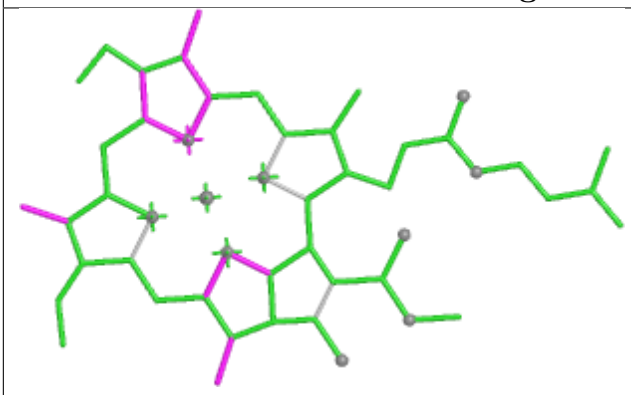


Rings

Ligand CLA 10 308



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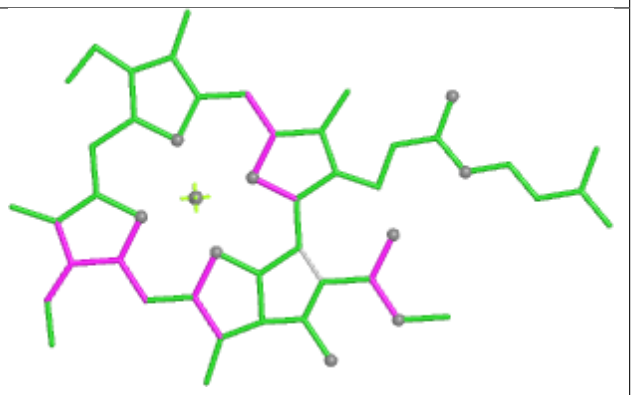

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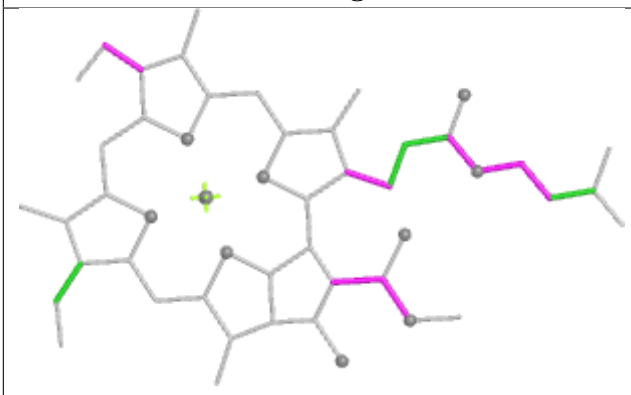

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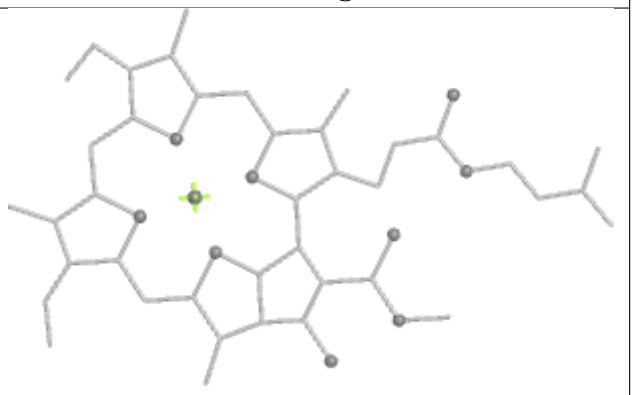
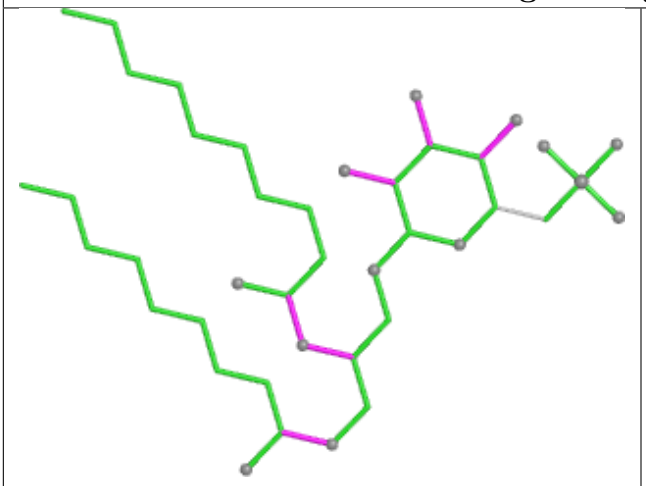


Rings

Ligand SQD 10 320



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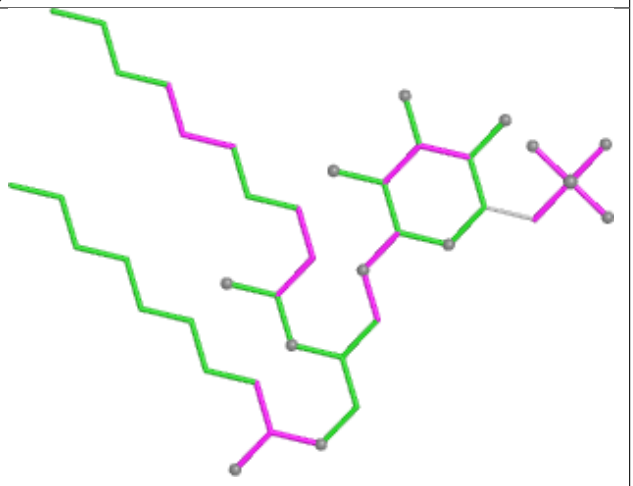
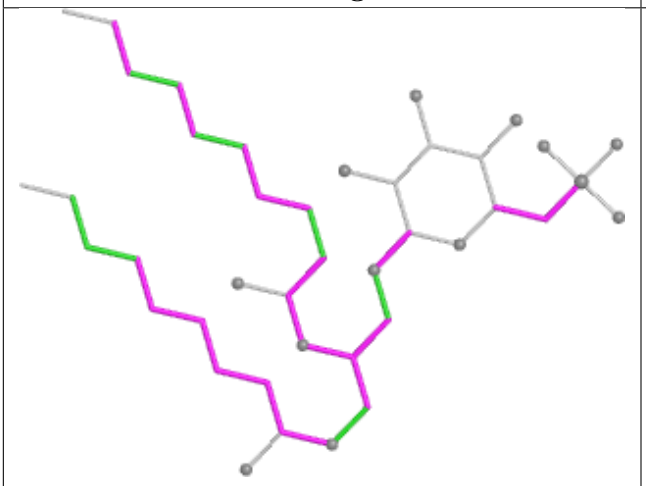


Bond angles



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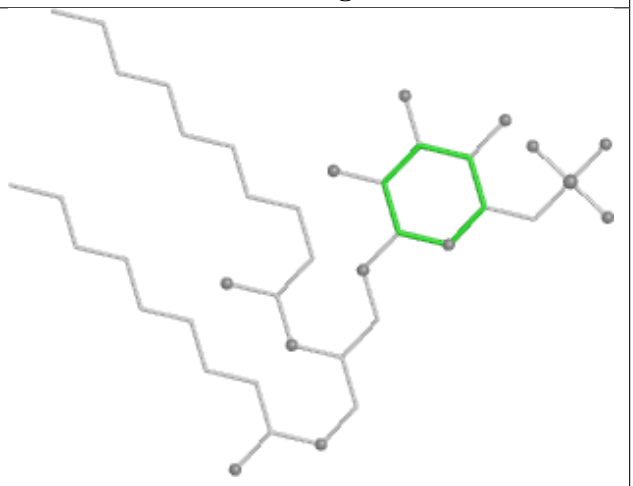
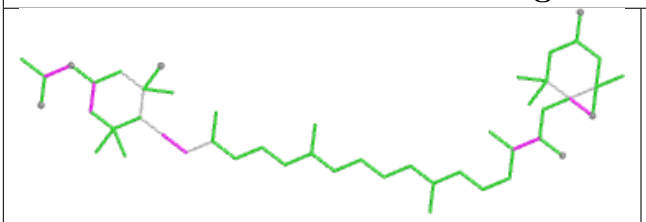


Rings

Ligand A86 0 301



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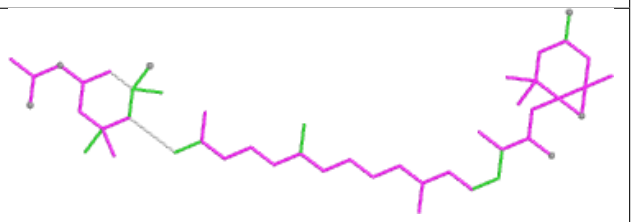

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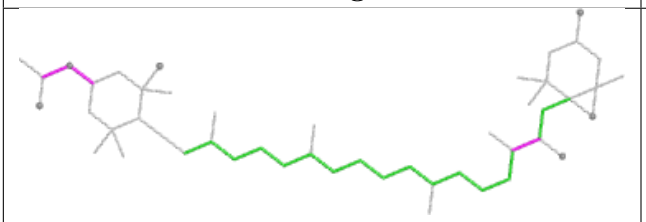

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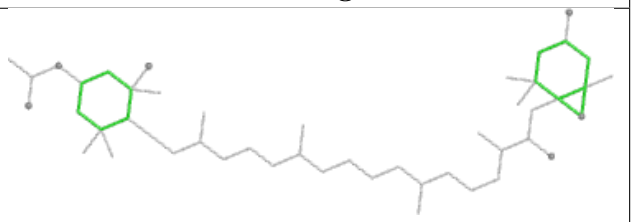
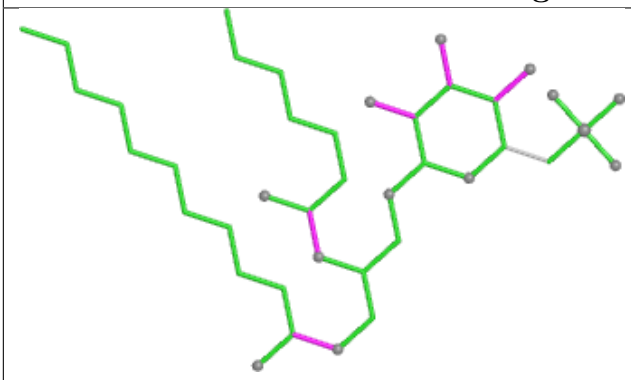


Rings

Ligand SQD i 101



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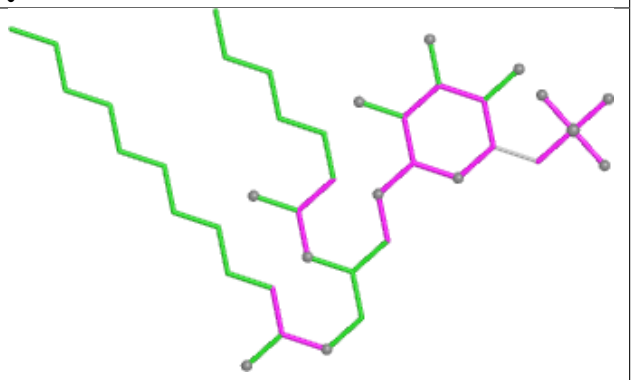

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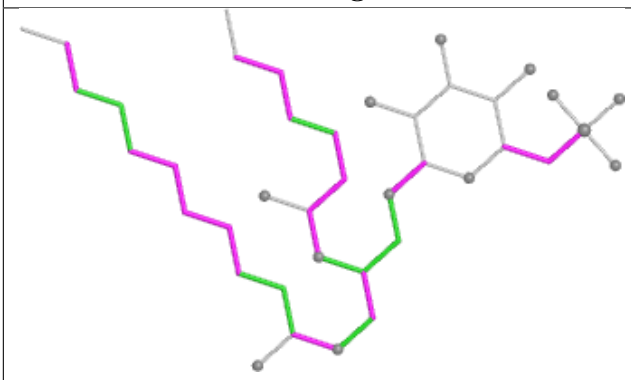

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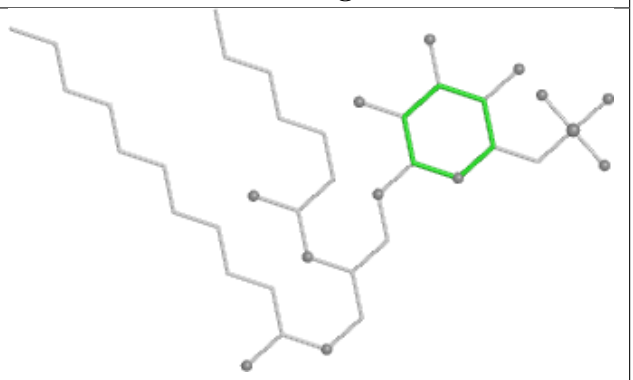
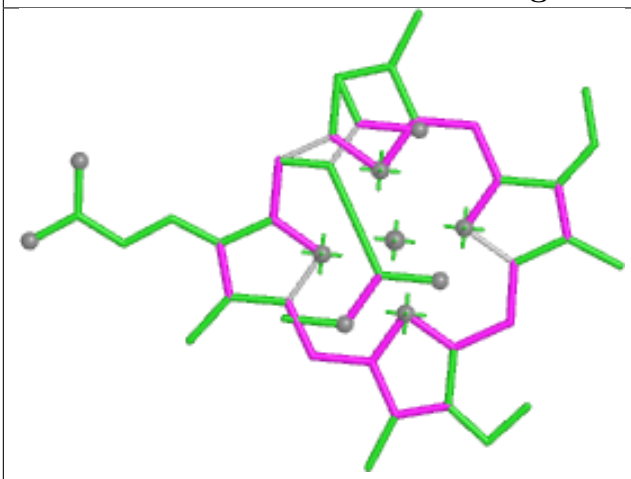


Rings

Ligand KC1 7 314



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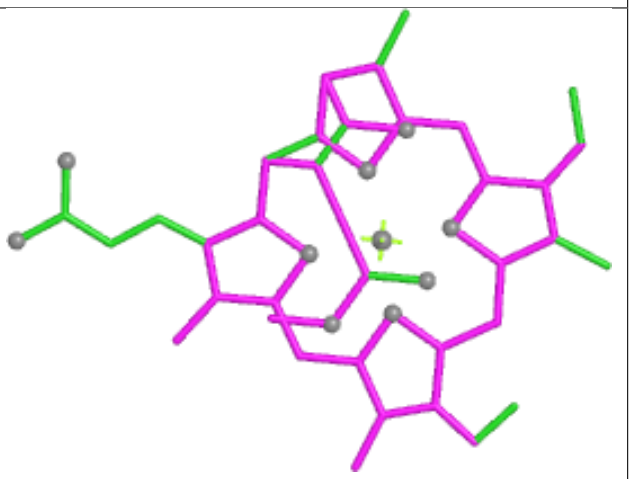
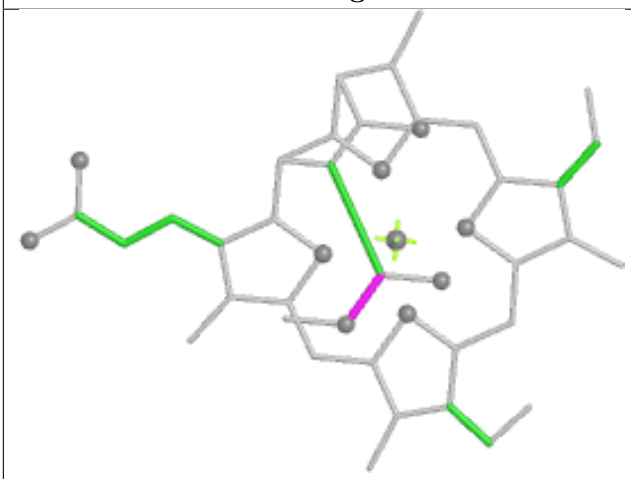


Bond angles



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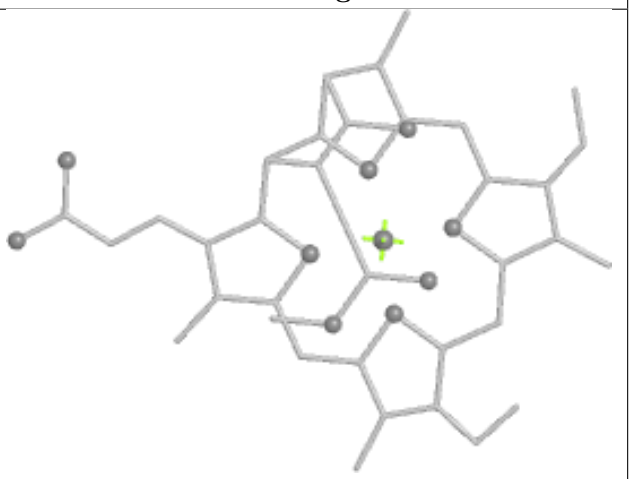
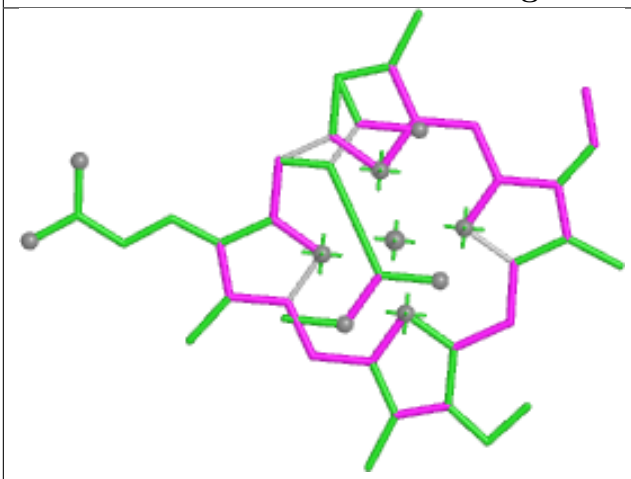


Rings

Ligand KC2 12 311



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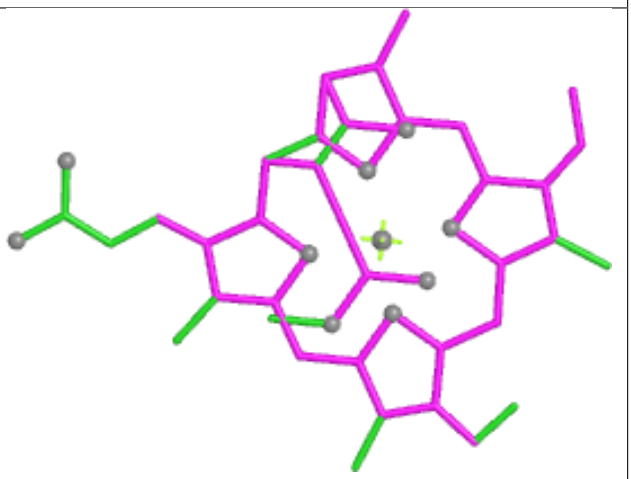
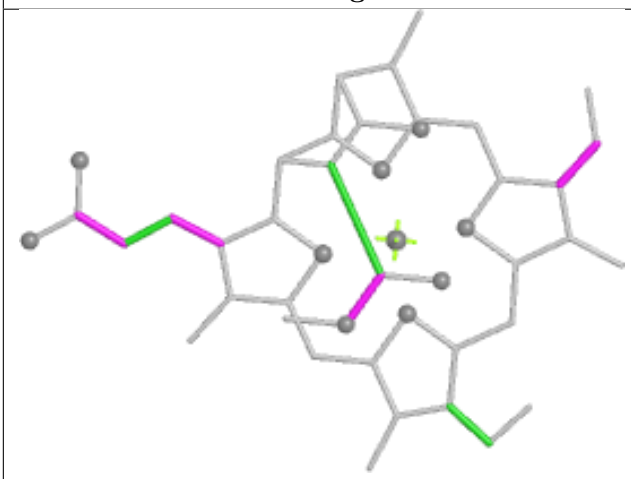


Bond angles



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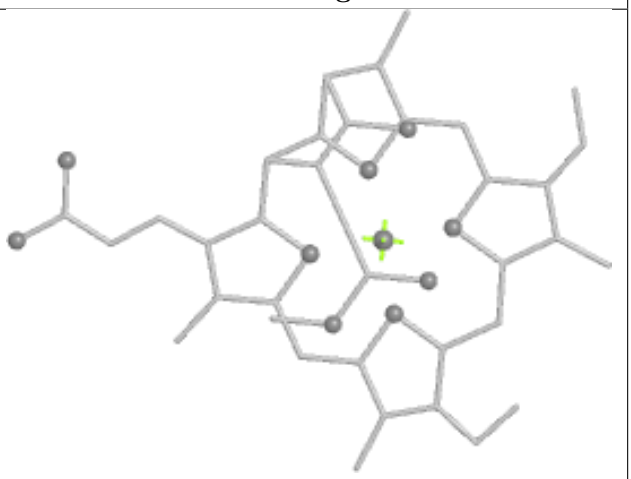
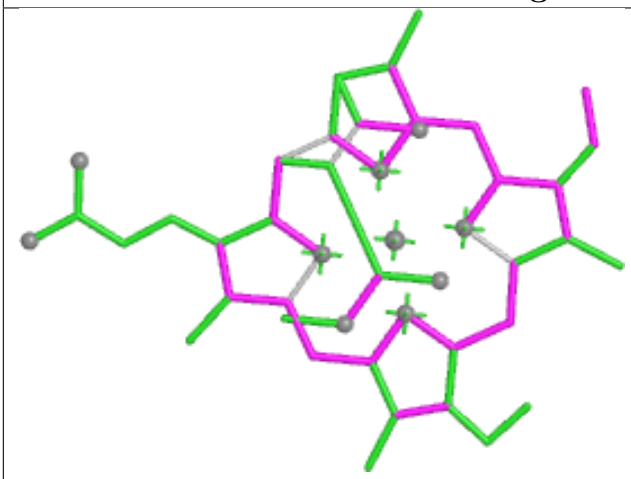


Rings

Ligand KC2 7 311



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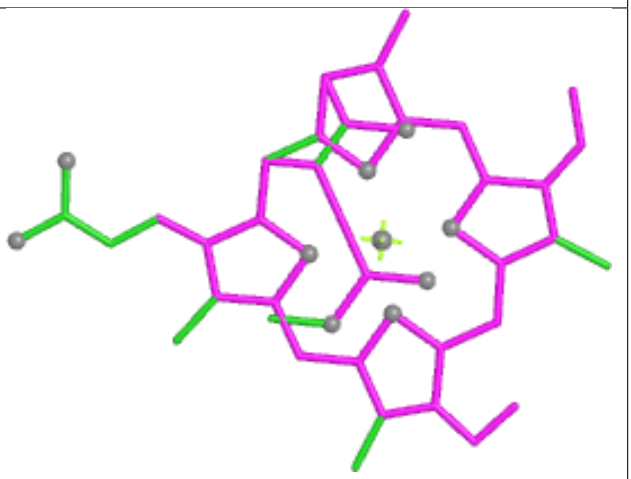
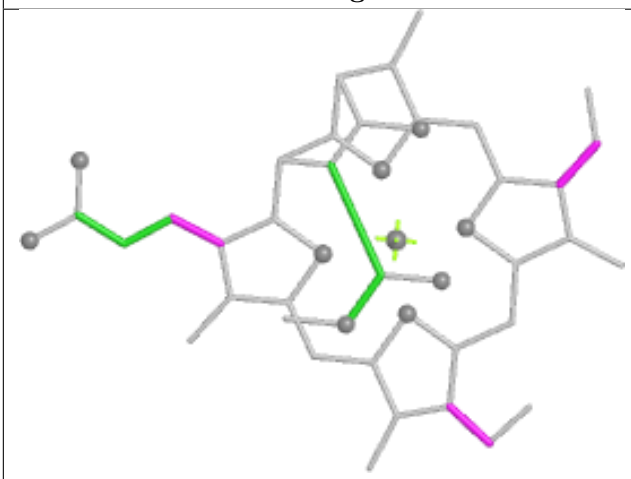


Bond angles



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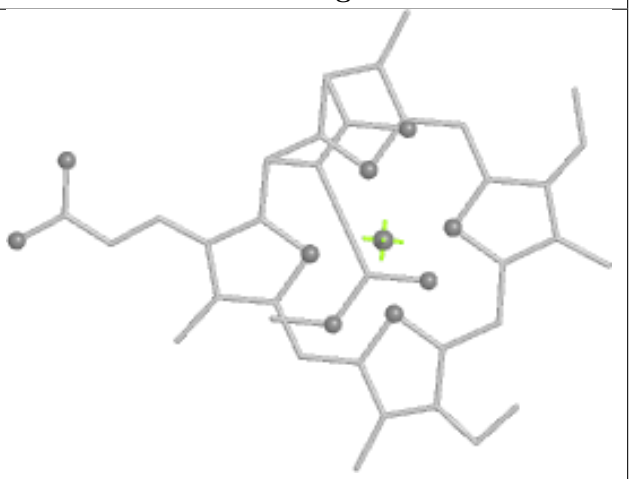
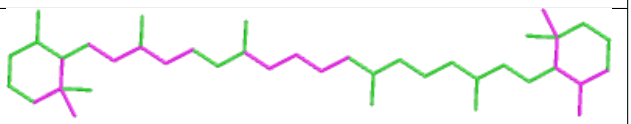


Rings

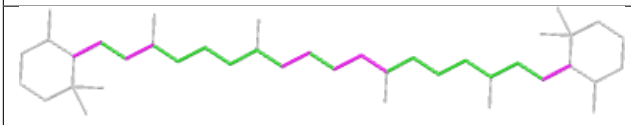
Ligand BCR B 618



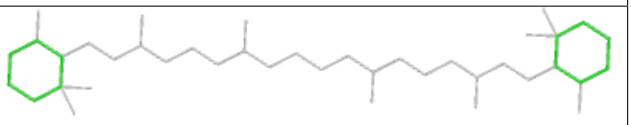
Bond lengths



Bond angles

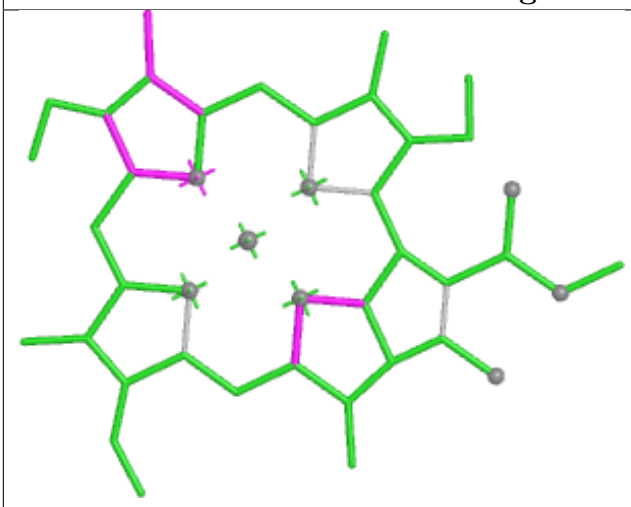


Torsions

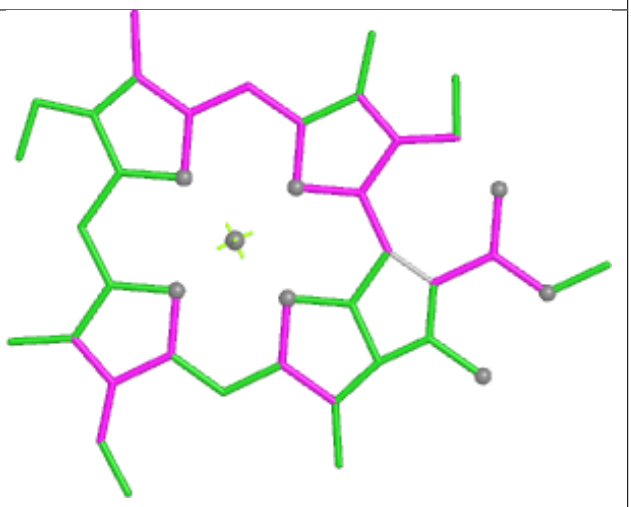


Rings

Ligand CLA 13 307



Bond lengths



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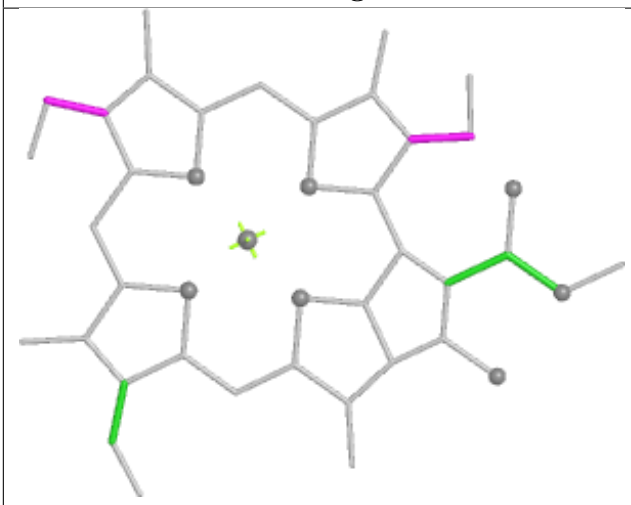
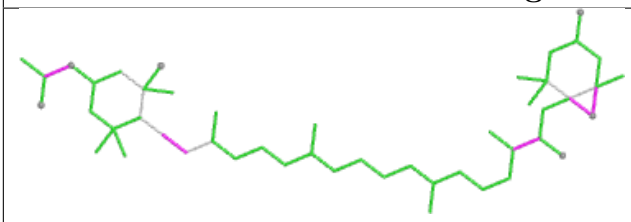


Torsions



Rings

Ligand A86 16 303



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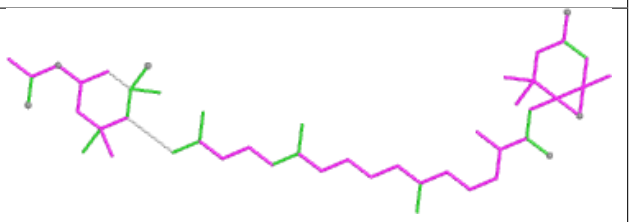

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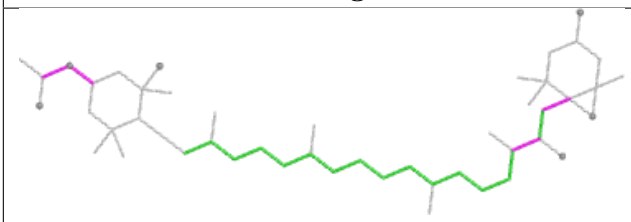

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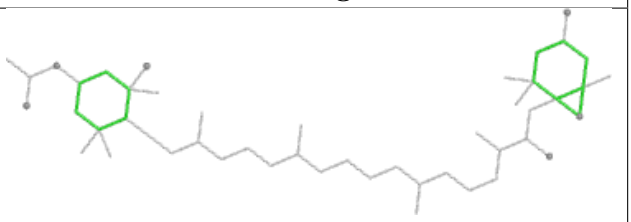
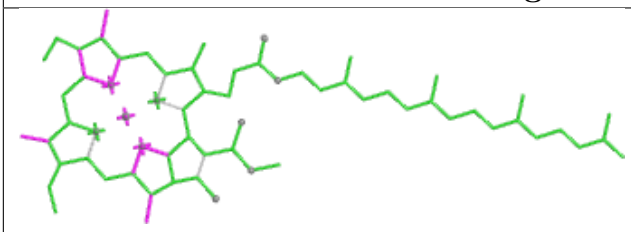


Rings

Ligand CLA B 616



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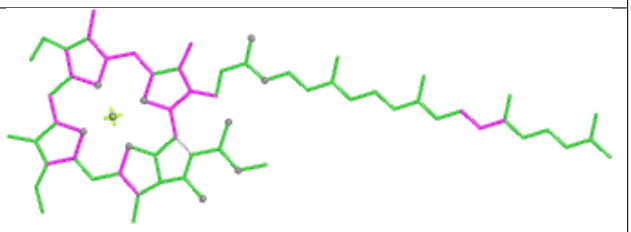
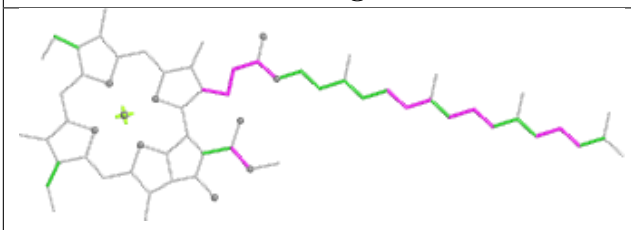


Bond angles



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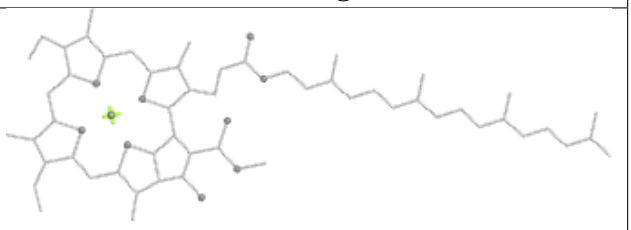
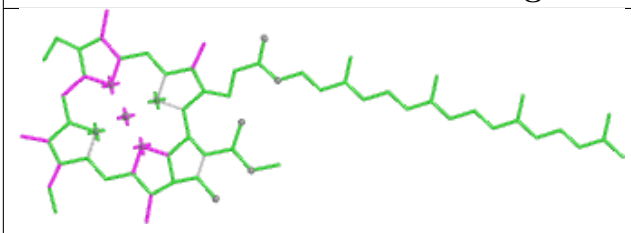


Rings

Ligand CLA B 604



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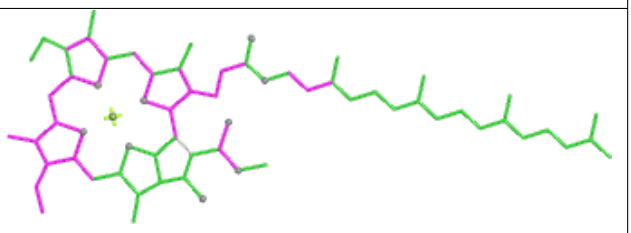

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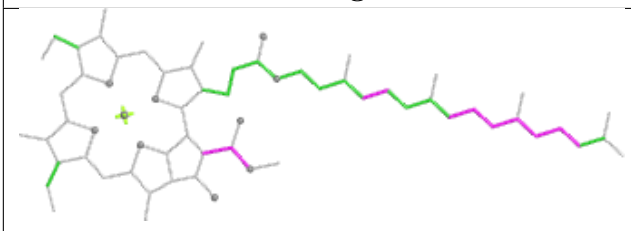

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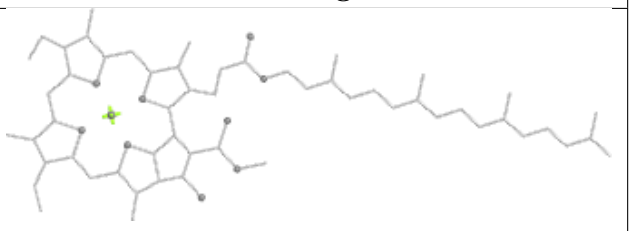
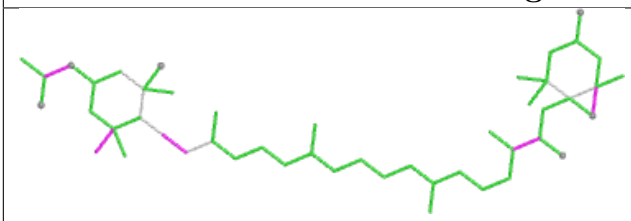


Rings

Ligand A86 11 305



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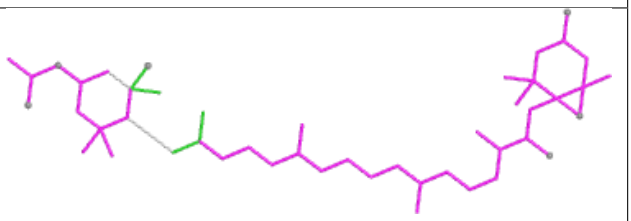
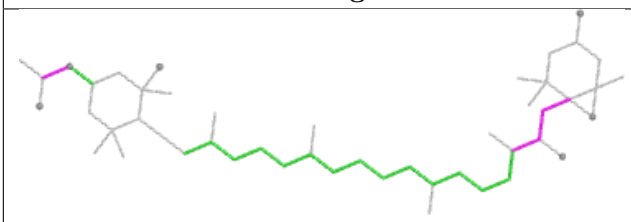


Bond angles



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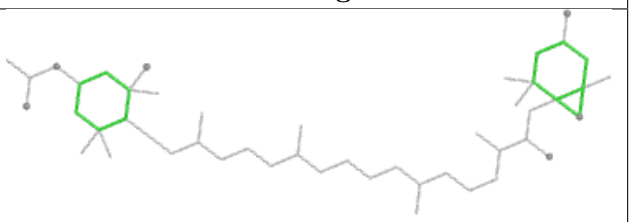
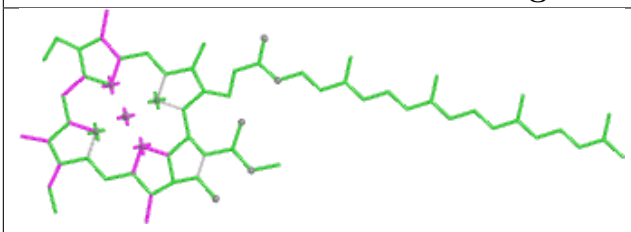


Rings

Ligand CLA c 503



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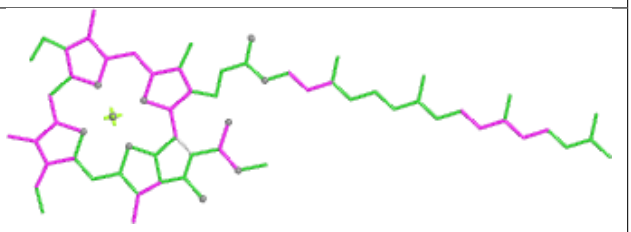
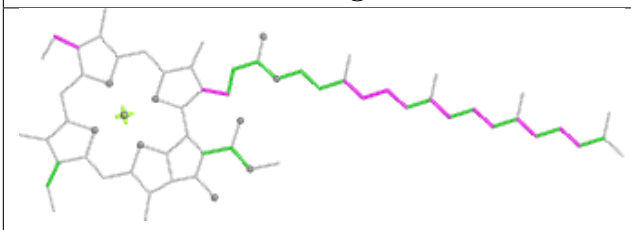


Bond angles



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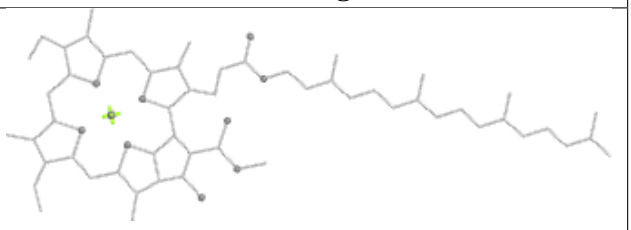
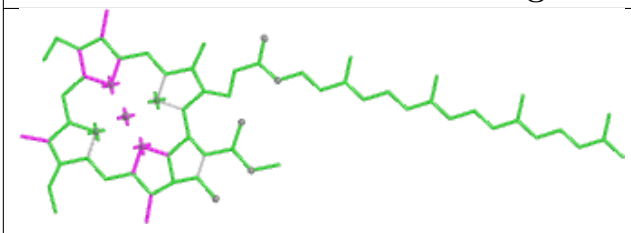


Rings

Ligand CLA b 609



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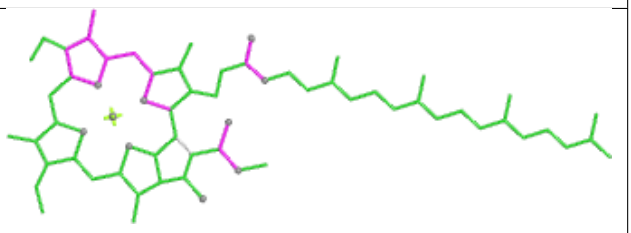
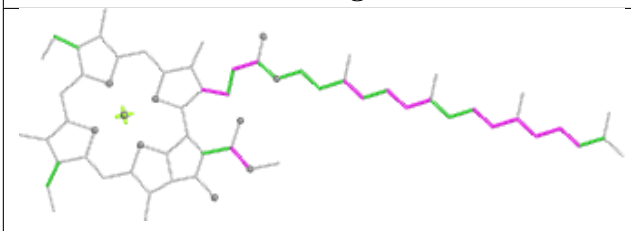


Bond angles



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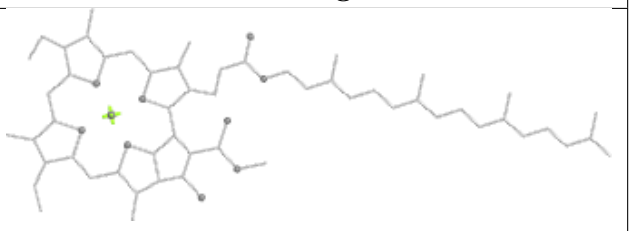
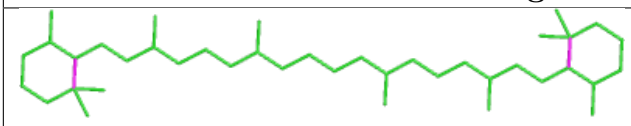


Rings

Ligand BCR c 517



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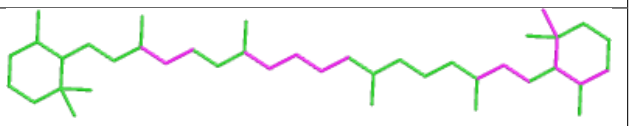
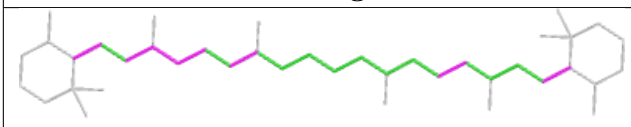


Bond angles



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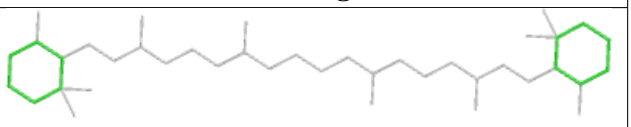
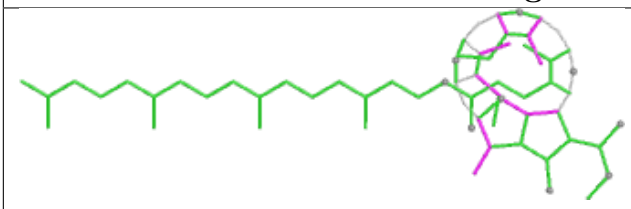


Rings

Ligand PHO d 403



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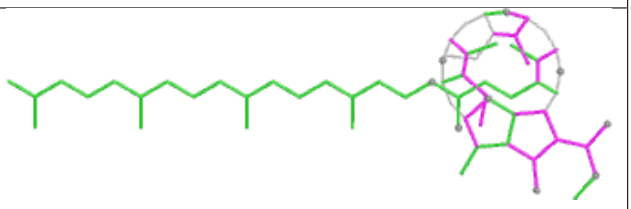

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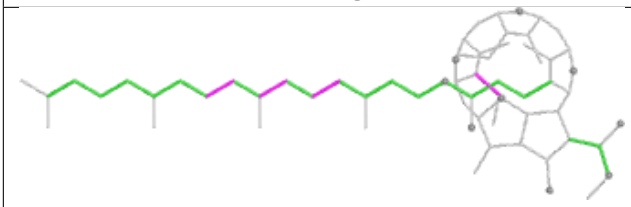

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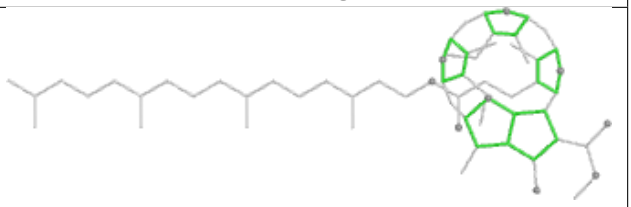
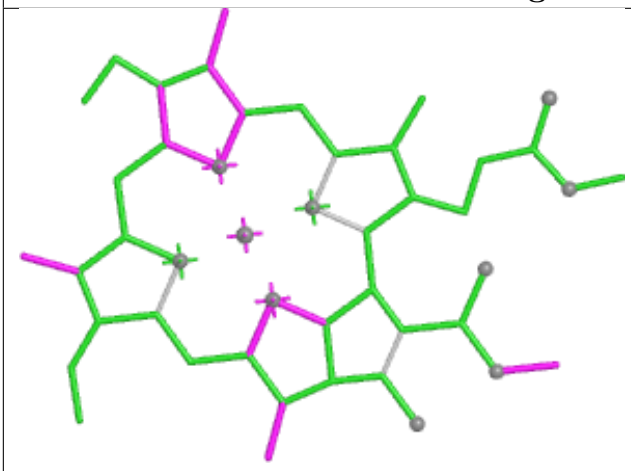


Rings

Ligand CLA 1 312



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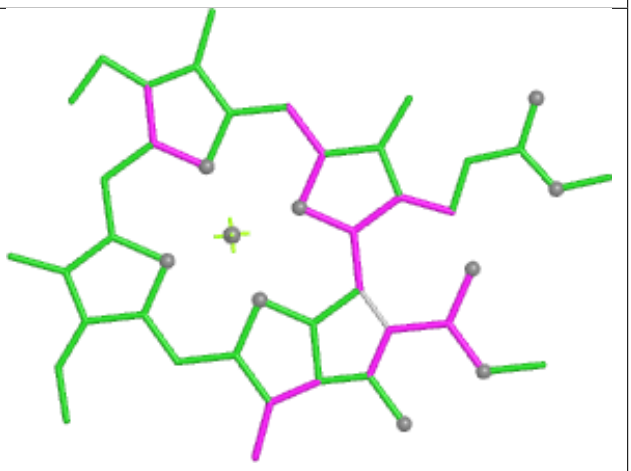

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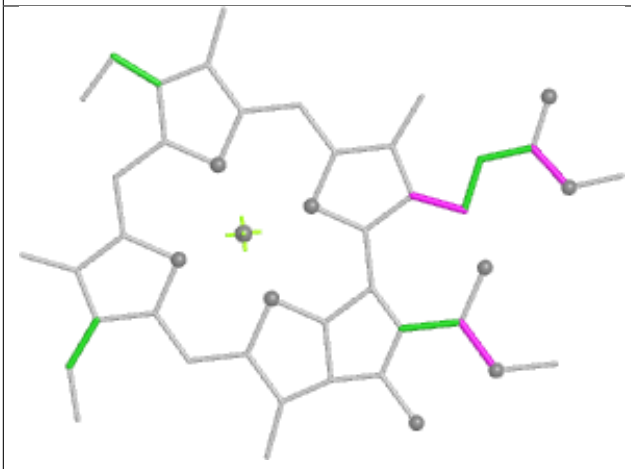

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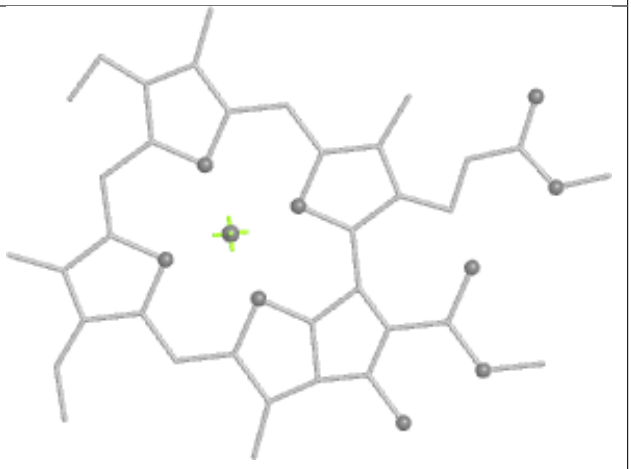
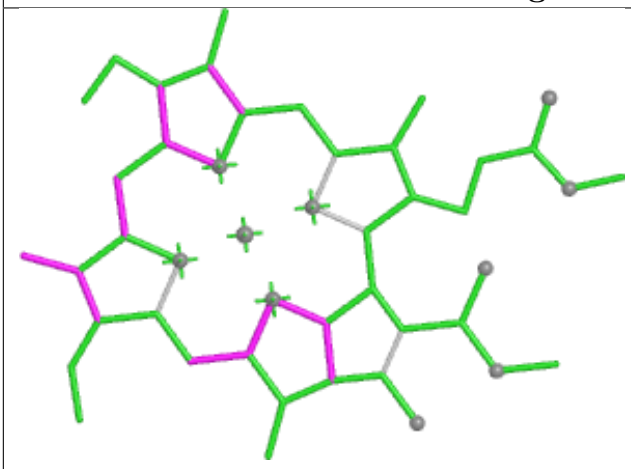


Rings

Ligand CLA 2 315



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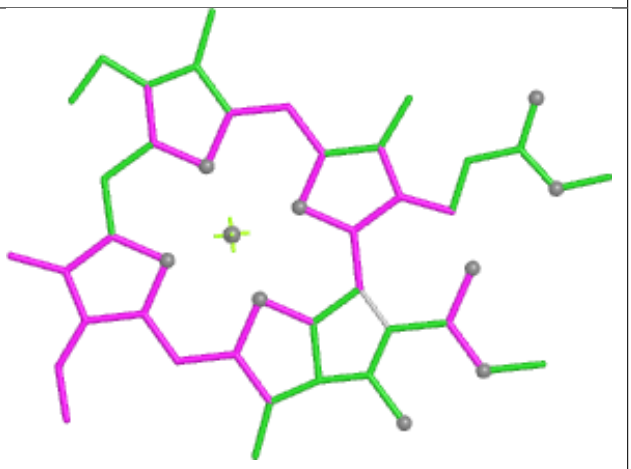
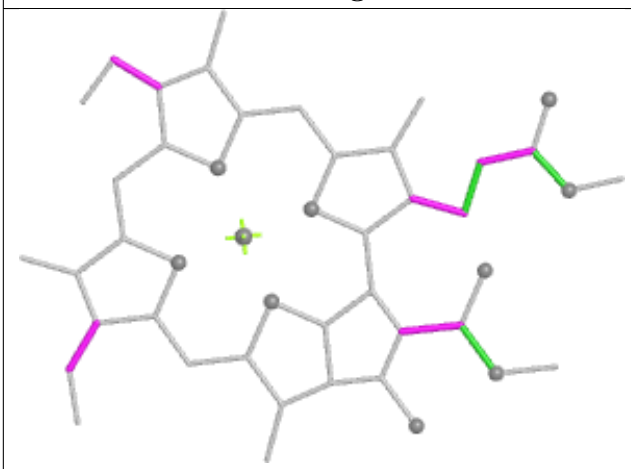


Bond angles



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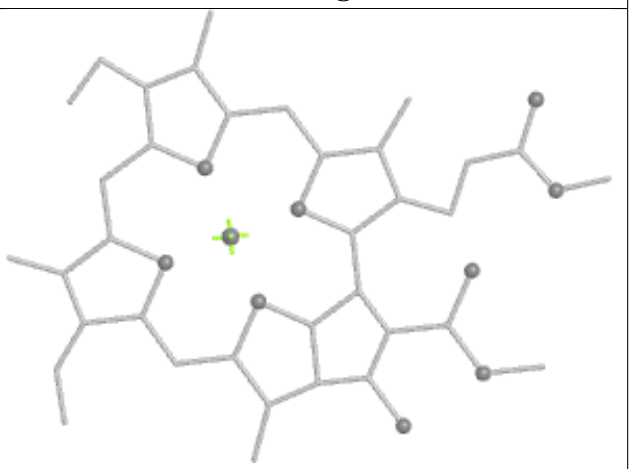
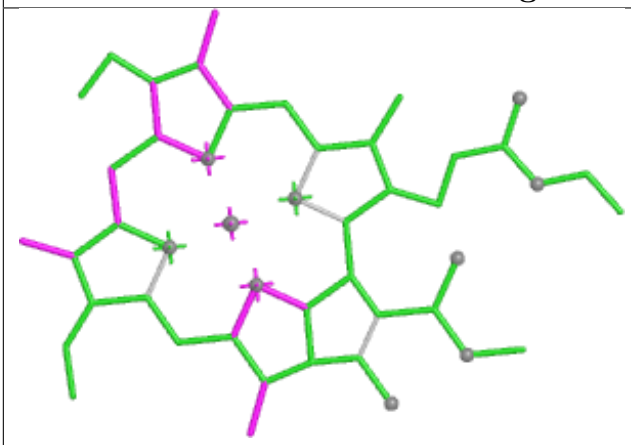


Rings

Ligand CLA 10 314



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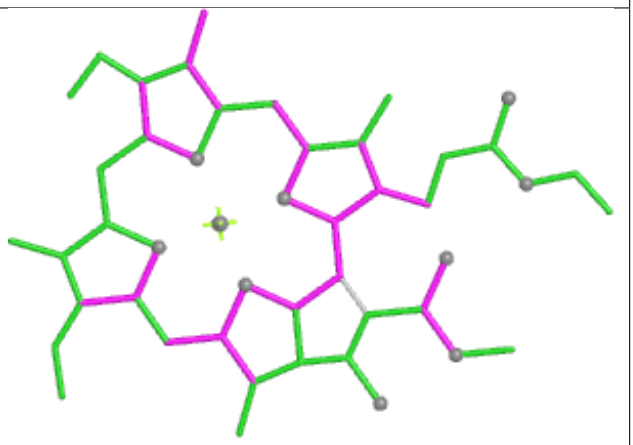
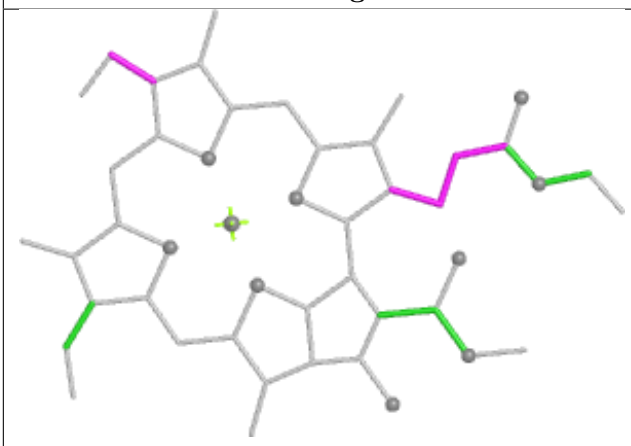


Bond angles



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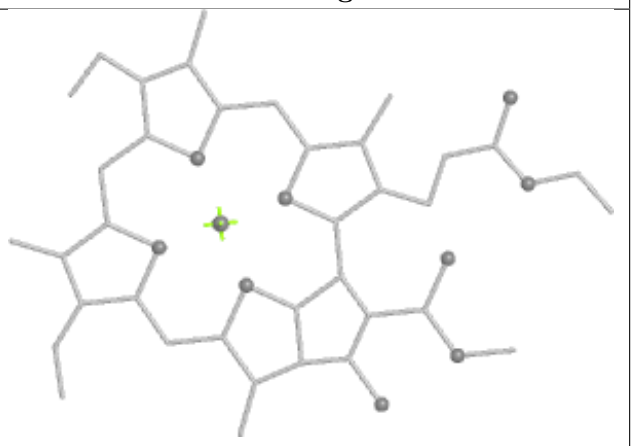
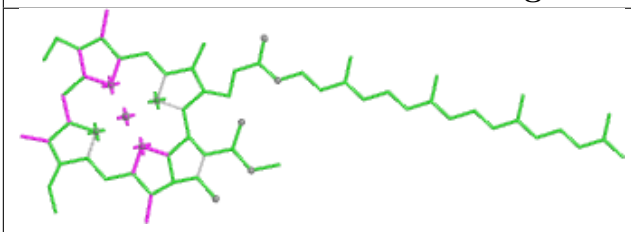


Rings

Ligand CLA C 509



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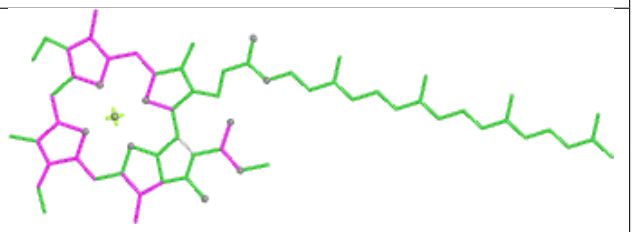
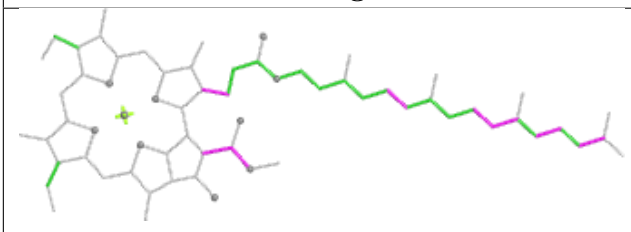


Bond angles



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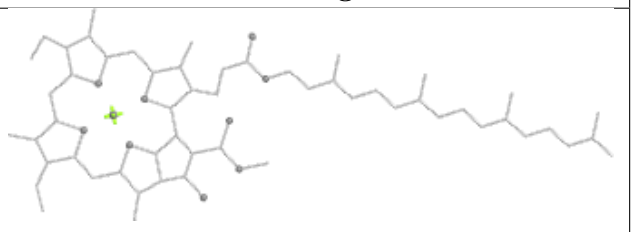
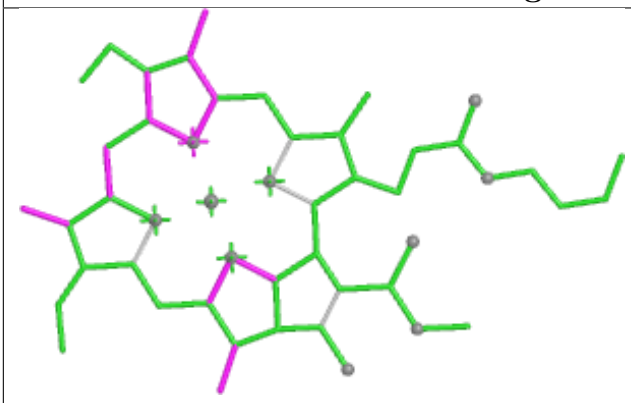


Rings

Ligand CLA C 514



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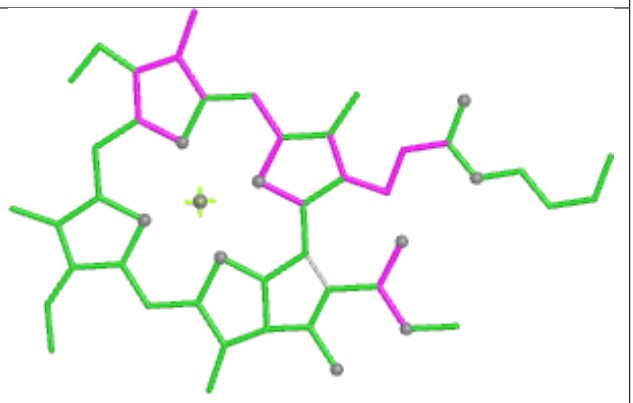
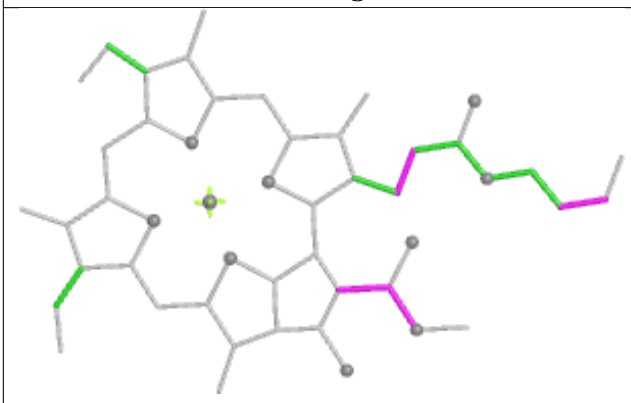


Bond angles



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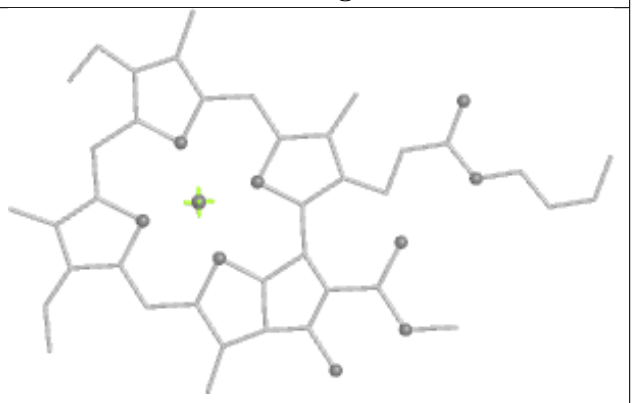
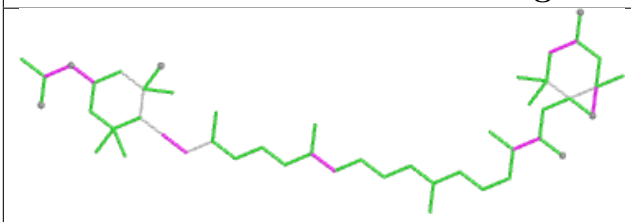
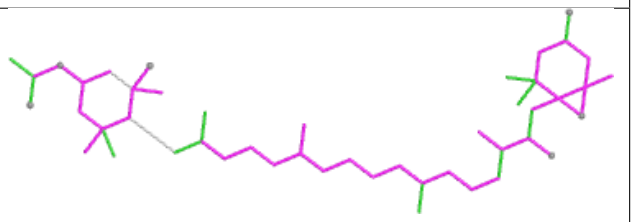


Rings

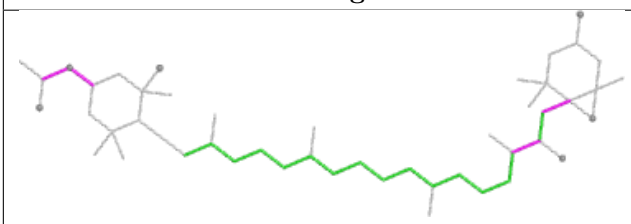
Ligand A86 1 303



Bond lengths



Bond angles



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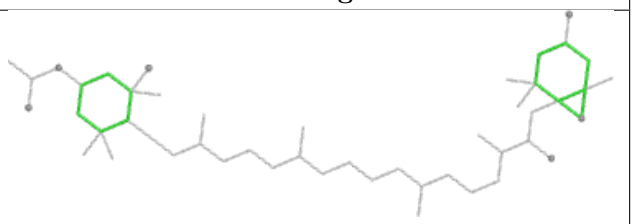
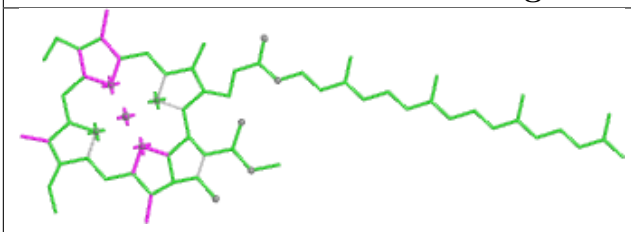


Rings

Ligand CLA C 513



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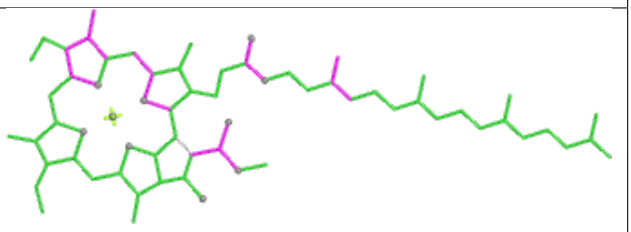

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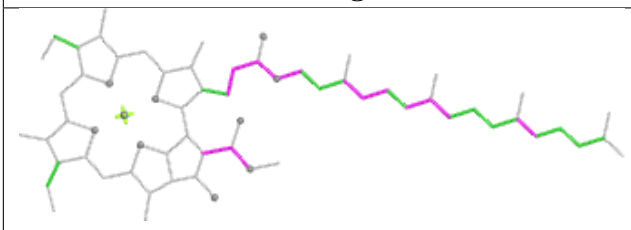

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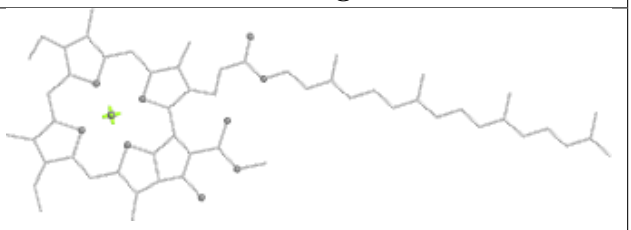

Rings

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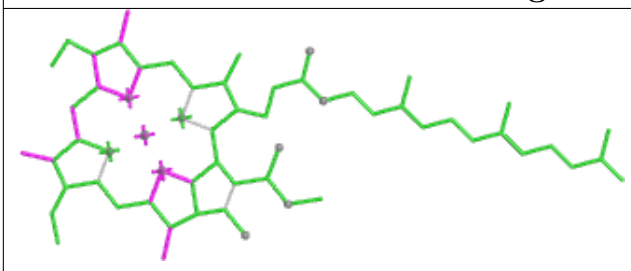

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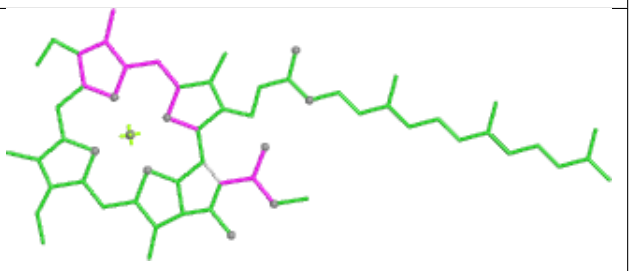

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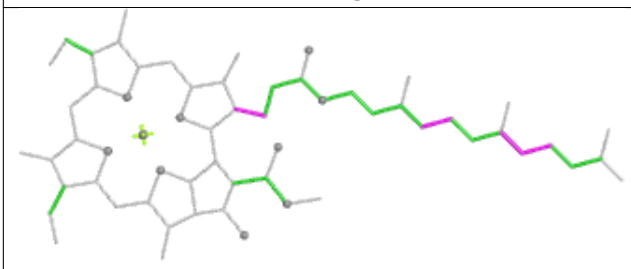

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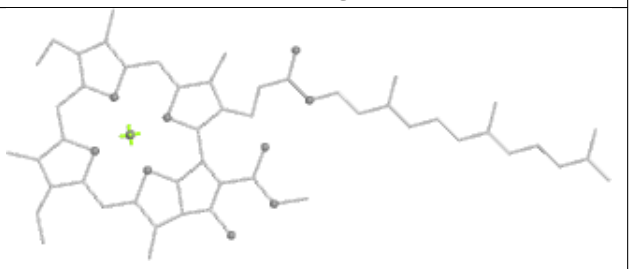
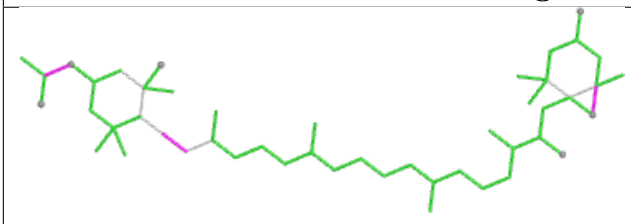


Rings

Ligand A86 1 302



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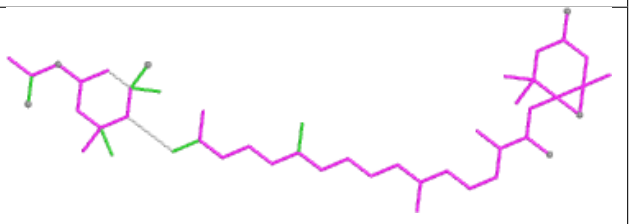

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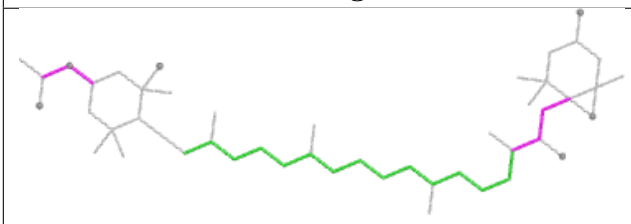

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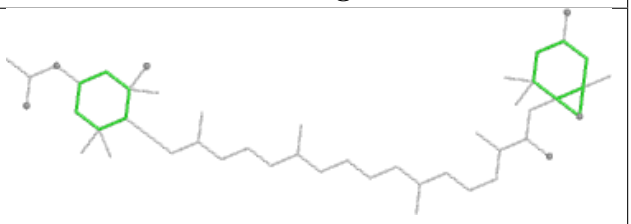
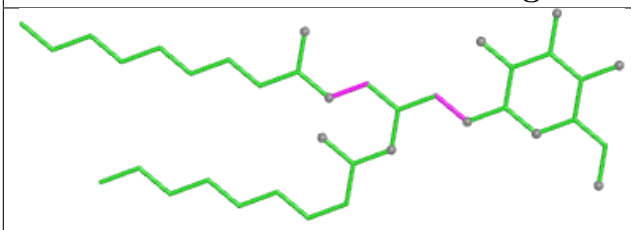


Rings

Ligand LMG d 409



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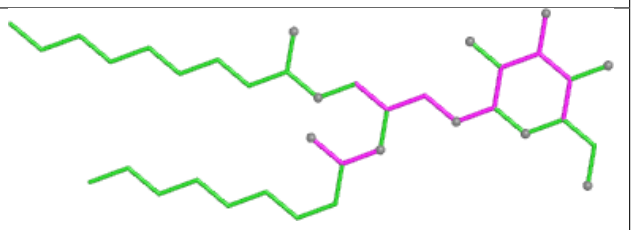

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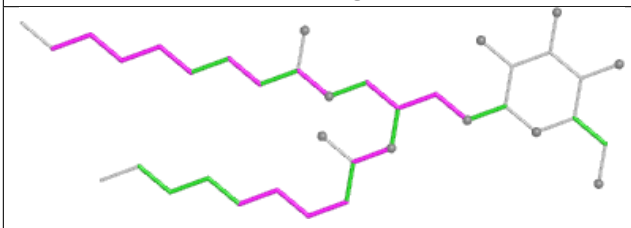

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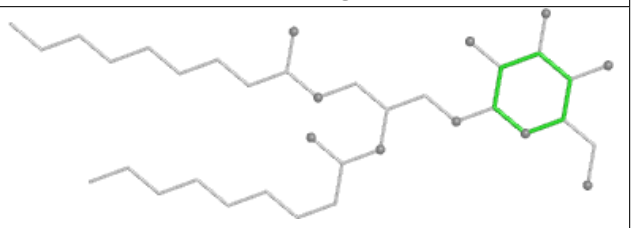

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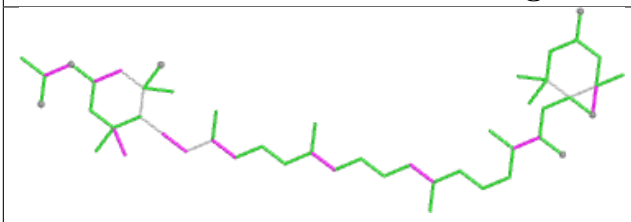

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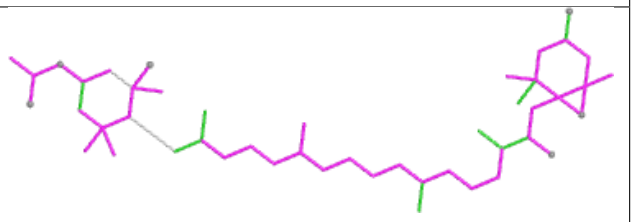

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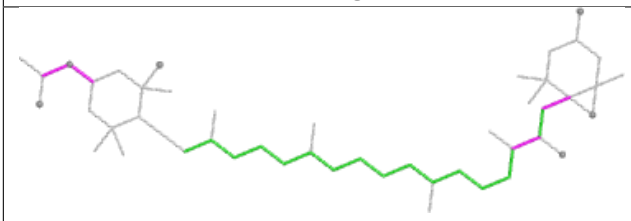

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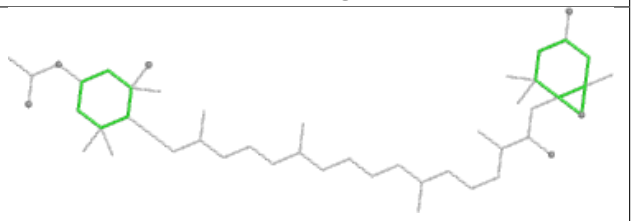

Rings

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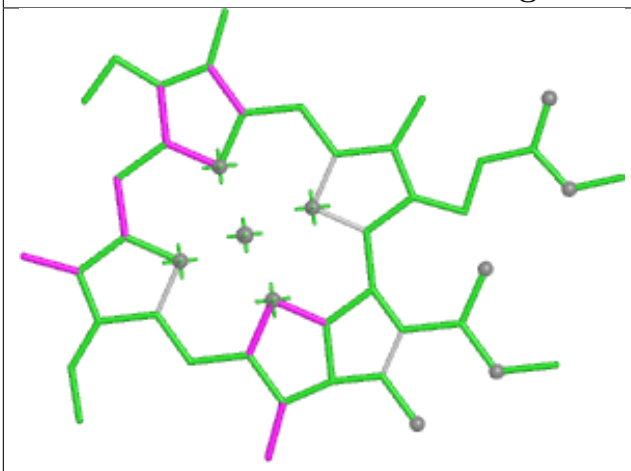

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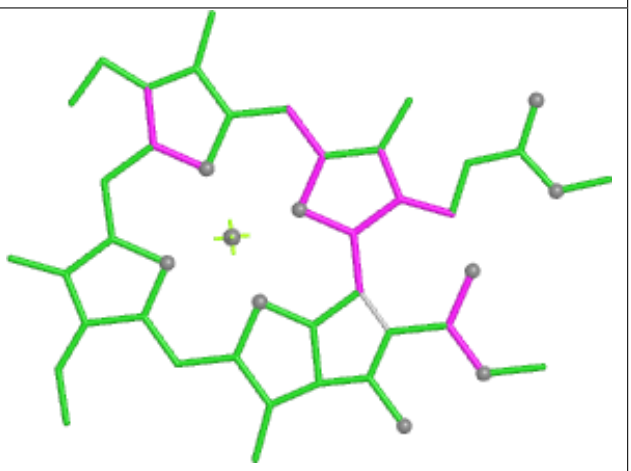

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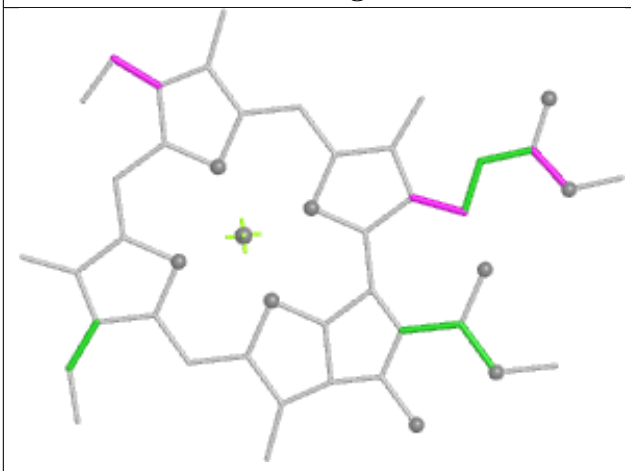

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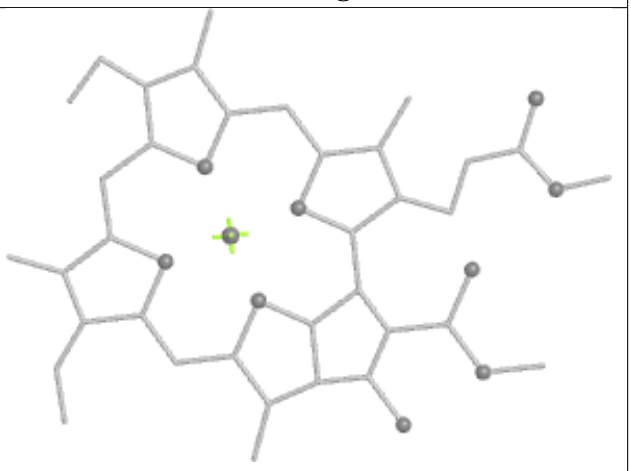

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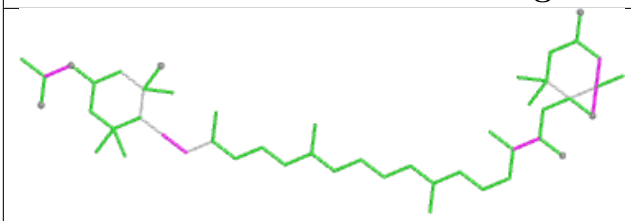

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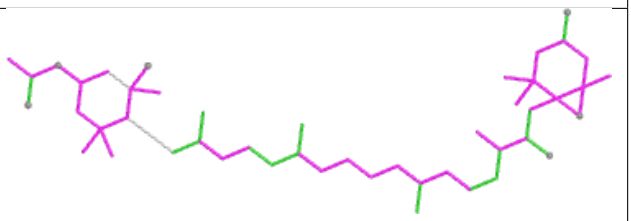

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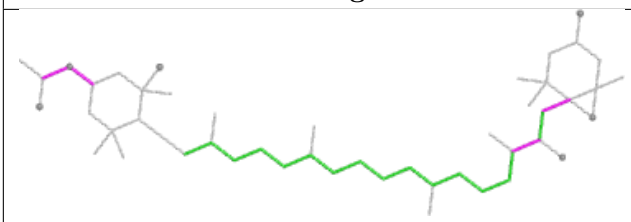

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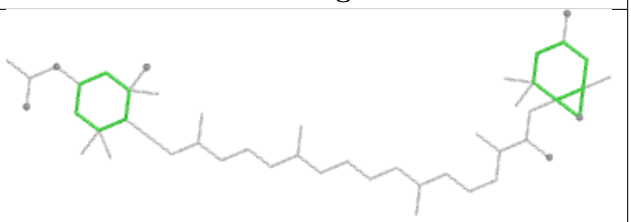
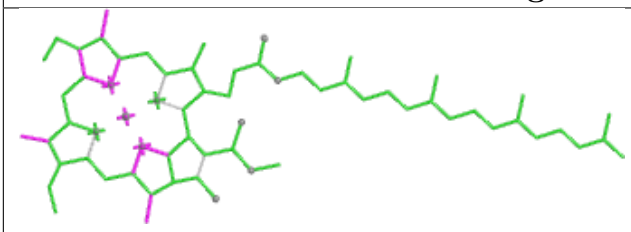


Rings

Ligand CLA b 617



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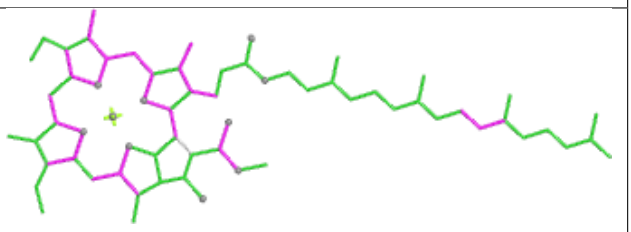

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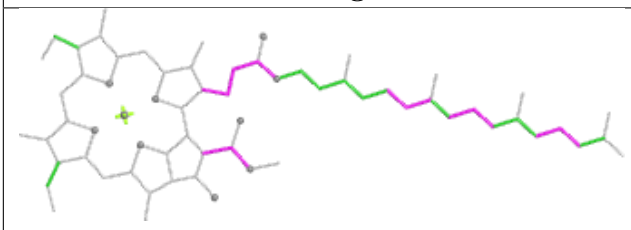

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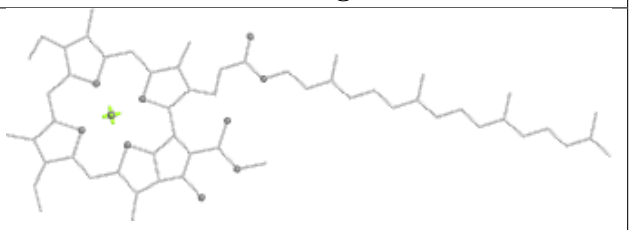
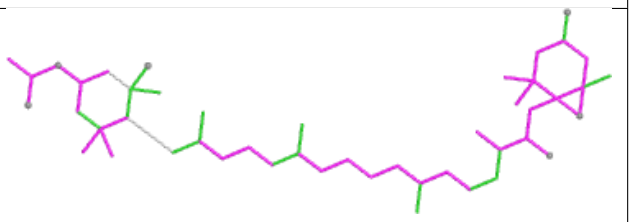


Rings

Ligand A86 2 305



Bond lengths



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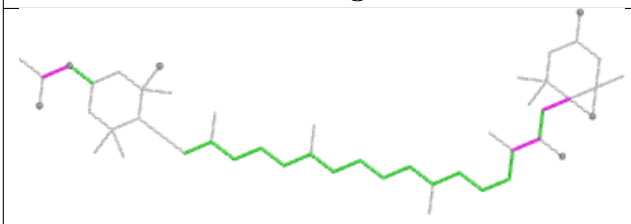

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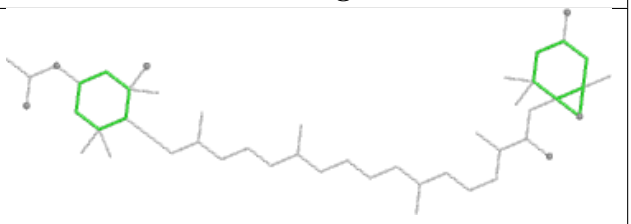

Rings

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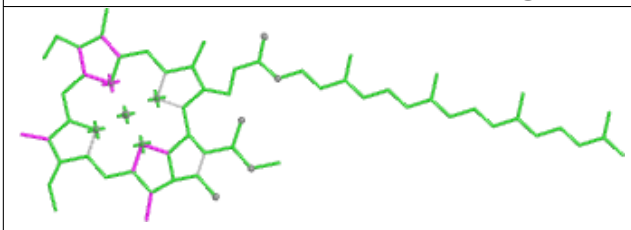

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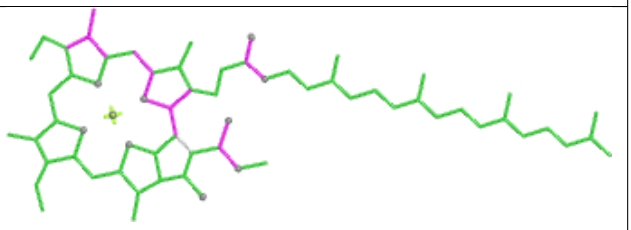

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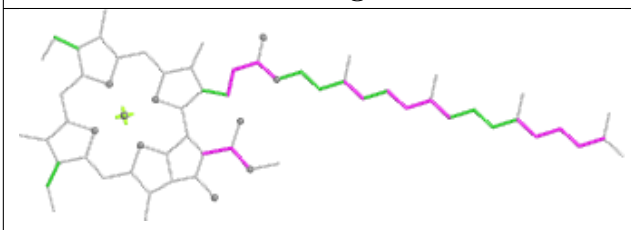

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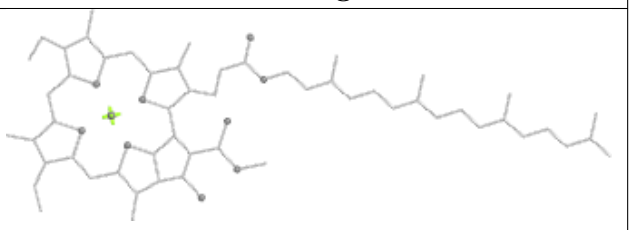
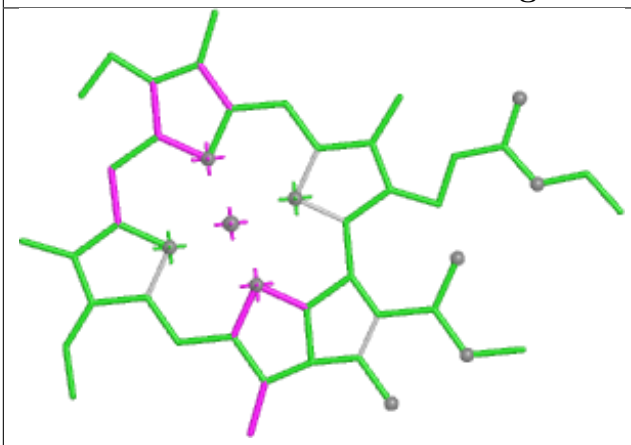


Rings

Ligand CLA 16 312



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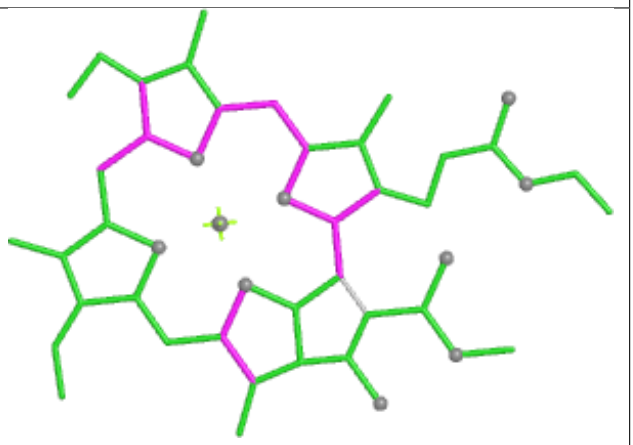

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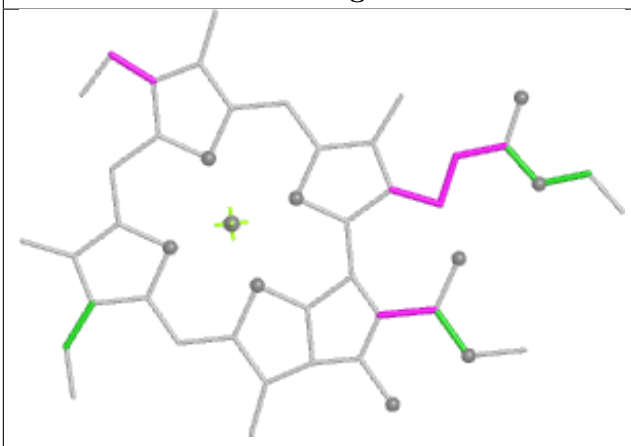

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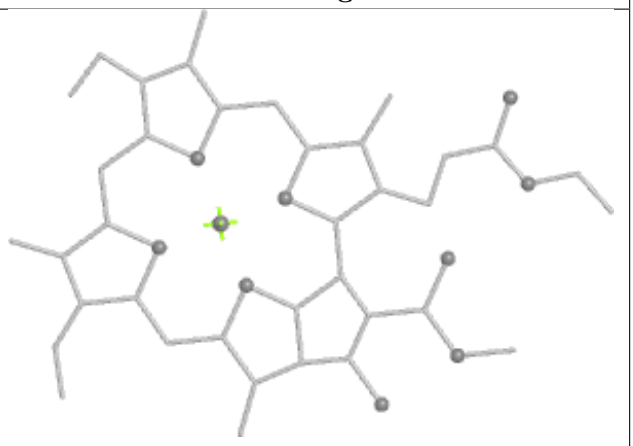

Rings

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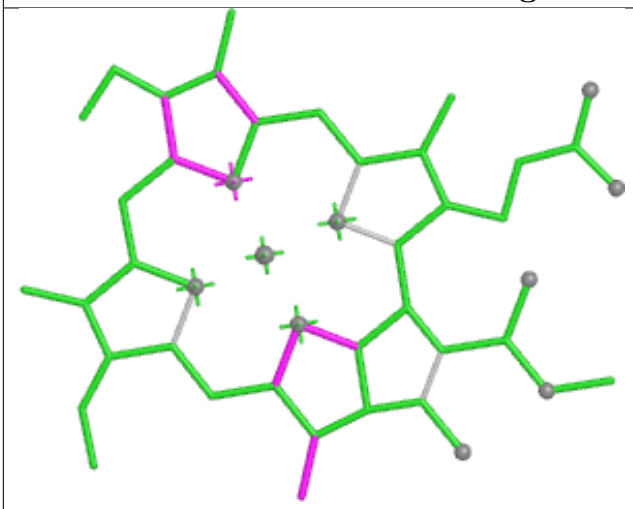

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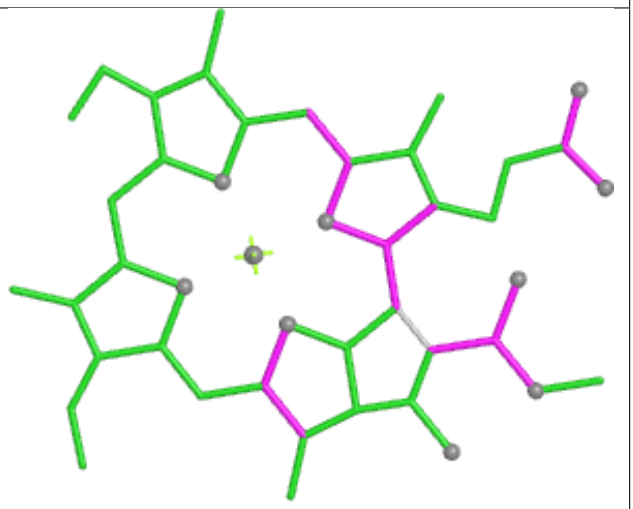

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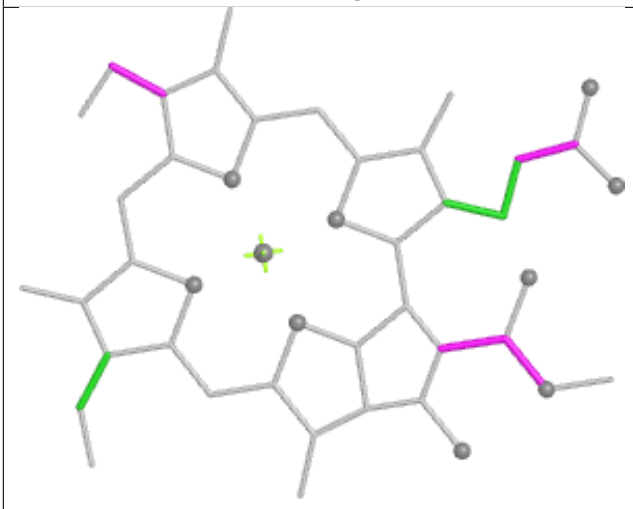
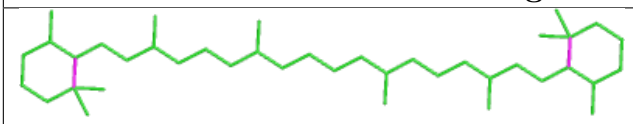


Torsions



Rings

Ligand BCR b 618



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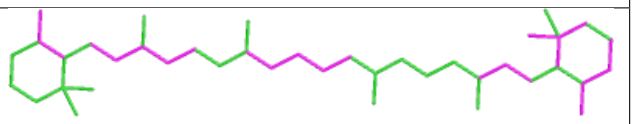

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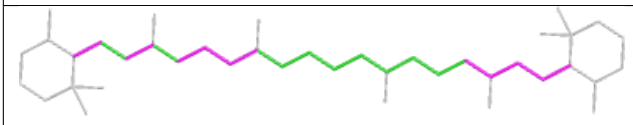

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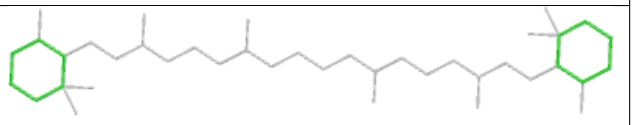
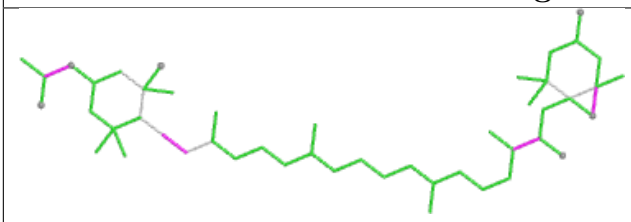


Rings

Ligand A86 0 305



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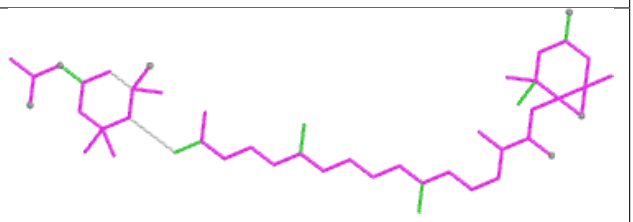
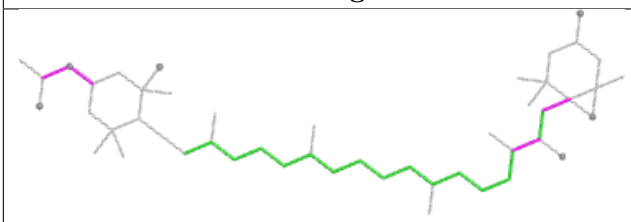


Bond angles



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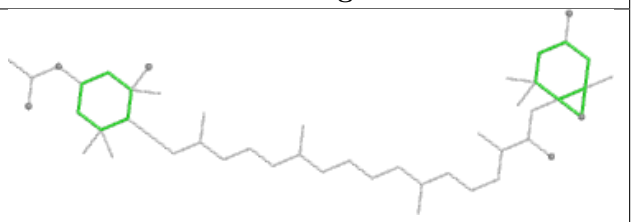

Rings

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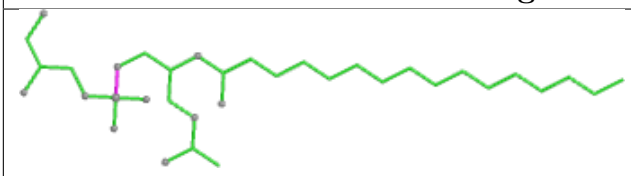
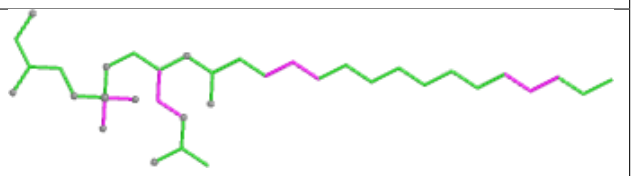
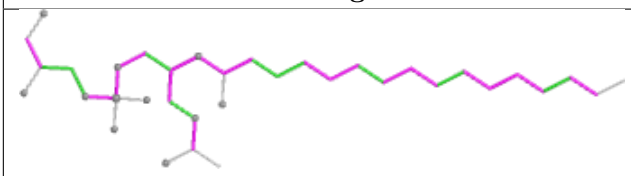


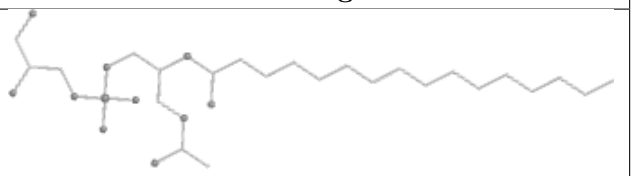
Bond lengths



Bond angles



Torsions

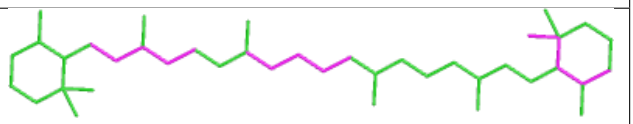


Rings

Ligand BCR A 407



Bond lengths



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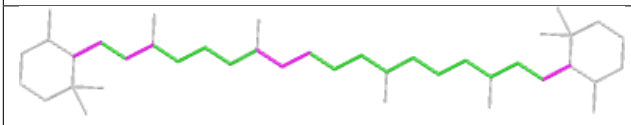

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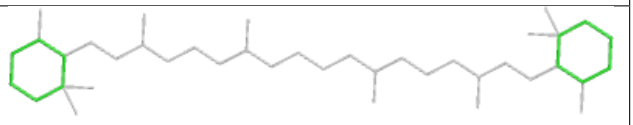
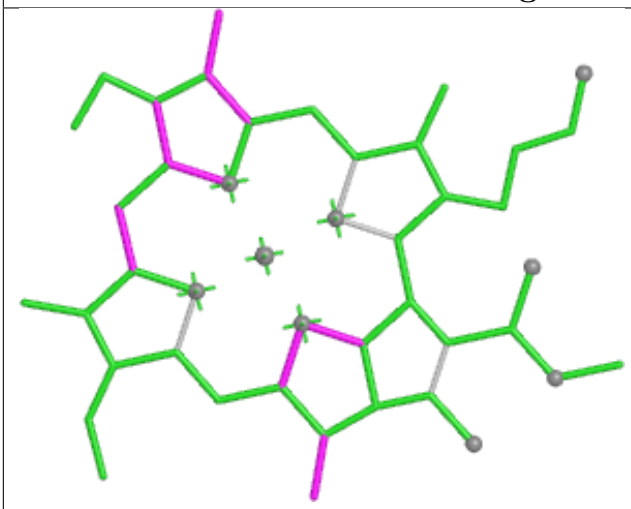


Rings

Ligand CLA 13 315



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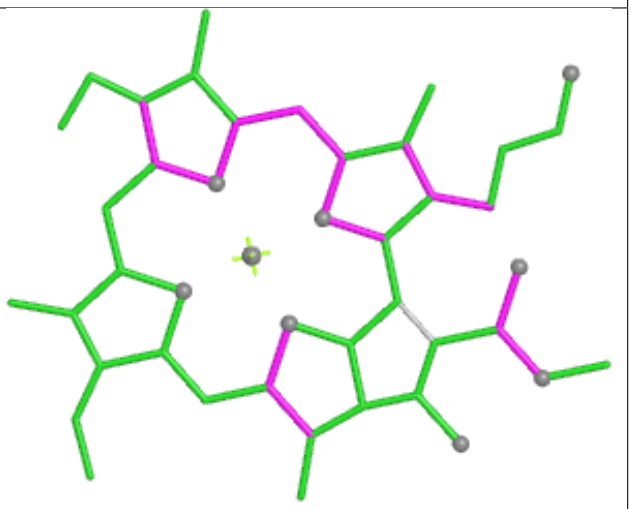

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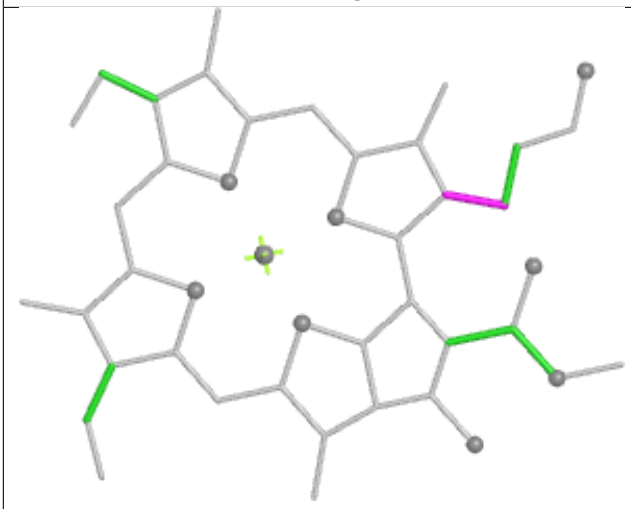

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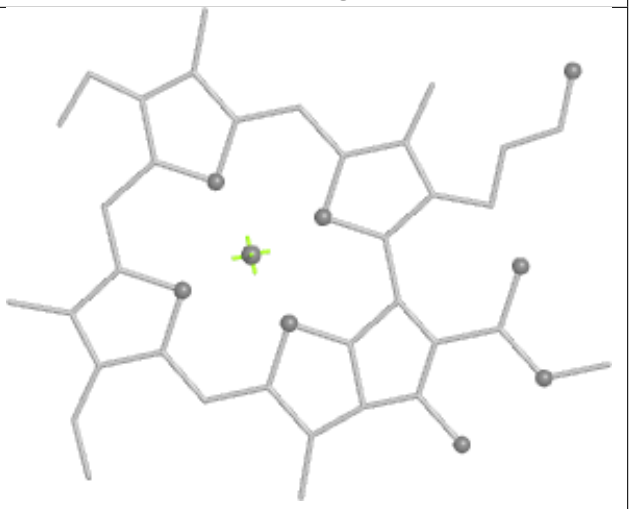
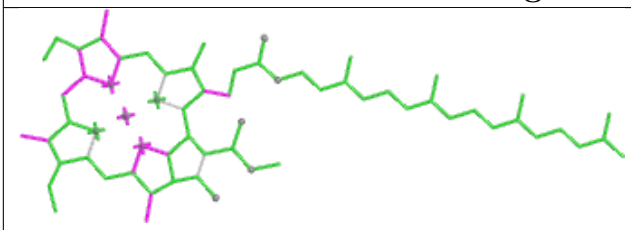


Rings

Ligand CLA B 602



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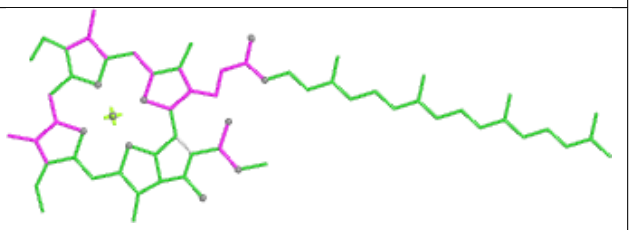

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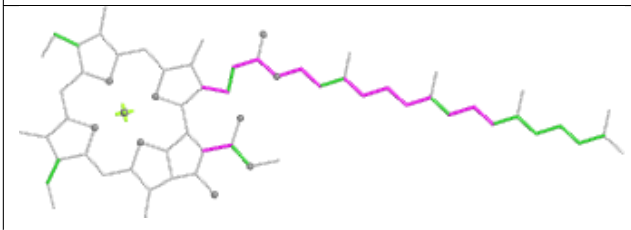

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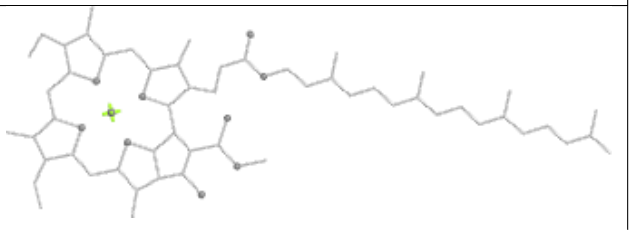
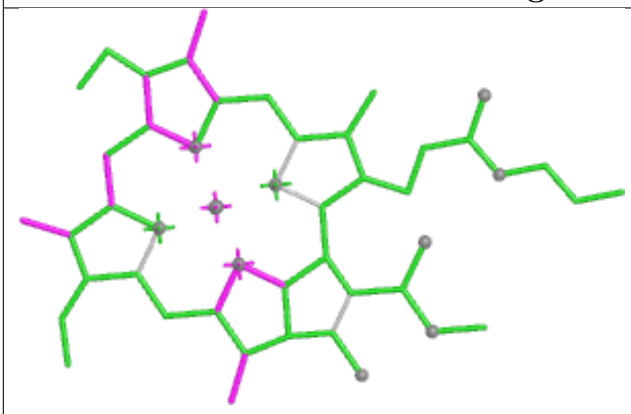


Rings

Ligand CLA p 604



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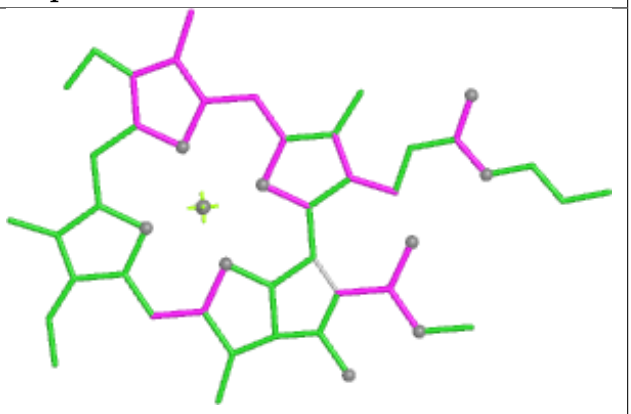

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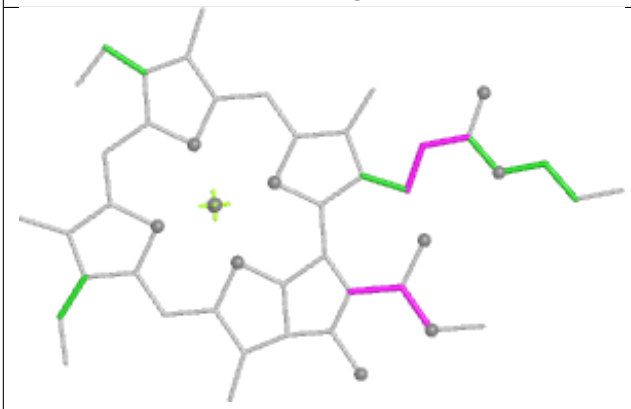

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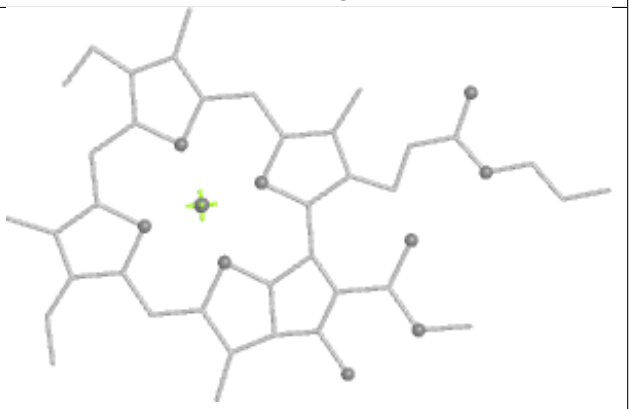
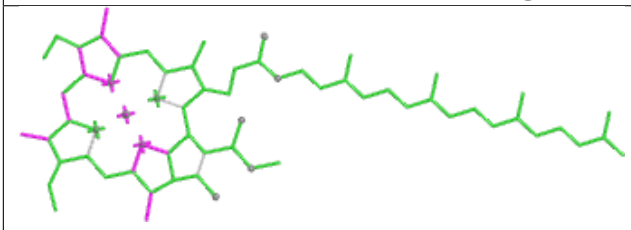


Rings

Ligand CLA 16 308



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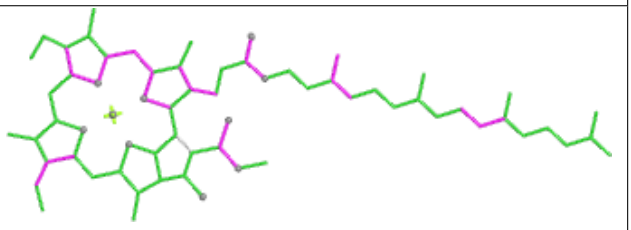
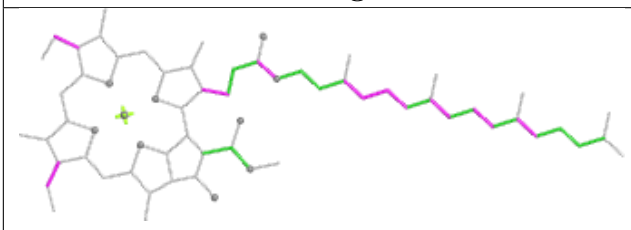


Bond angles



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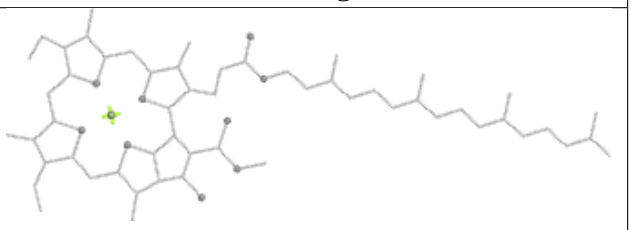
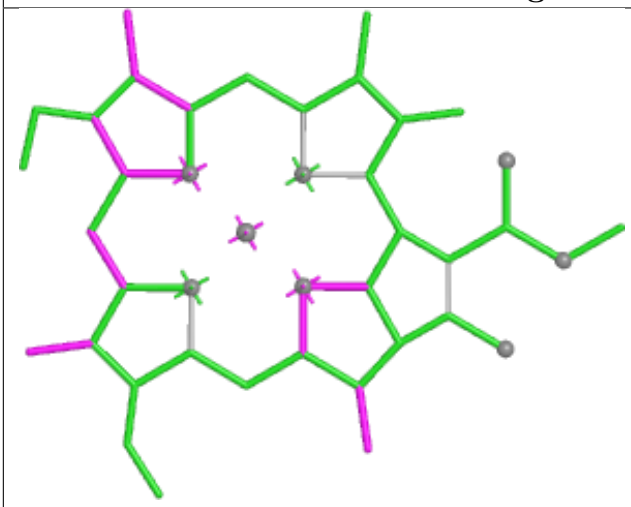


Rings

Ligand CLA p 610



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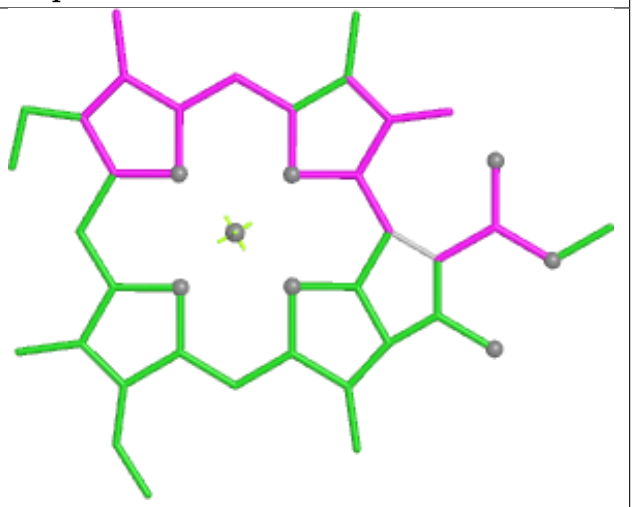
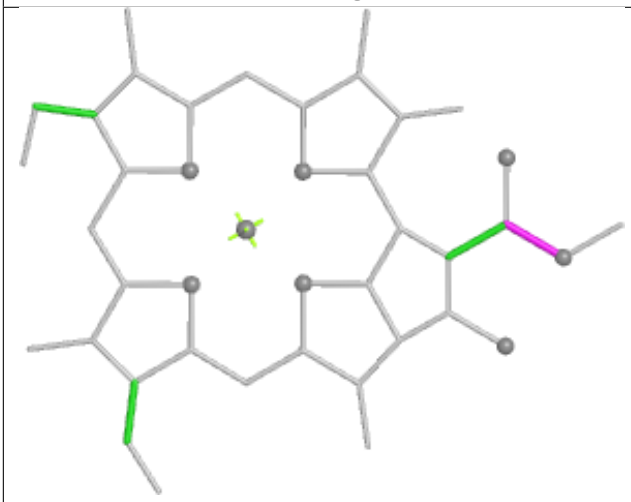


Bond angles



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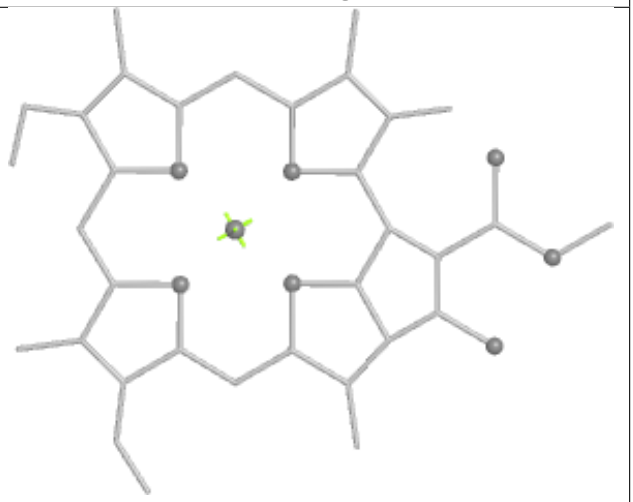
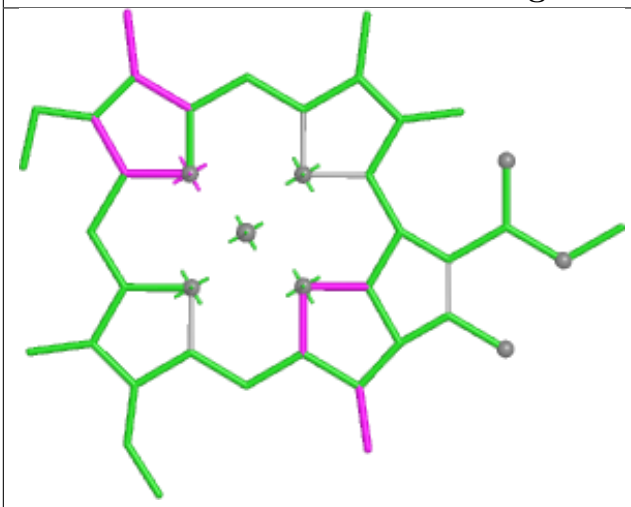


Rings

Ligand CLA 7 315



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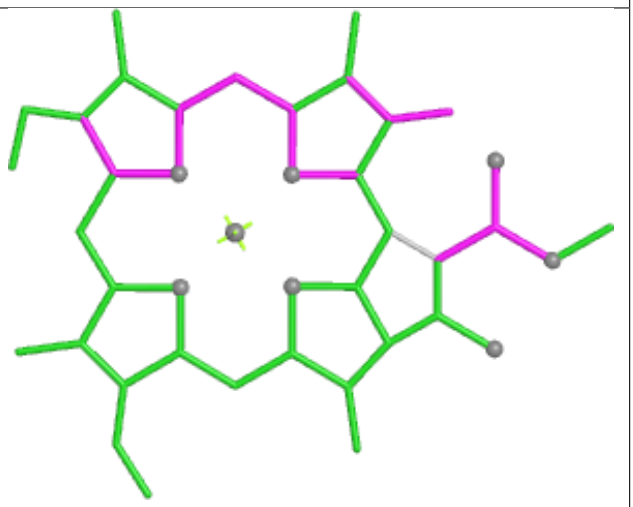
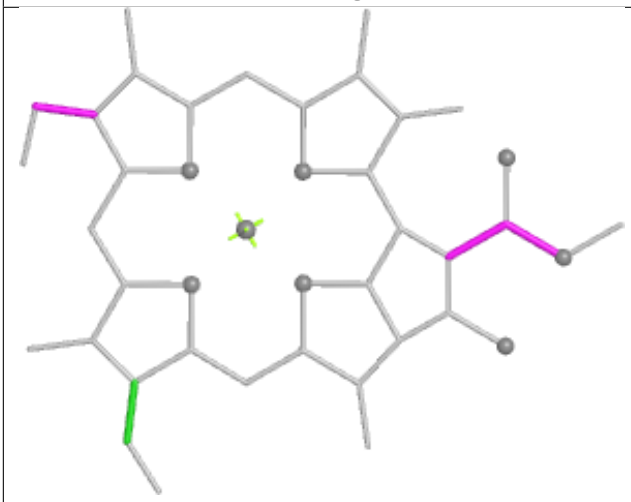


Bond angles



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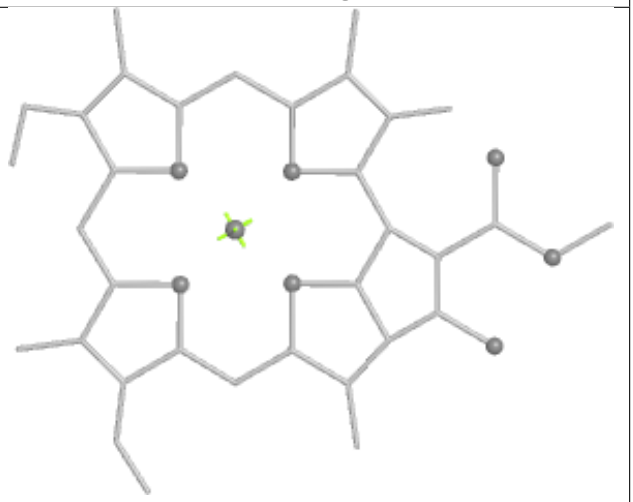
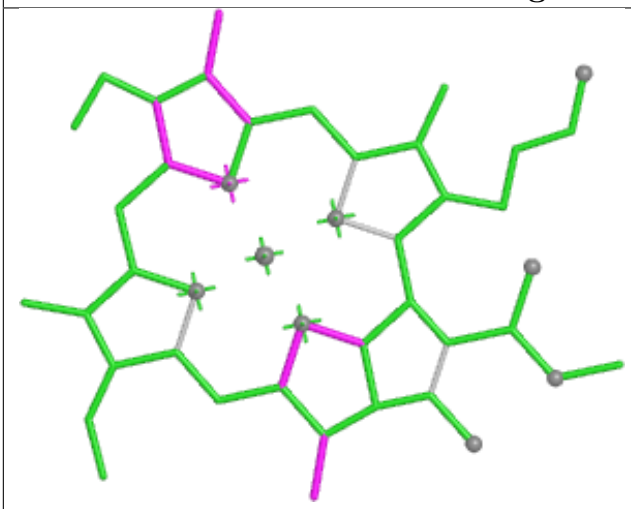


Rings

Ligand CLA 3 315



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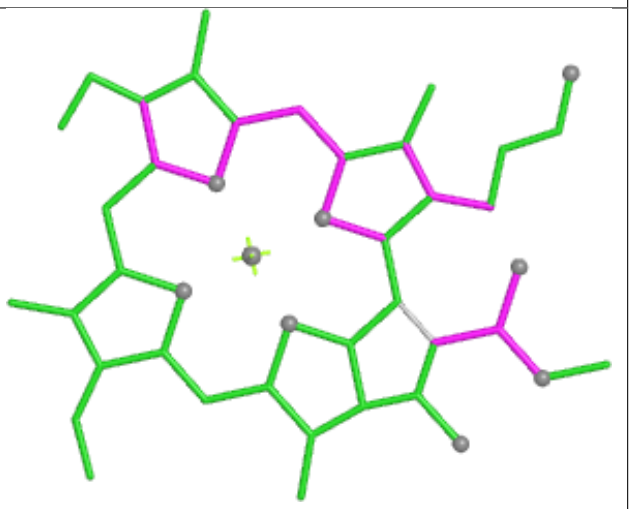

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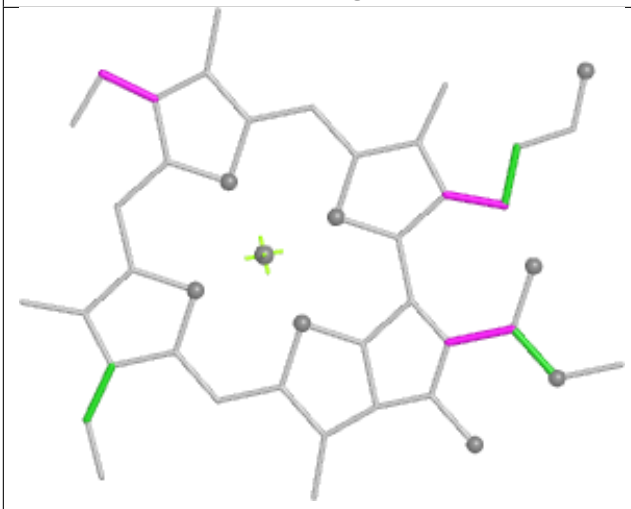

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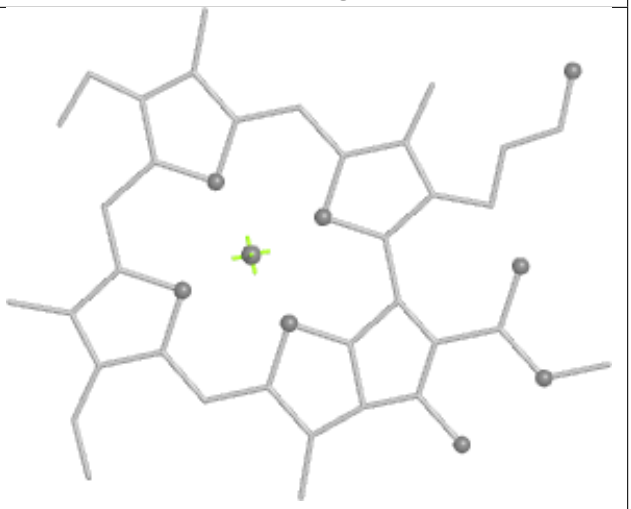
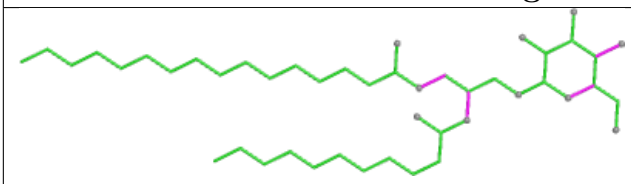


Rings

Ligand LMG k 101



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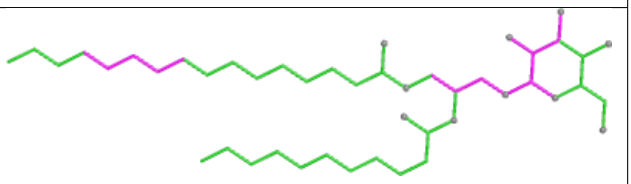
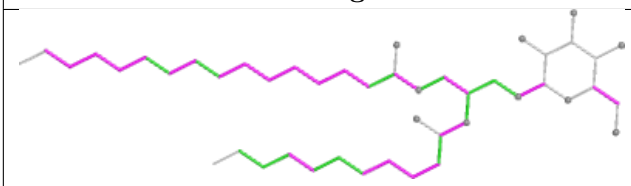


Bond angles



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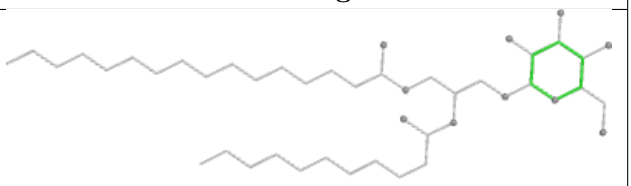
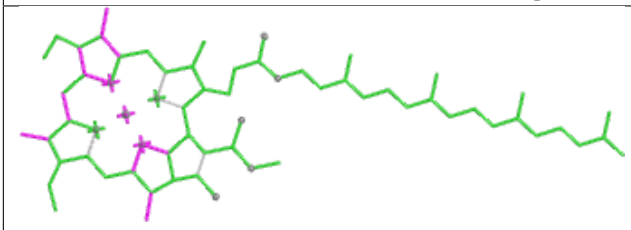


Rings

Ligand CLA 6 309



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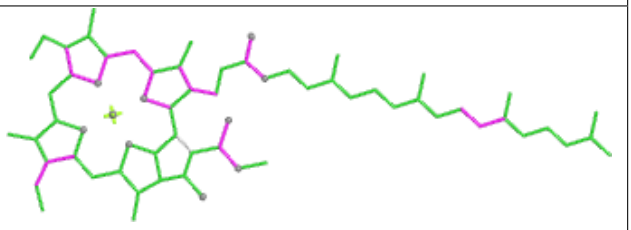
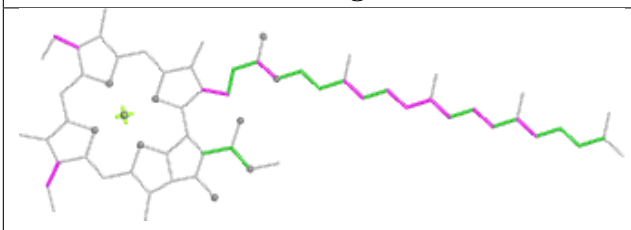


Bond angles



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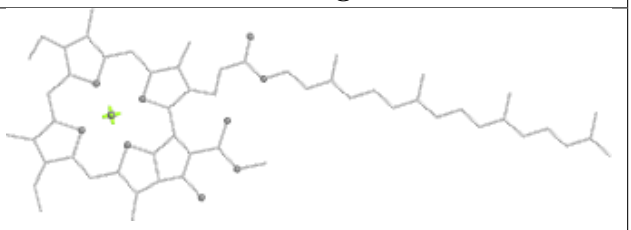
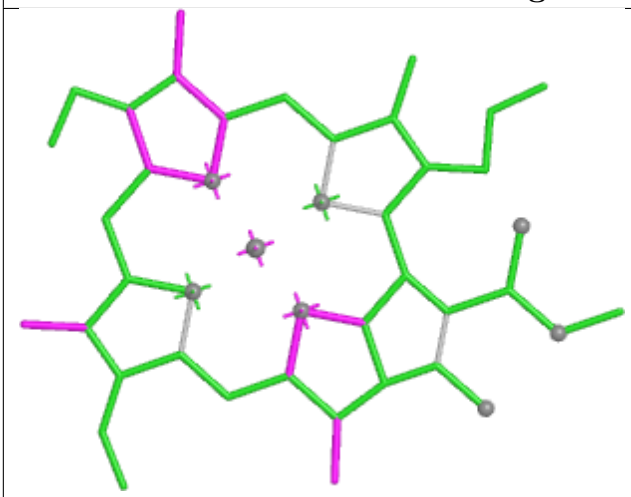


Rings

Ligand CLA 8 315



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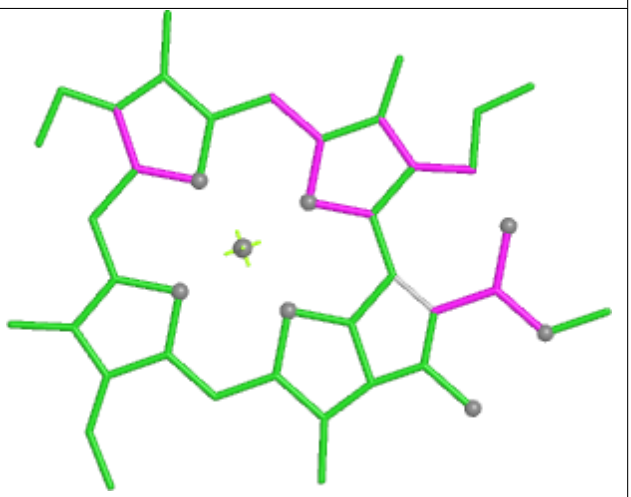

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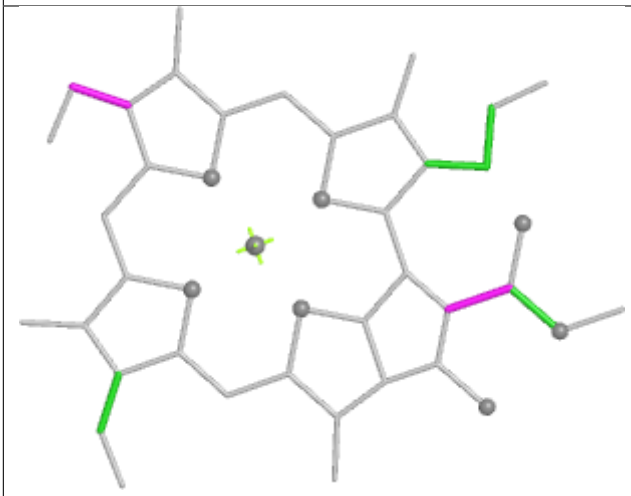

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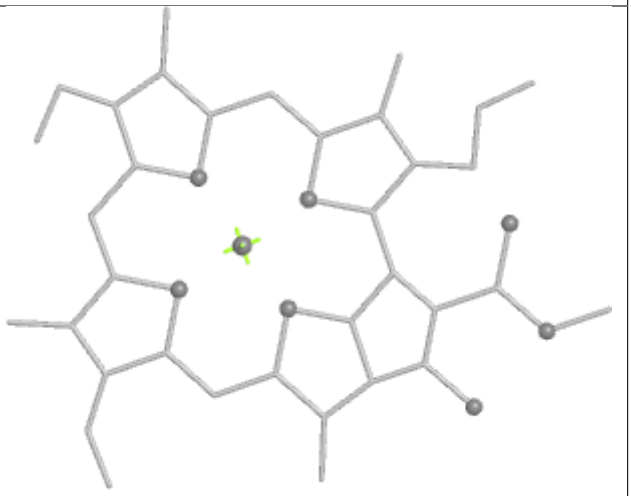
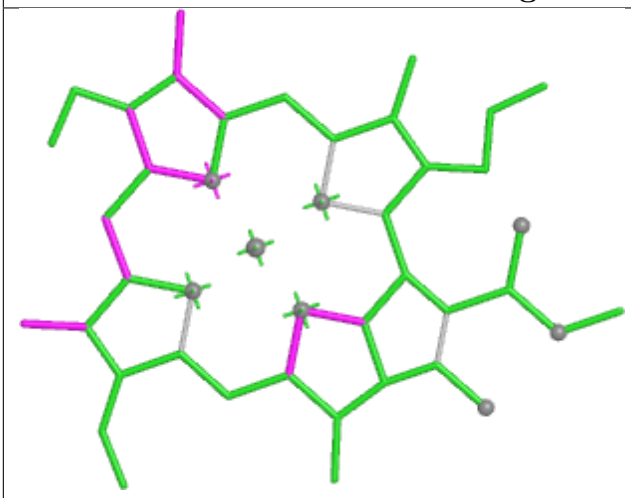


Rings

Ligand CLA 14 315



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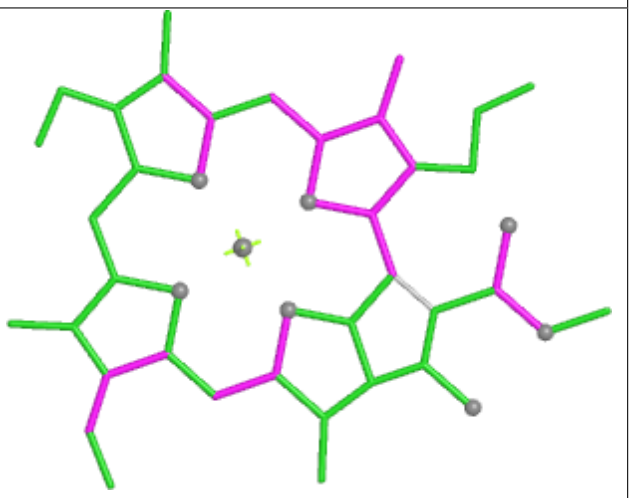
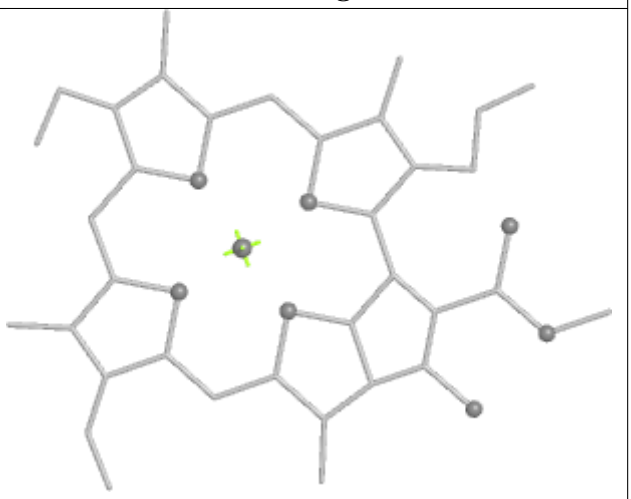


Bond angles

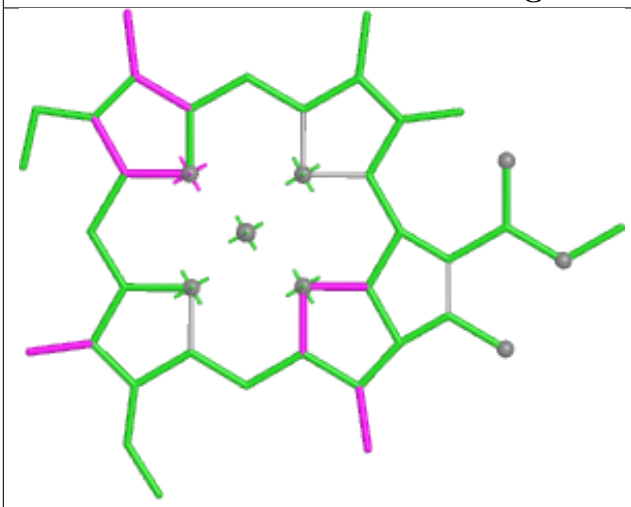


Torsions



Rings

Ligand CLA P 605



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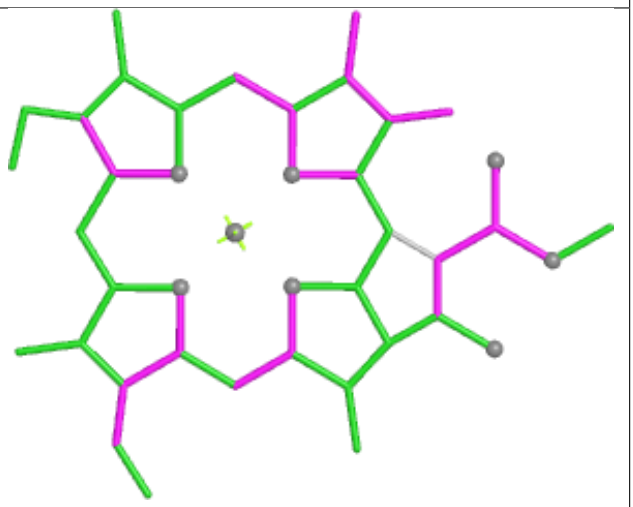
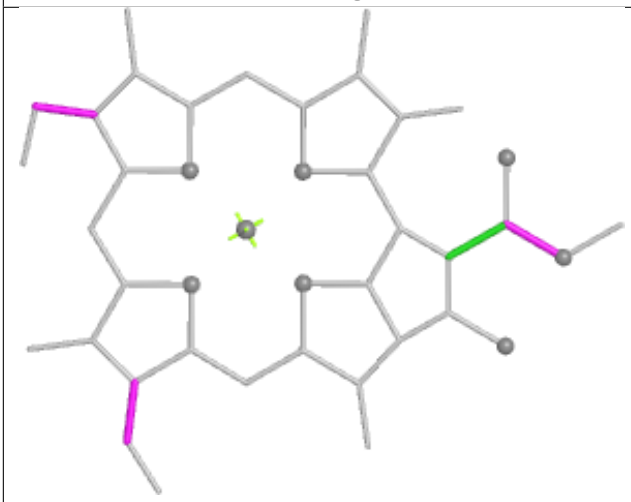


Bond angles



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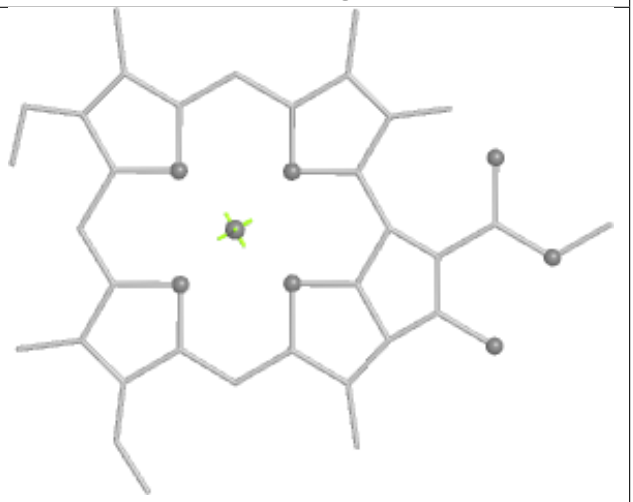
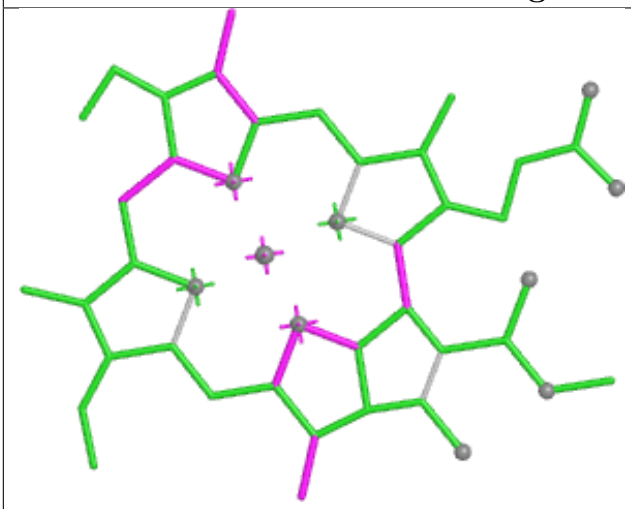


Rings

Ligand CLA 5 311



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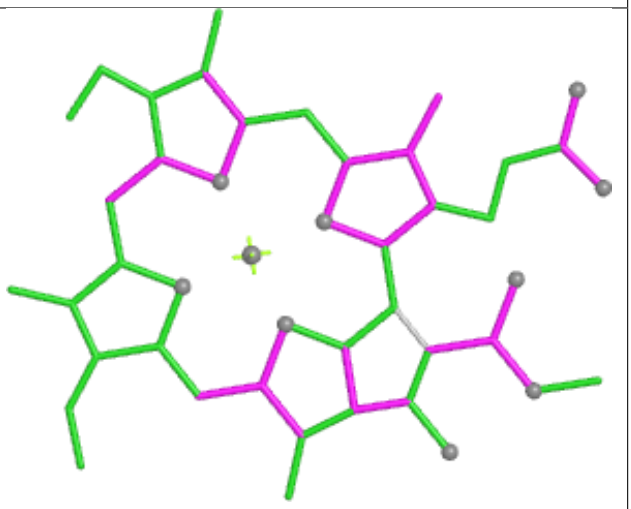
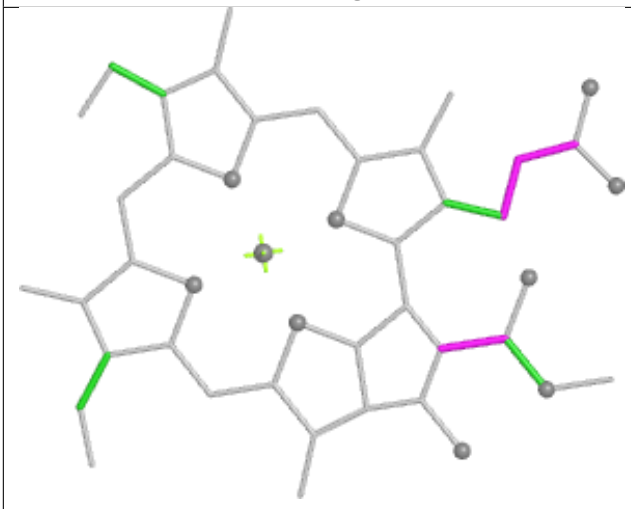


Bond angles

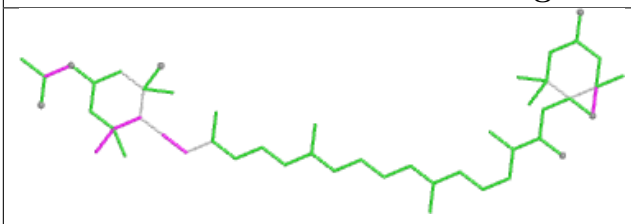


Torsions



Rings

Ligand A86 5 304



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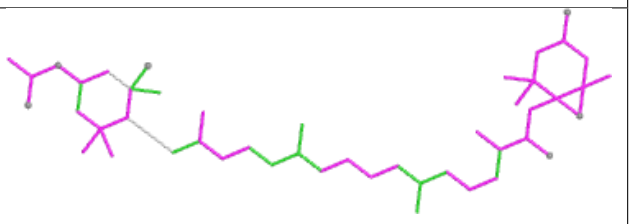
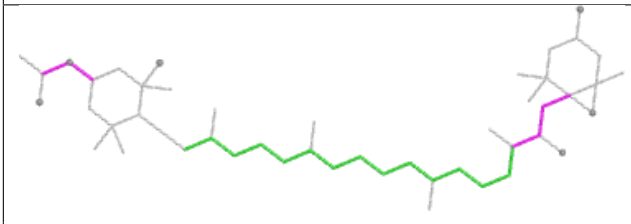
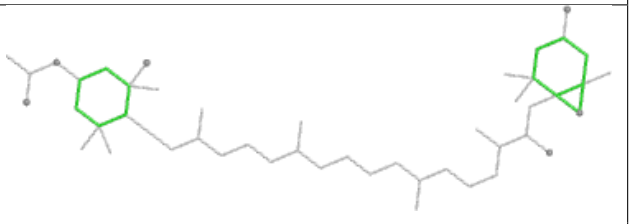


Bond angles

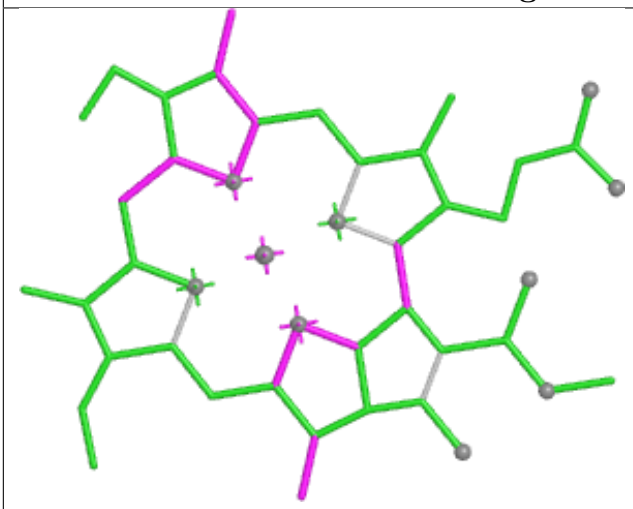


Torsions



Rings

Ligand CLA 15 311



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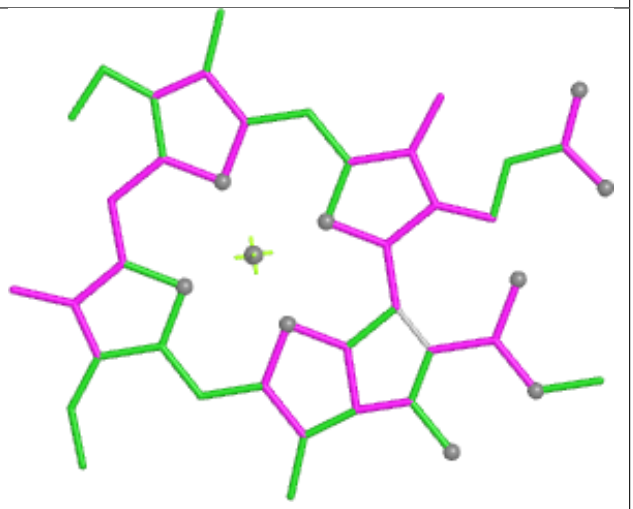

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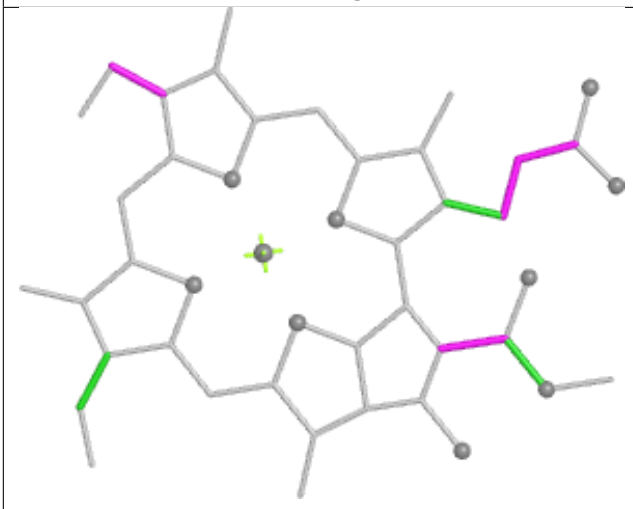
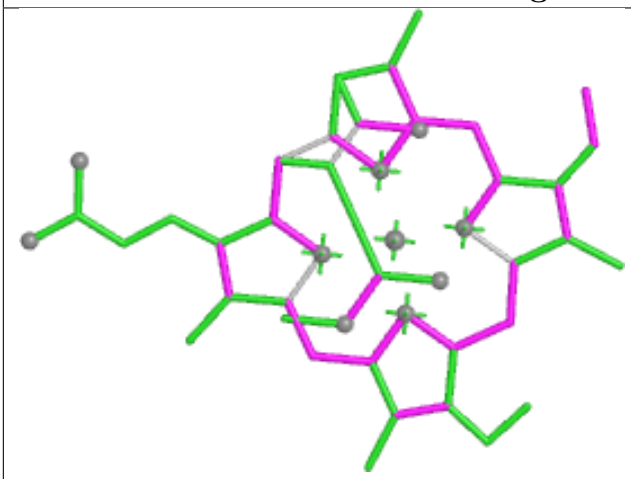


Torsions



Rings

Ligand KC2 4 310



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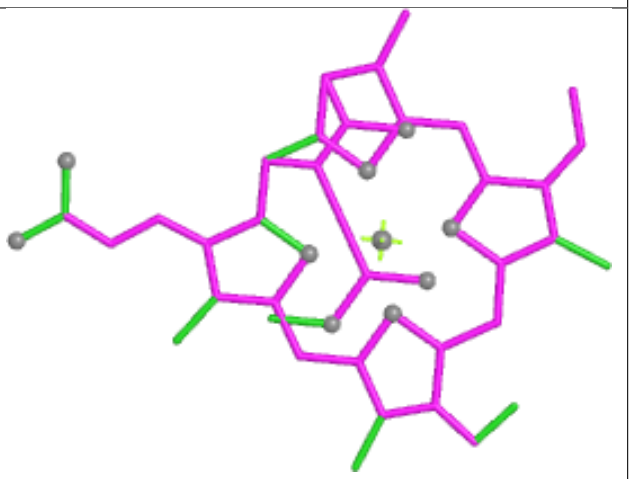

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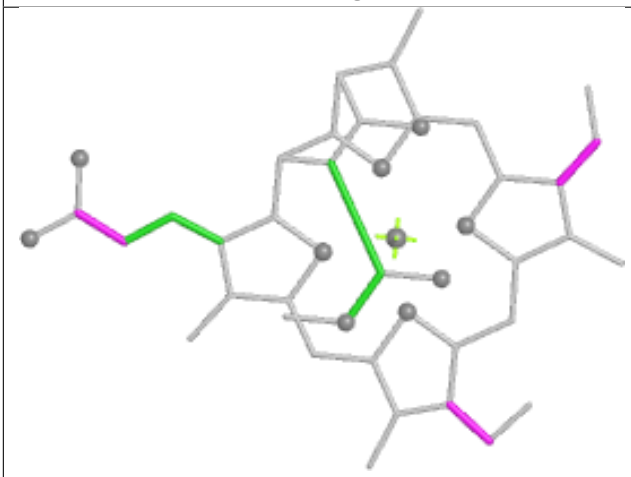

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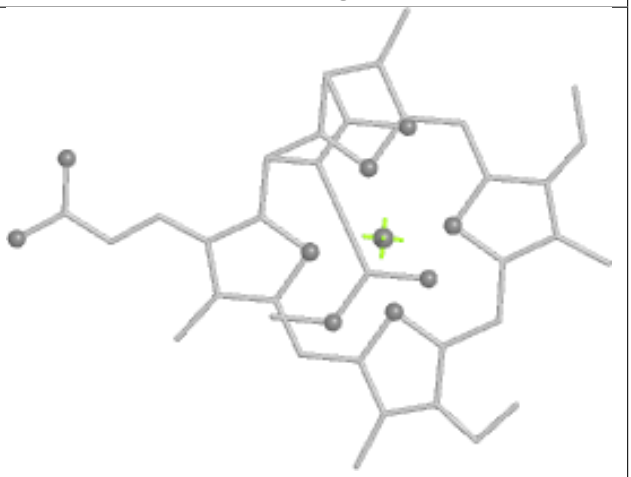
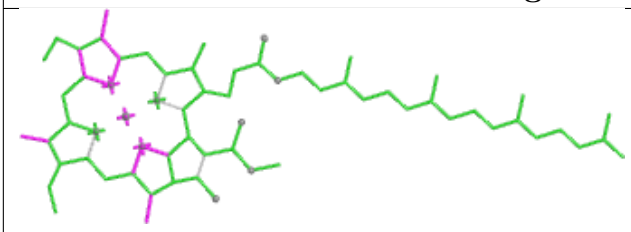


Rings

Ligand CLA C 502



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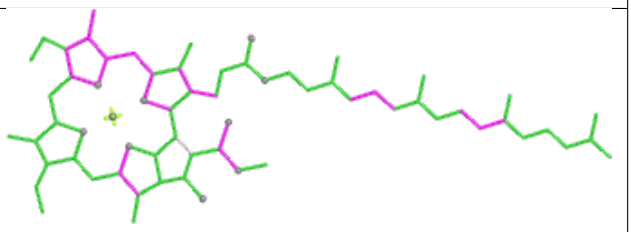

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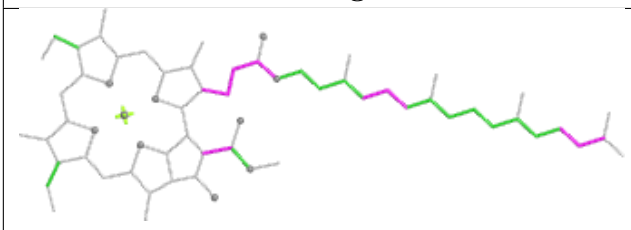

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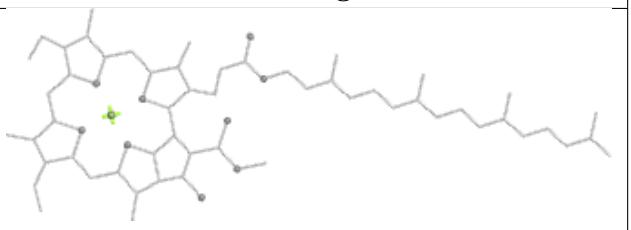
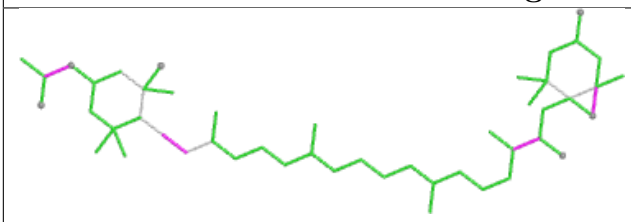


Rings

Ligand A86 14 303



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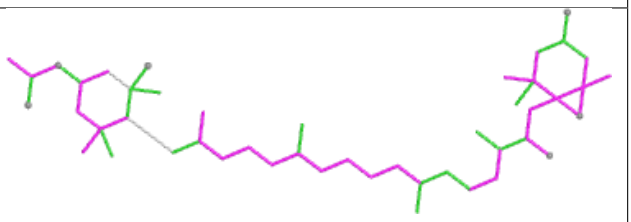

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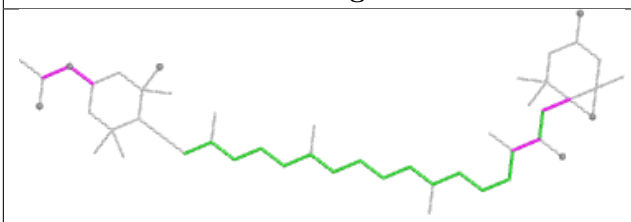

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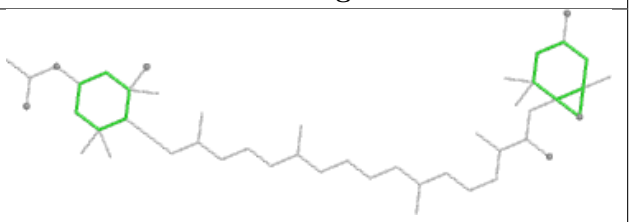
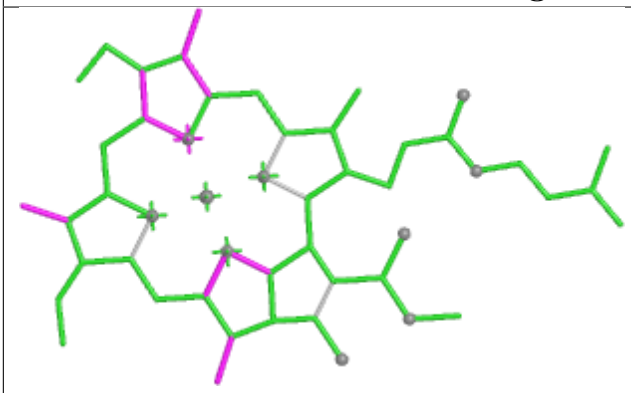


Rings

Ligand CLA 1 310



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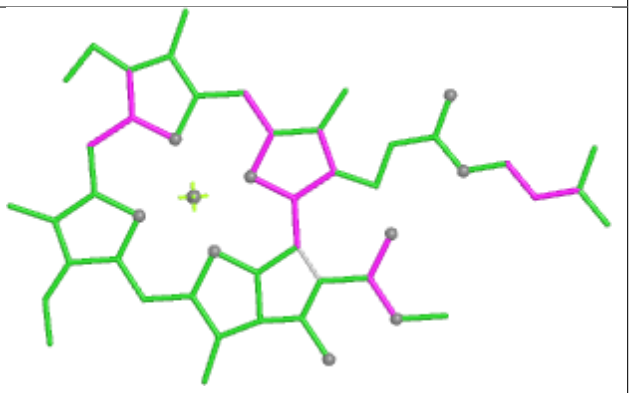

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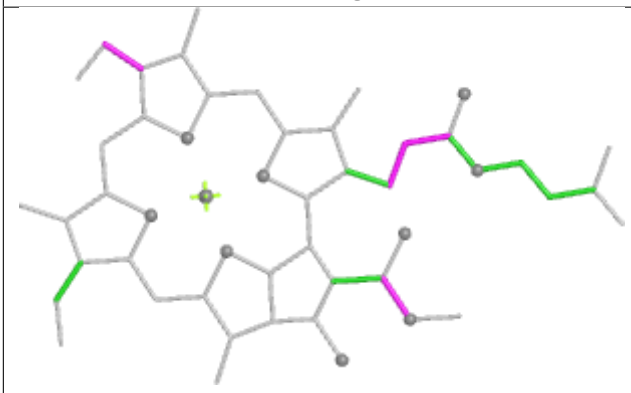

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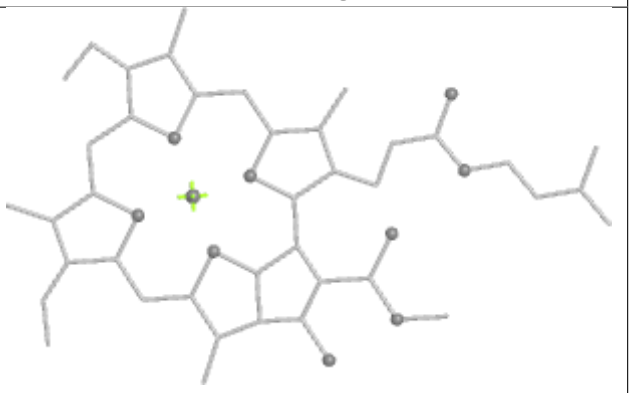

Rings

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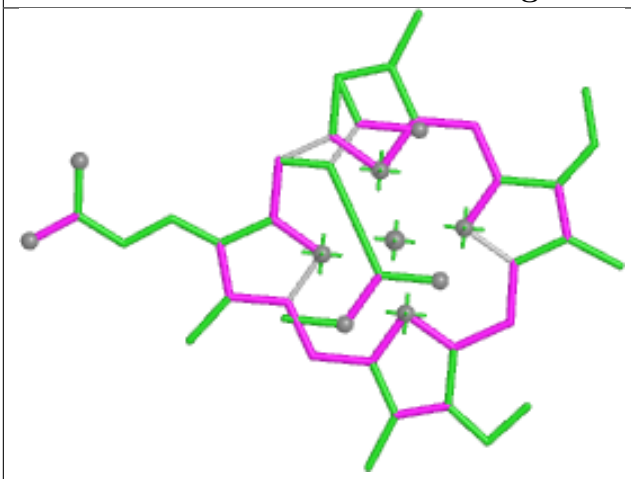

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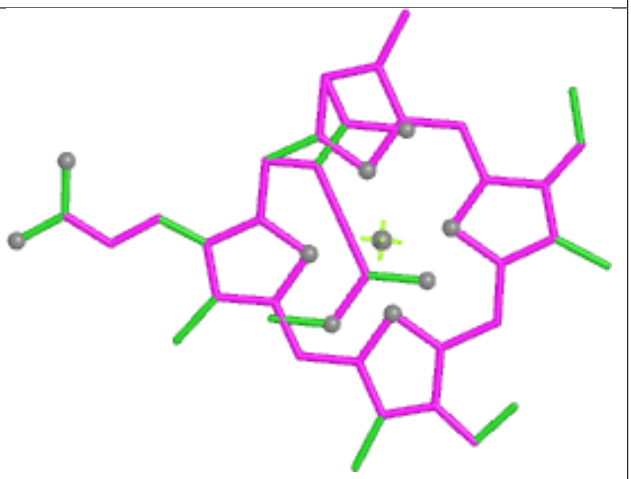

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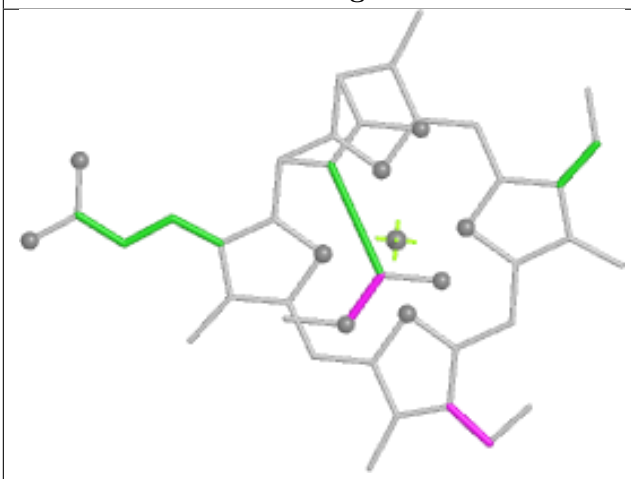

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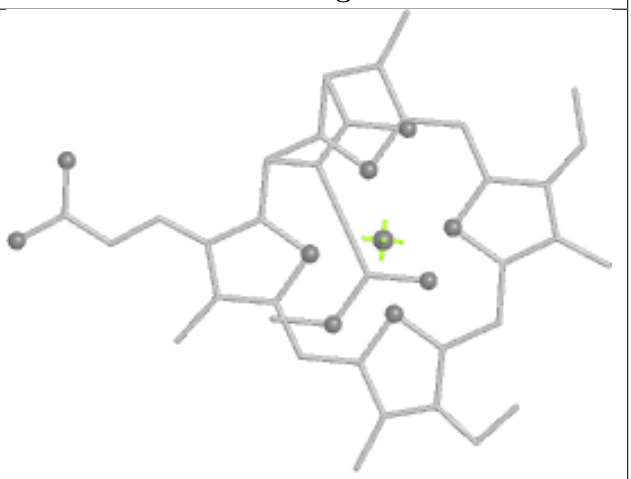
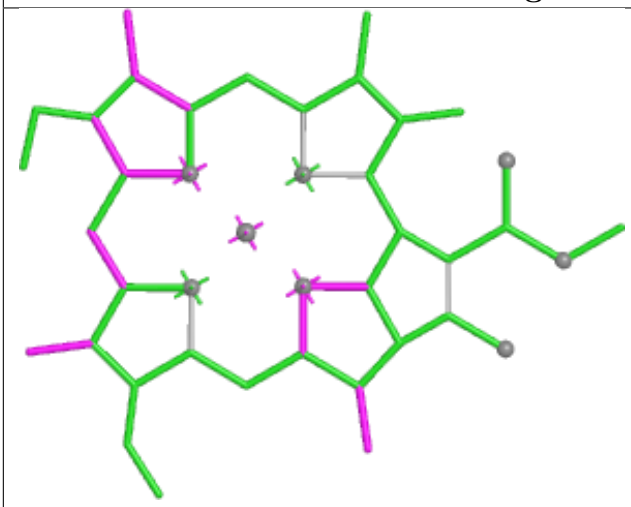


Rings

Ligand CLA P 610



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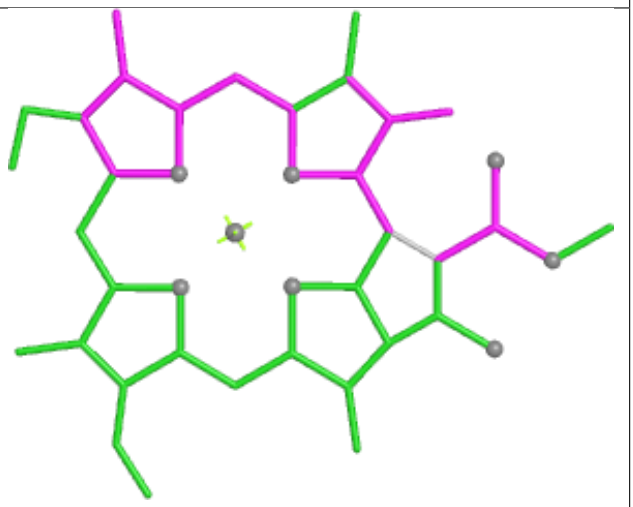
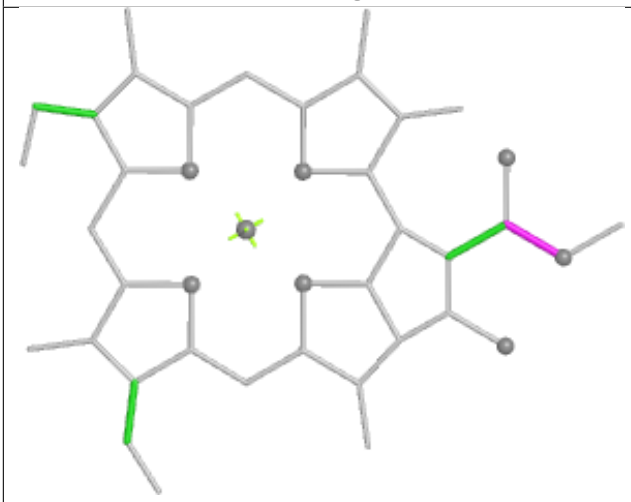


Bond angles



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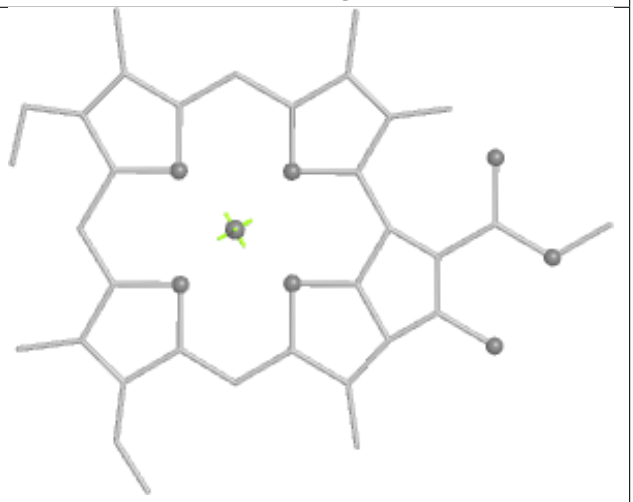
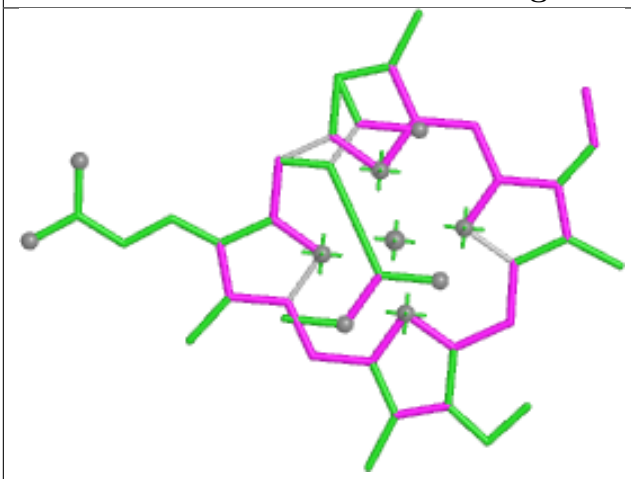


Rings

Ligand KC2 2 310



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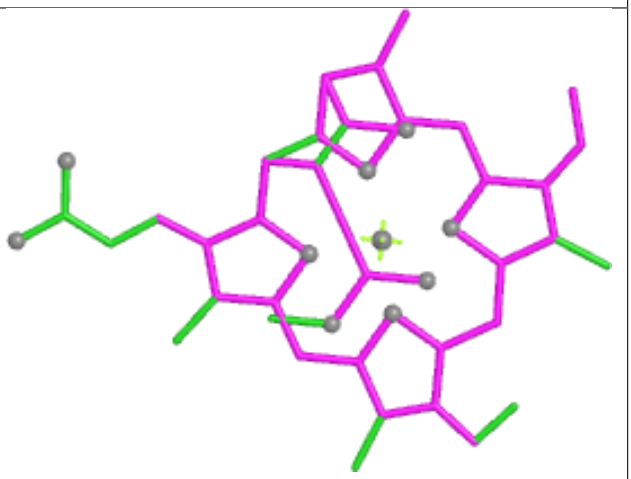

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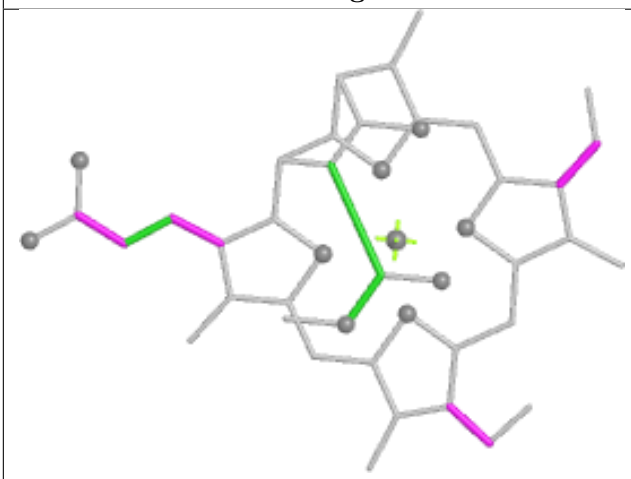

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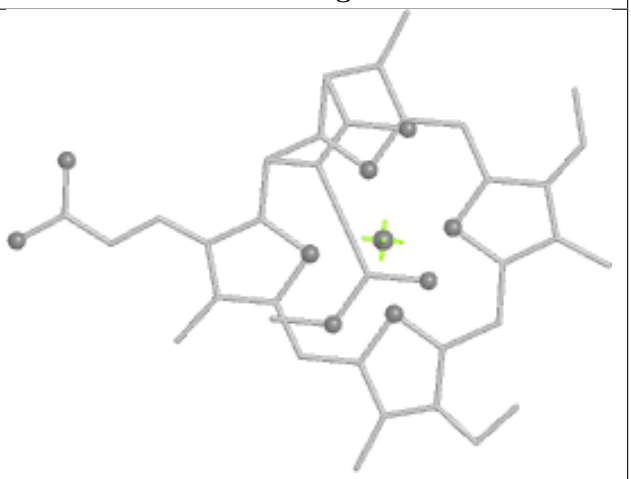

Rings

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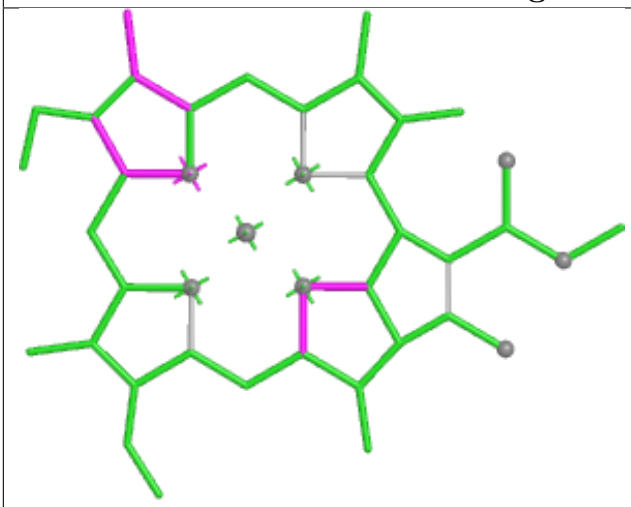

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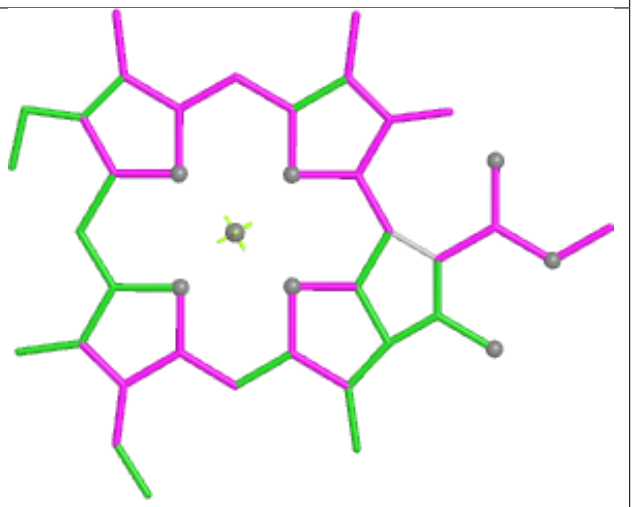

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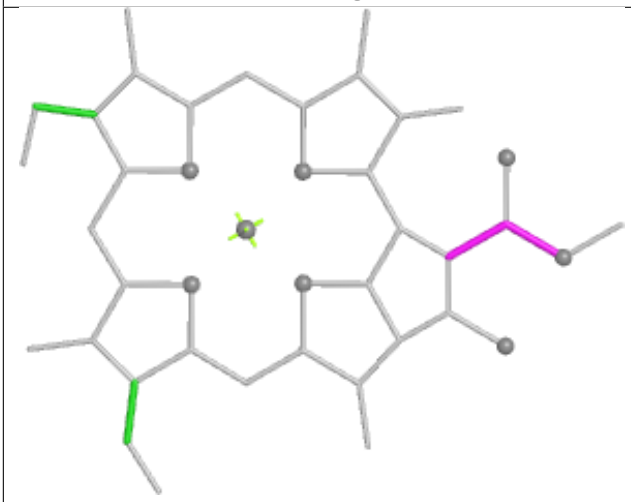

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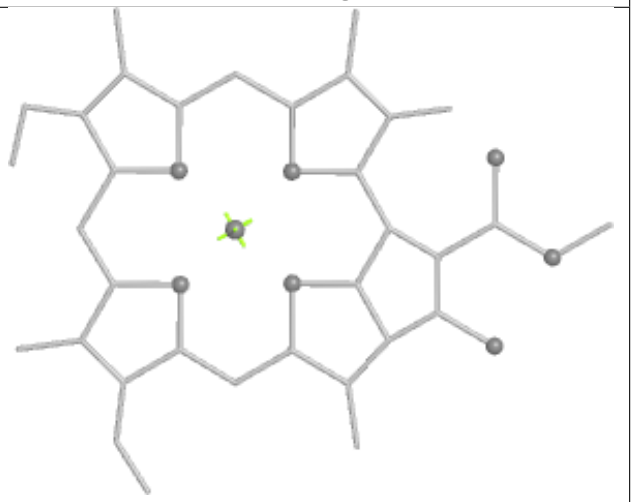

Rings

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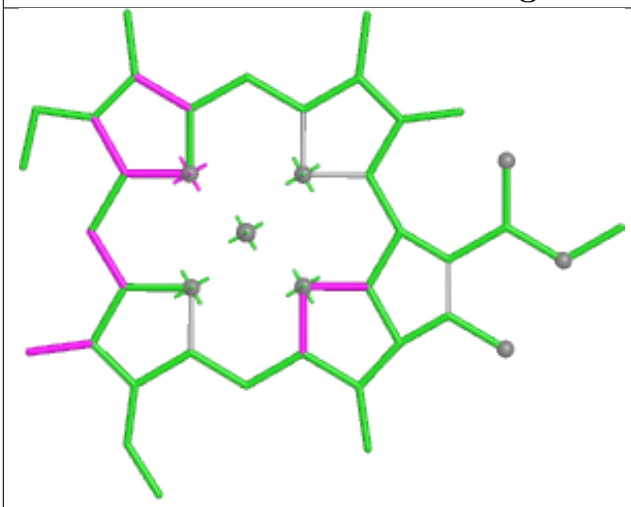

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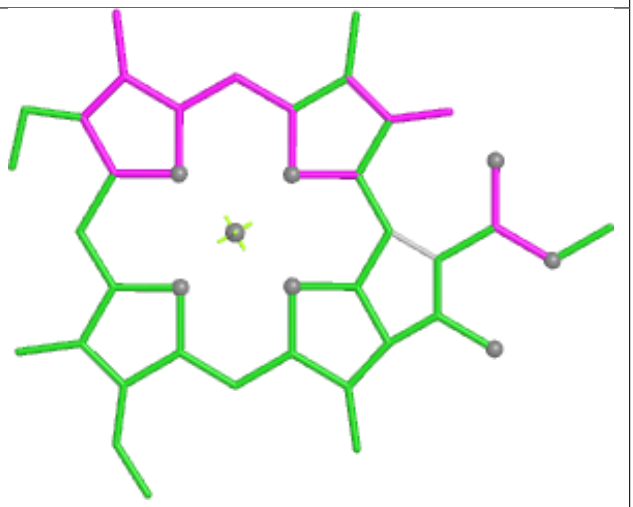

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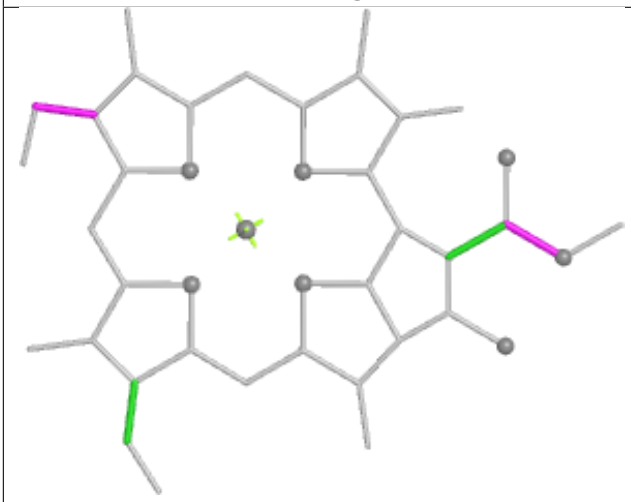

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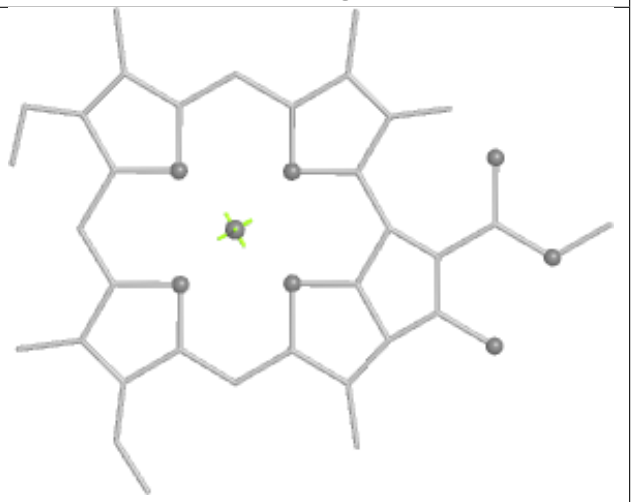
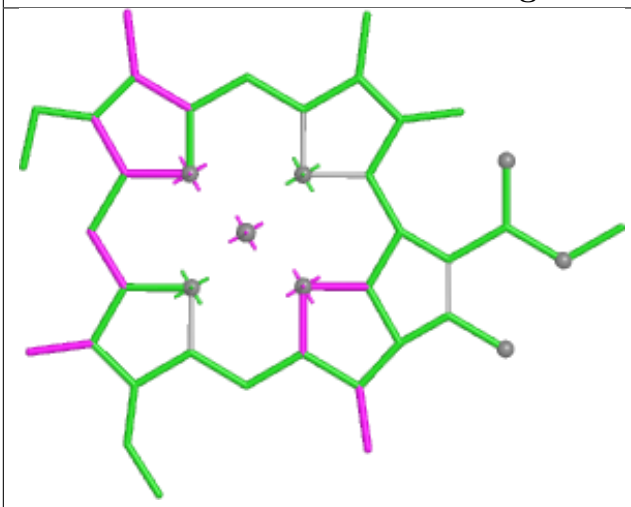


Rings

Ligand CLA 17 308



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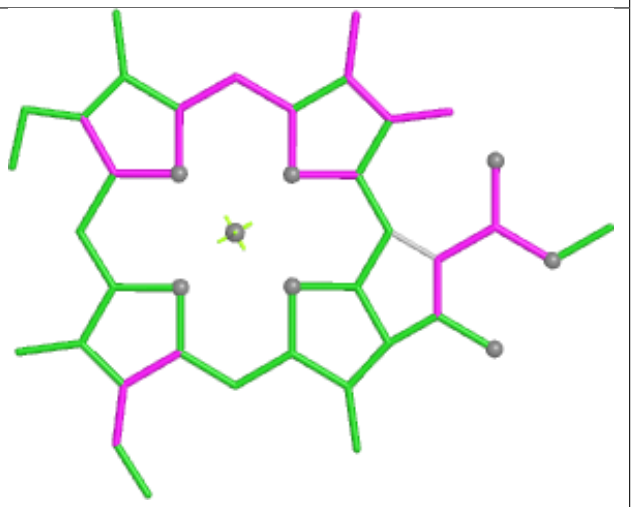

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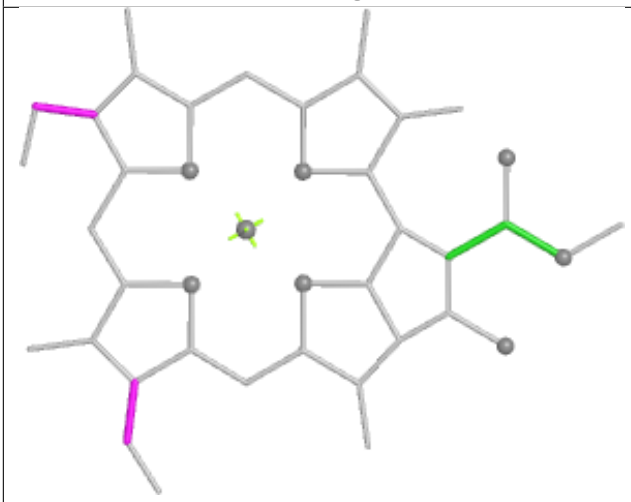

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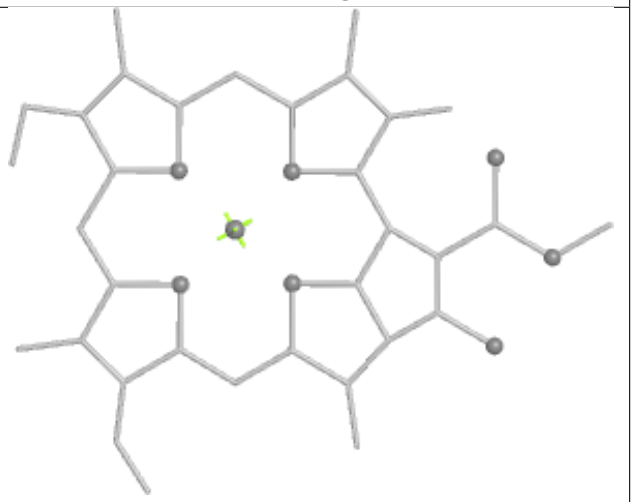
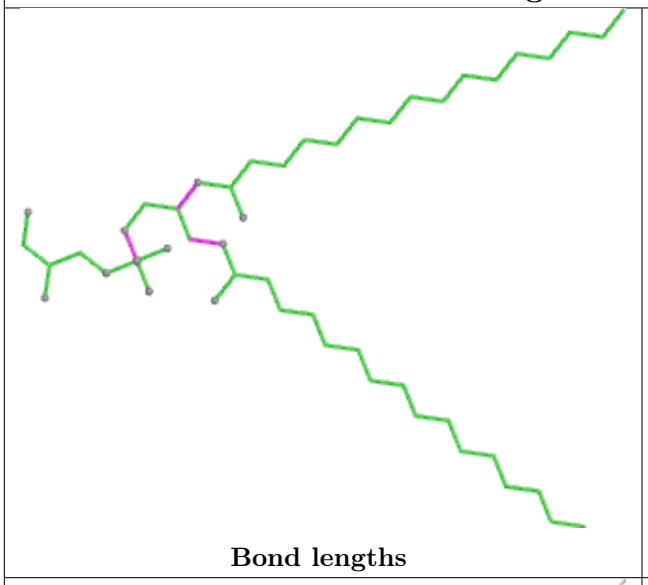


Rings

Ligand LHG L 101



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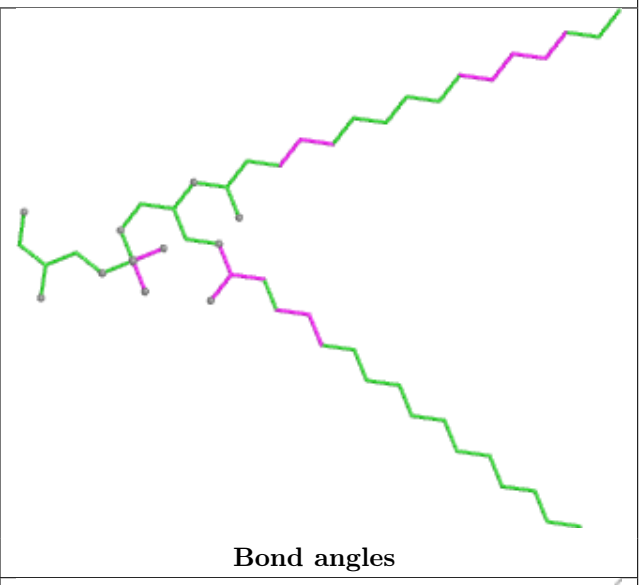

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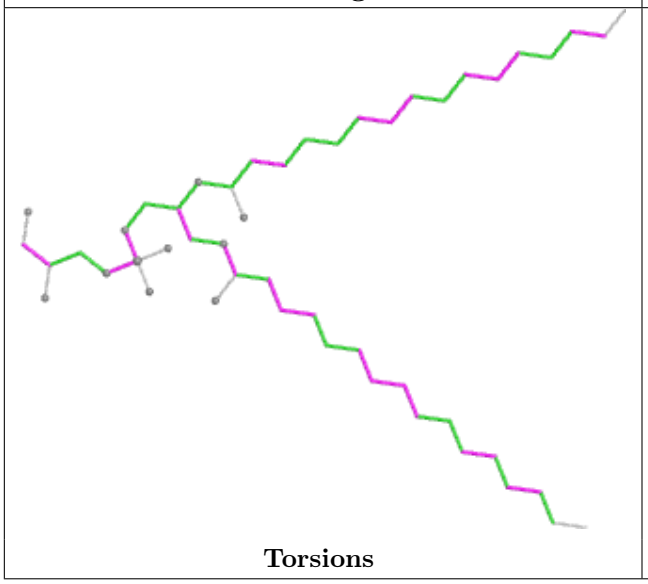

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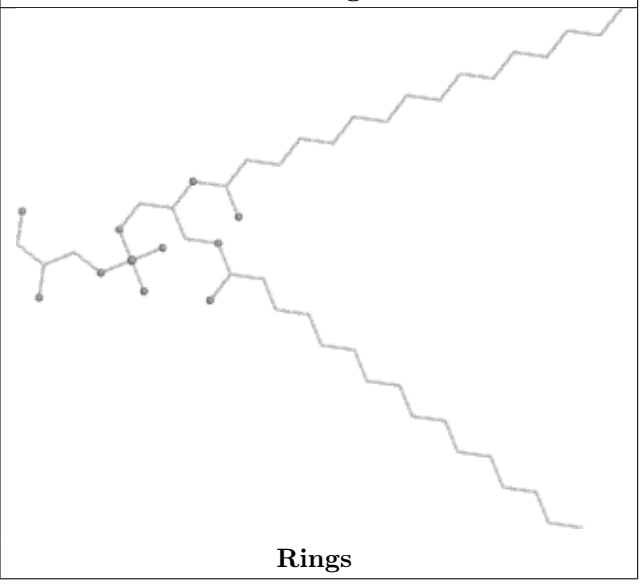
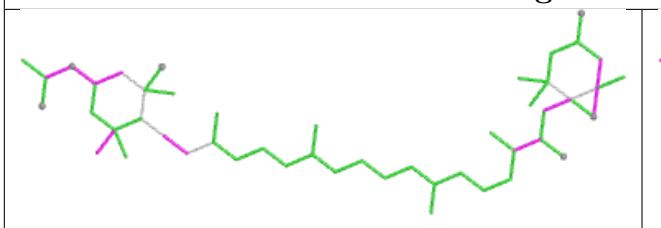


Rings

Ligand A86 3 305



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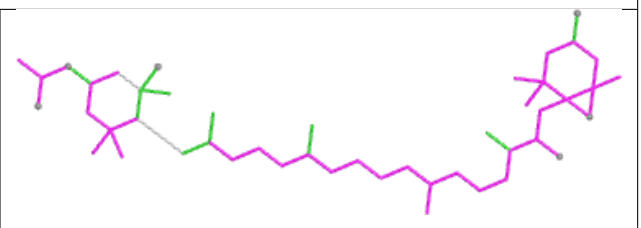

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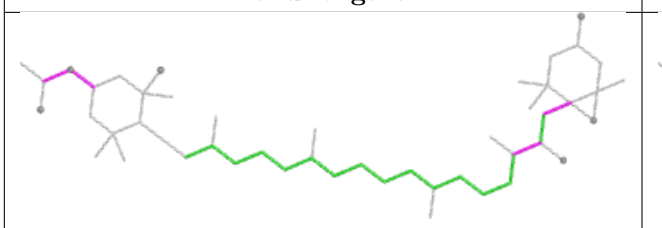

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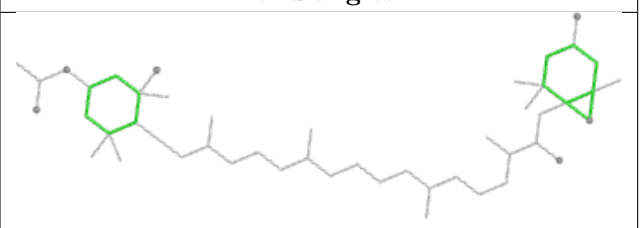
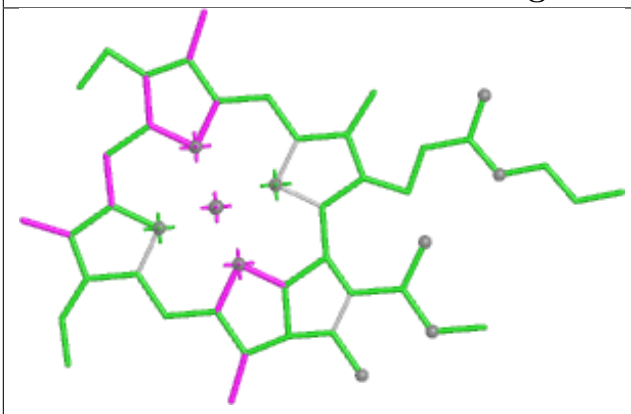


Rings

Ligand CLA 2 312



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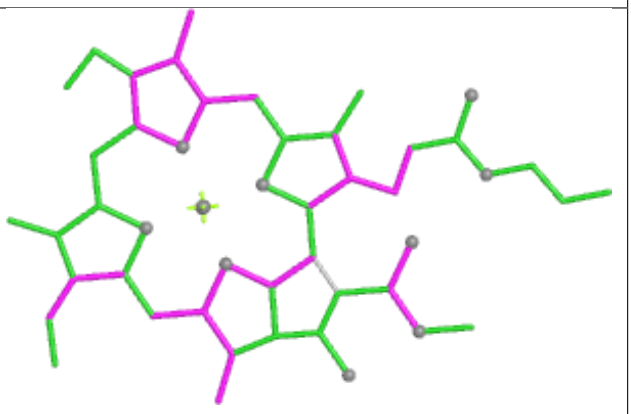
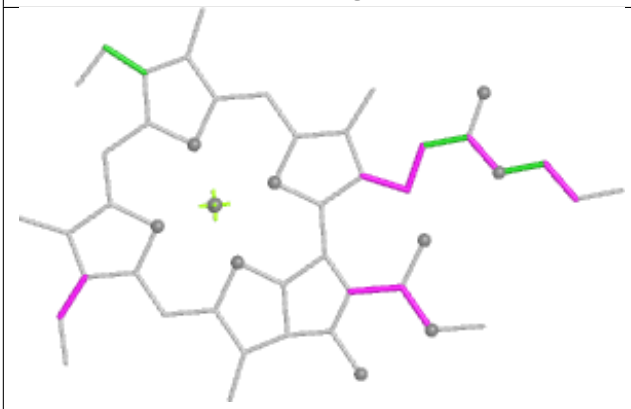


Bond angles



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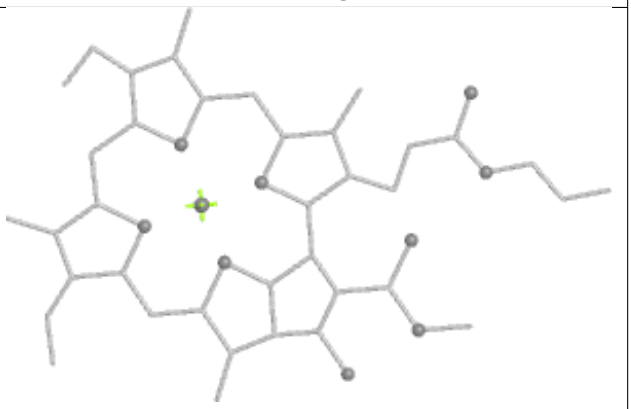
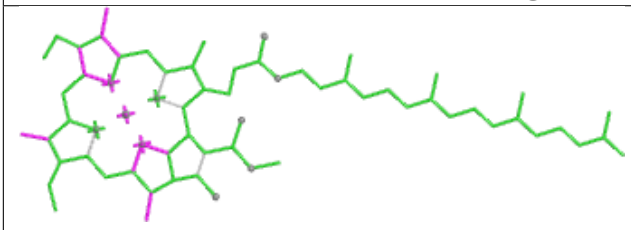
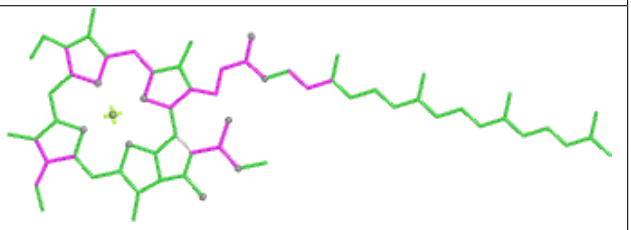


Rings

Ligand CLA w 203



Bond lengths



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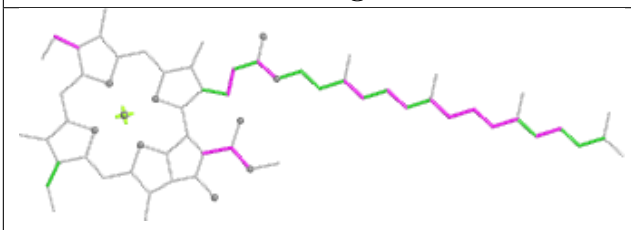

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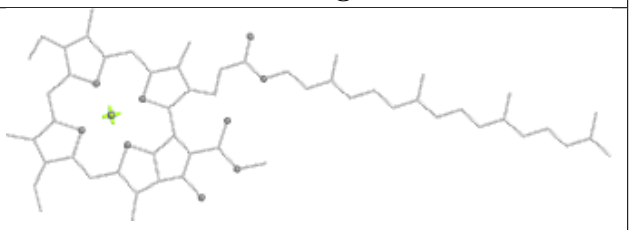

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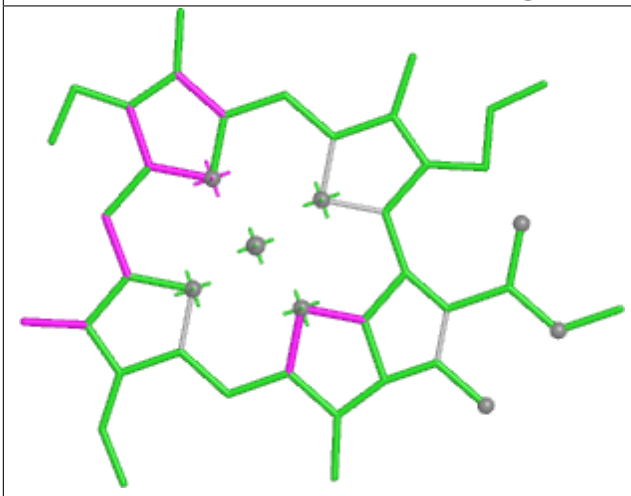

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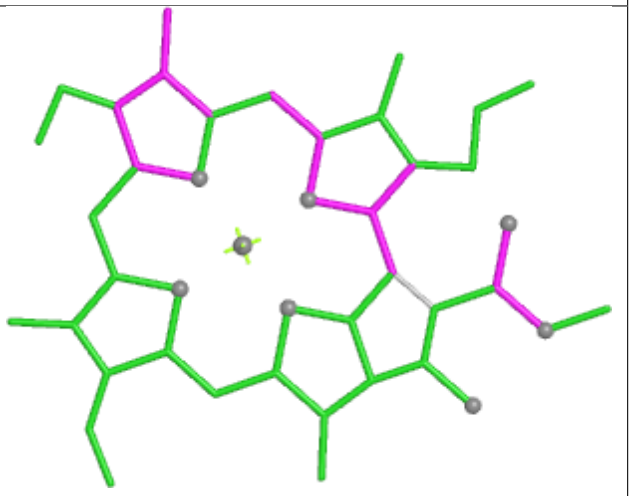

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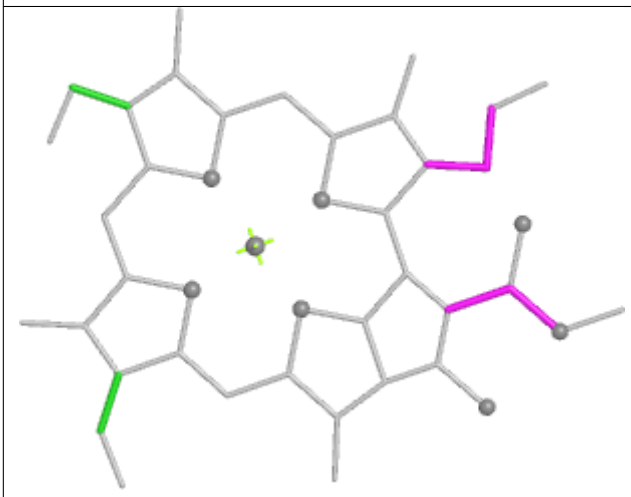

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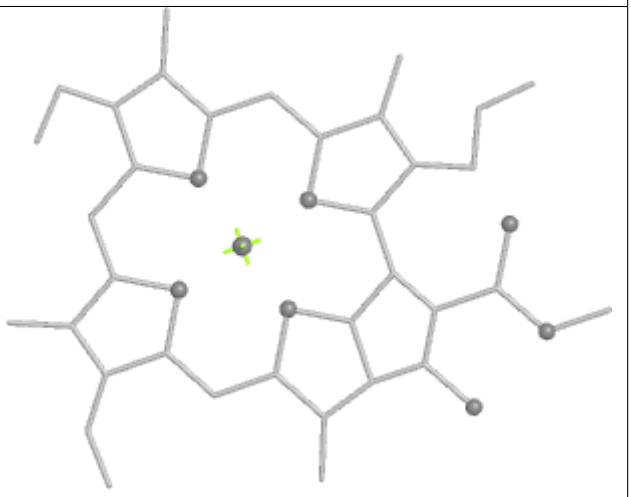

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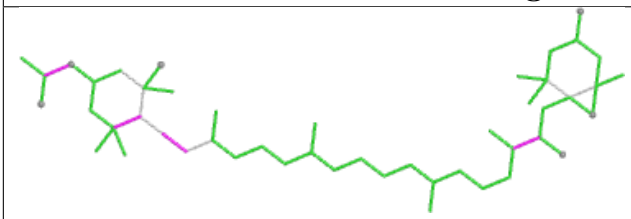

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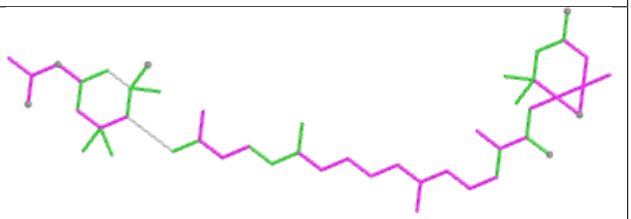

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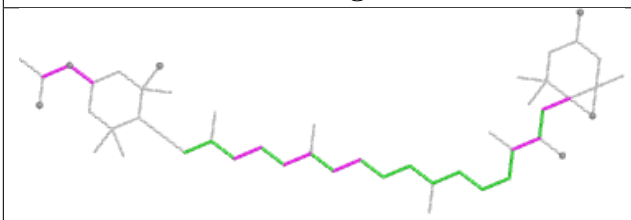

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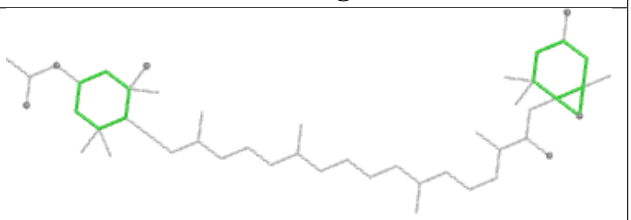

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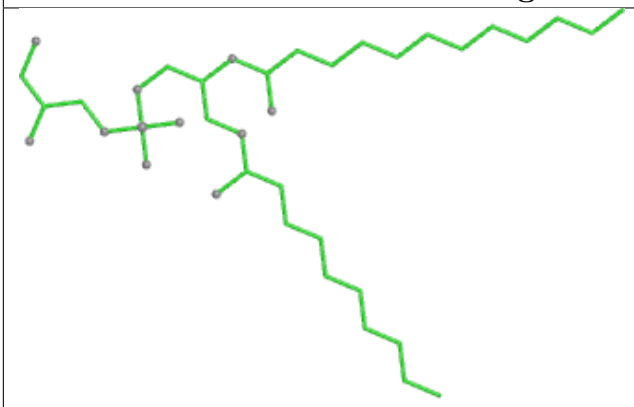

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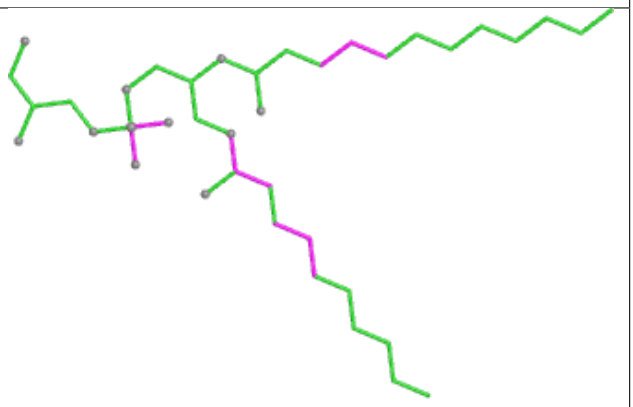

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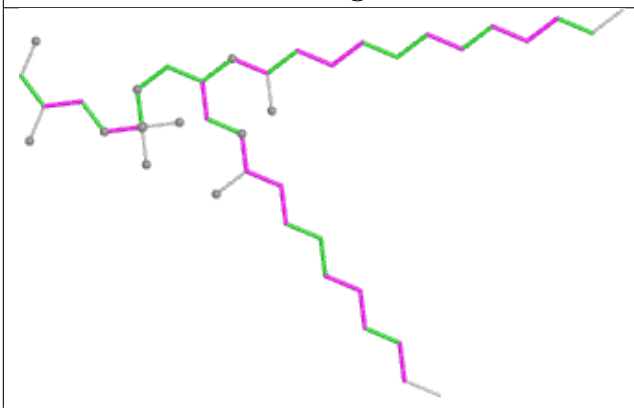

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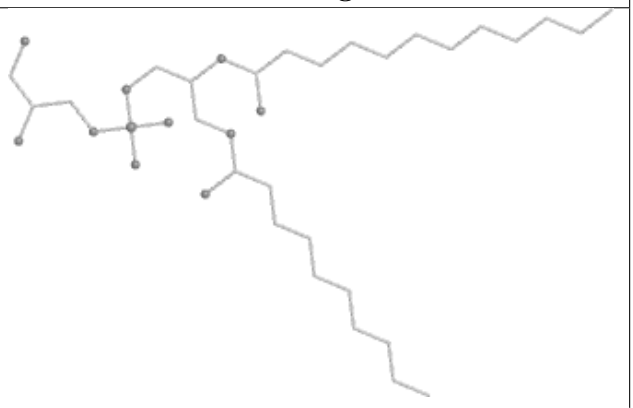

Rings

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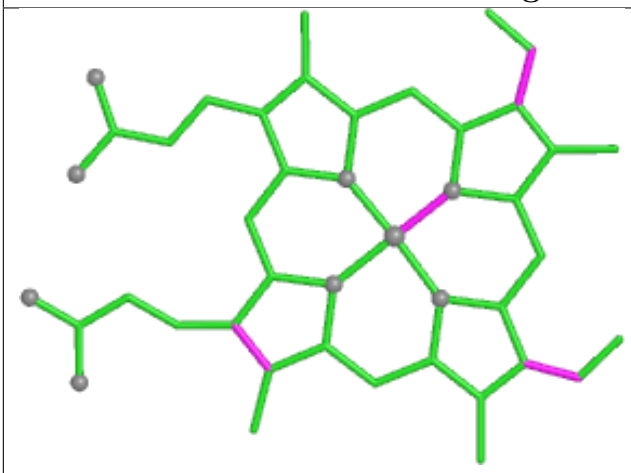

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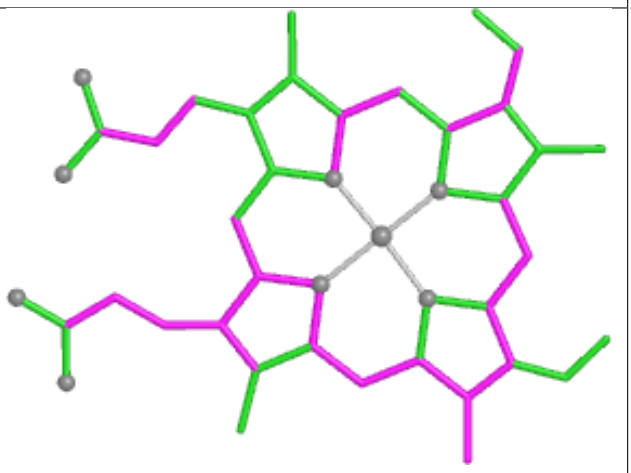

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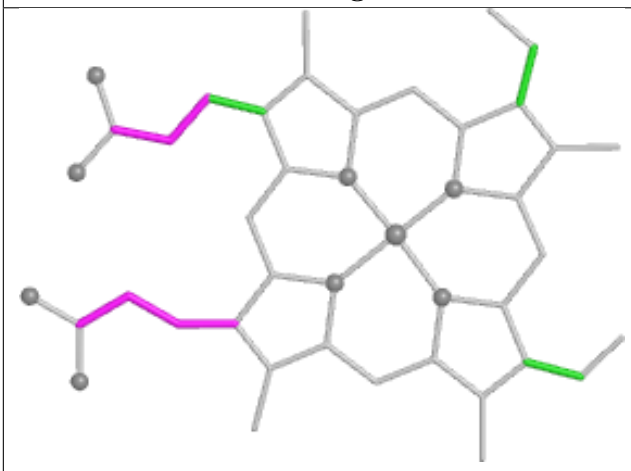

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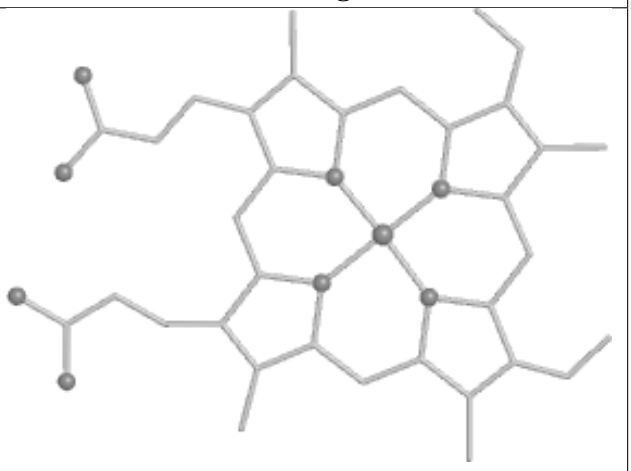

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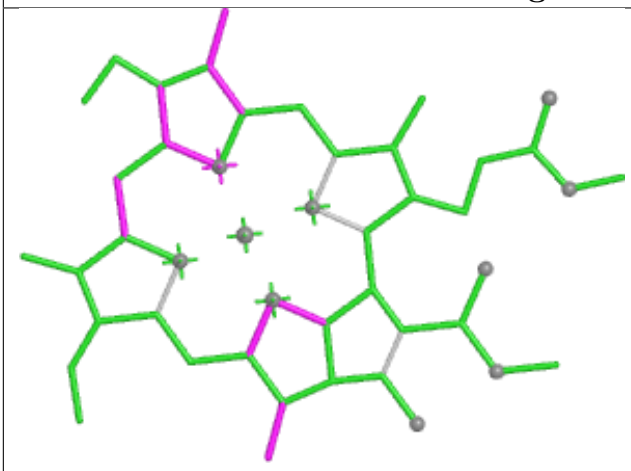

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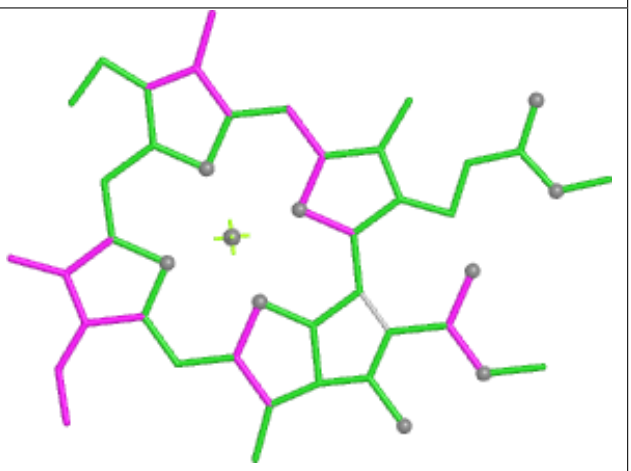

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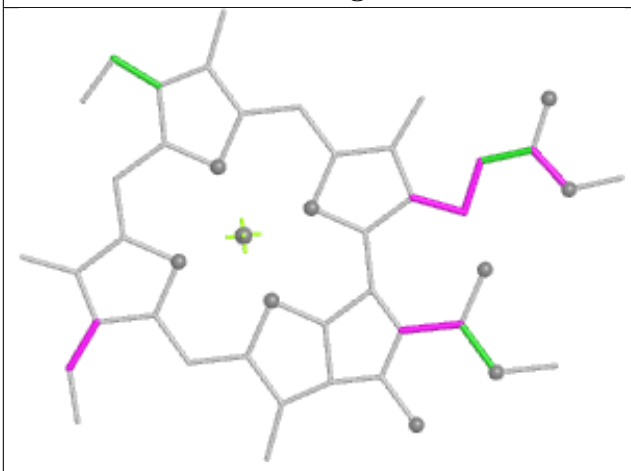

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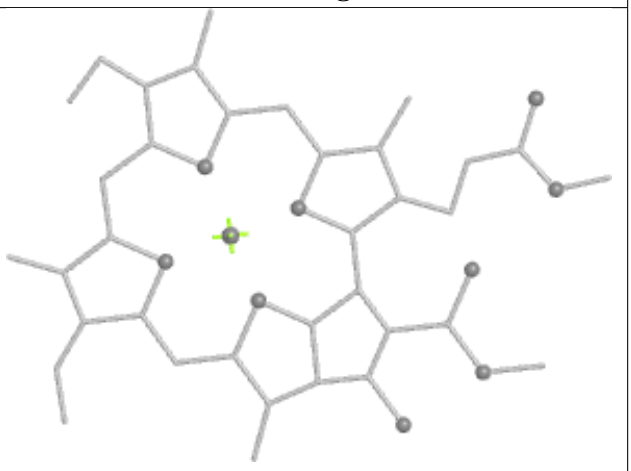

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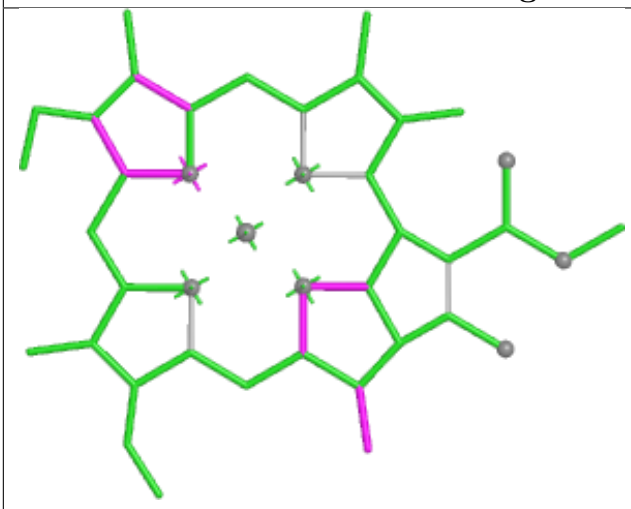

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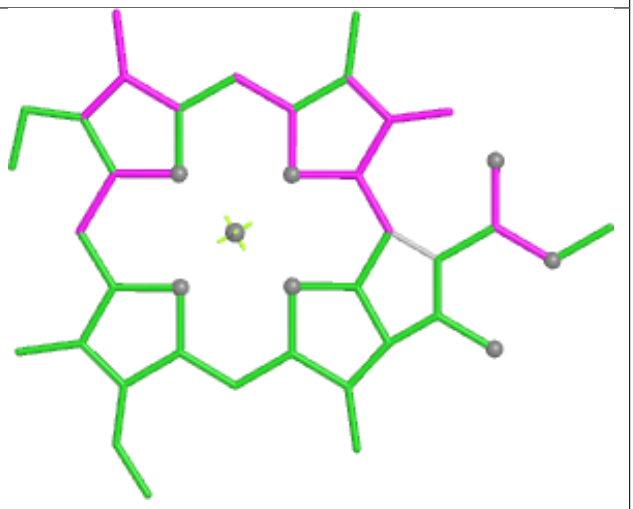

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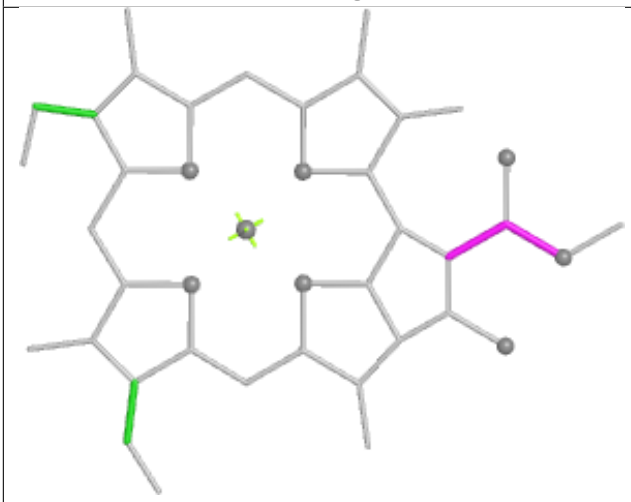

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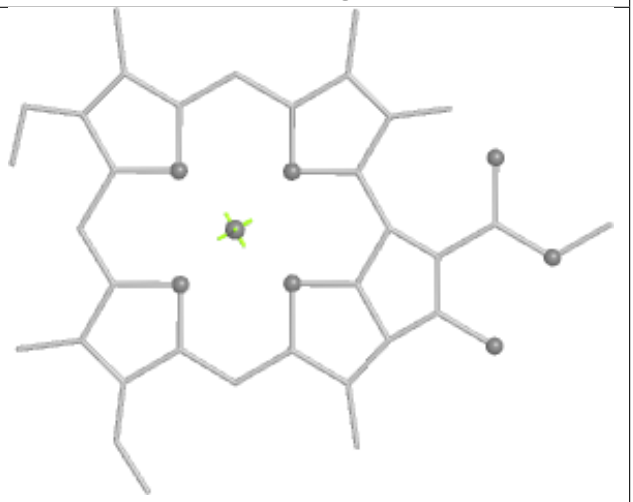

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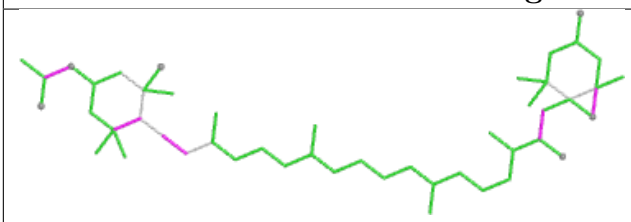

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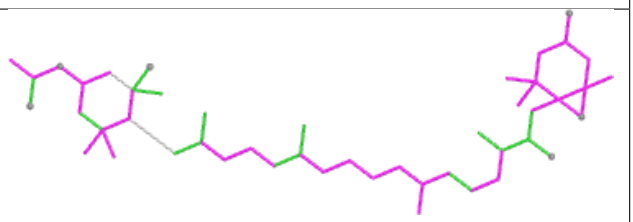

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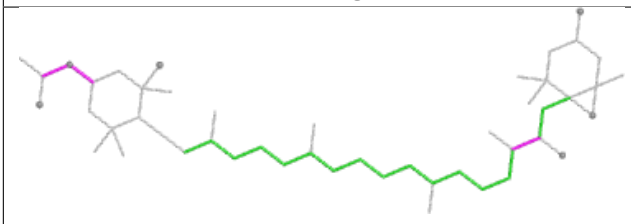

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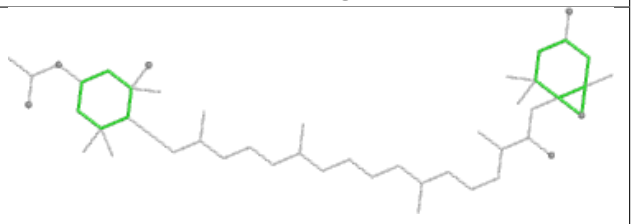

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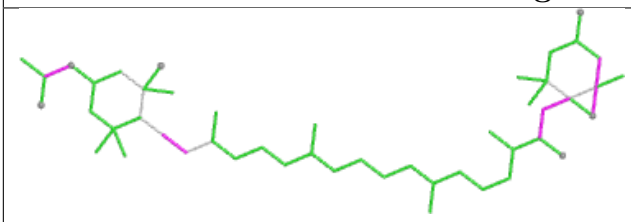

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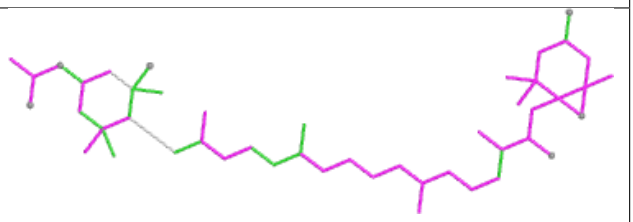

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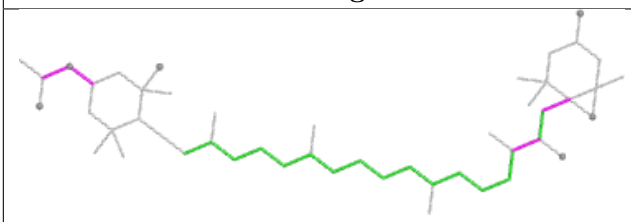

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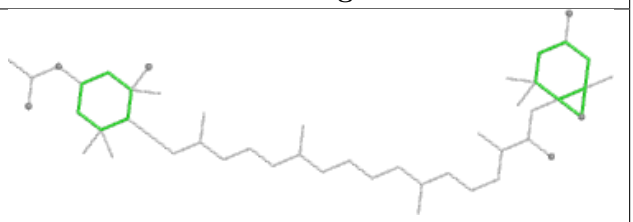

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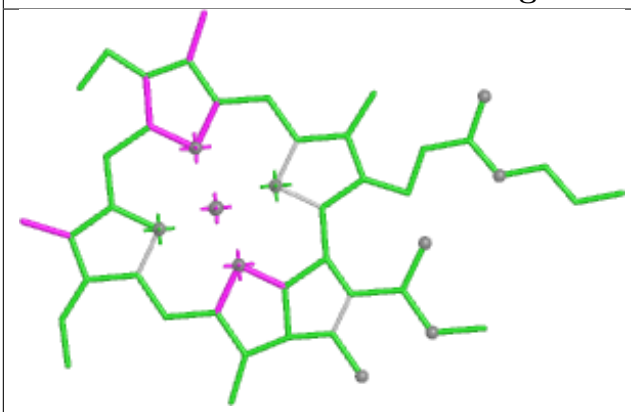

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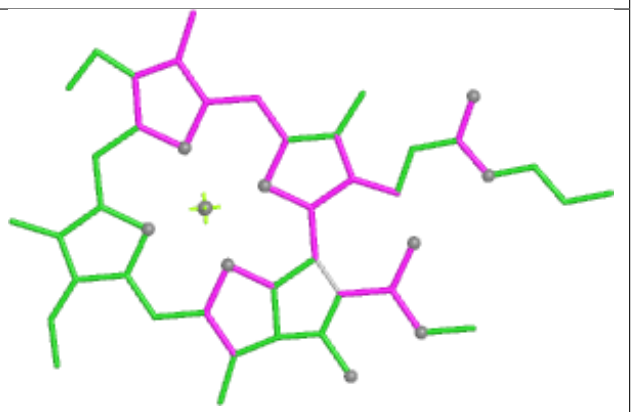

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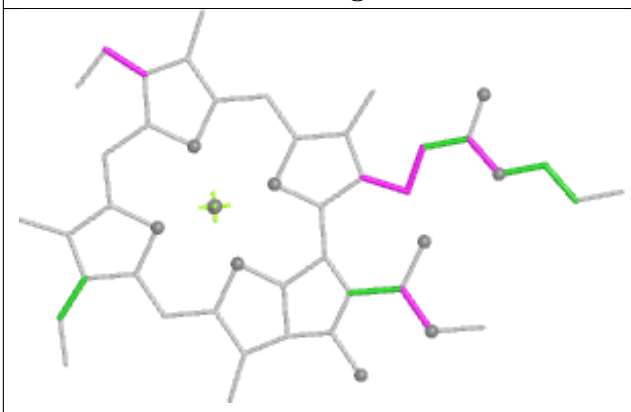

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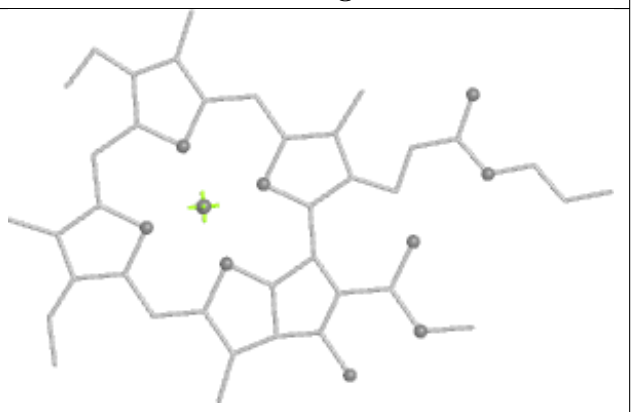

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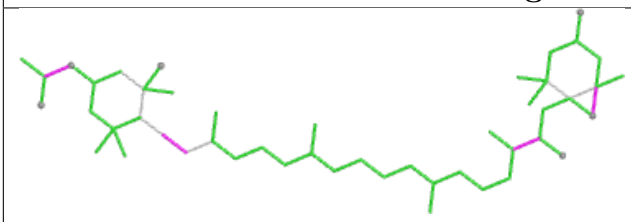

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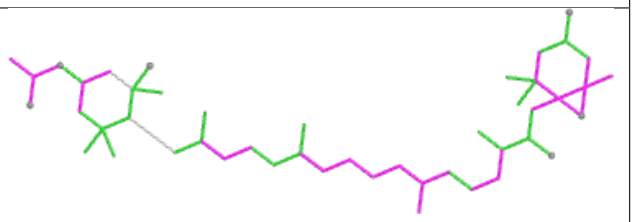

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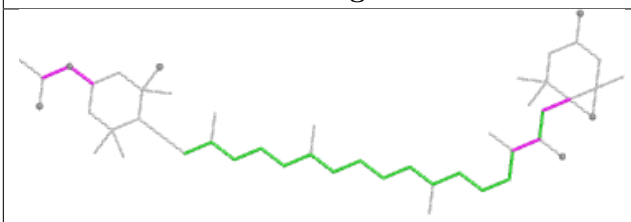

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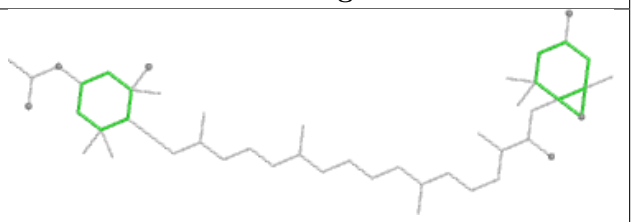

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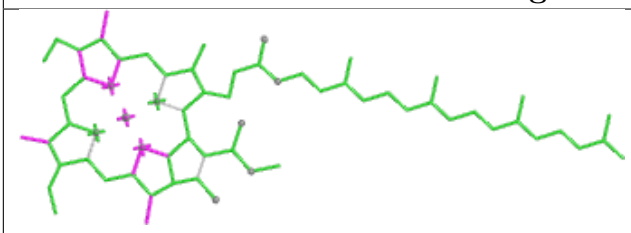

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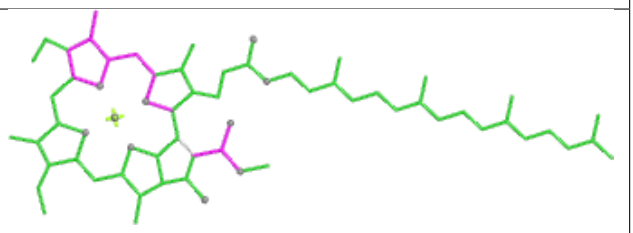

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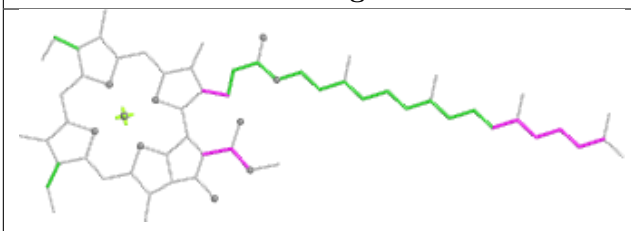

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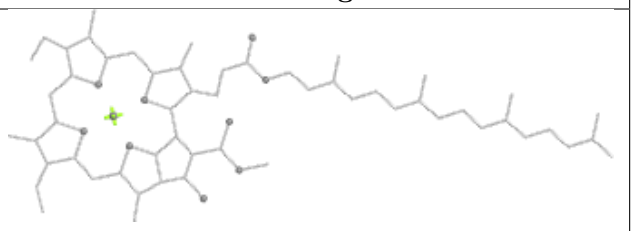

Rings

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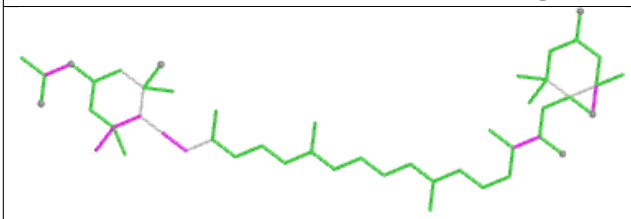

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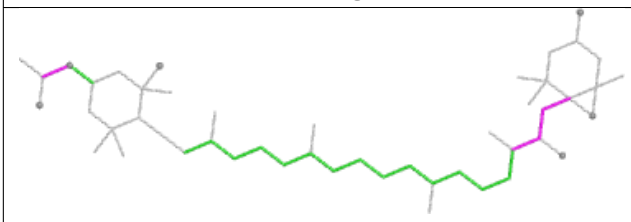
Bond angles



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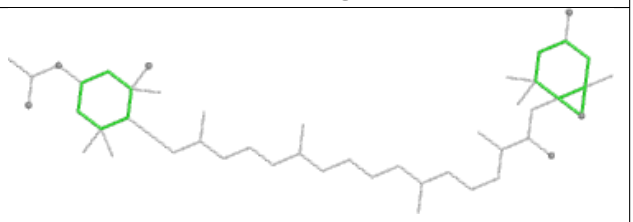

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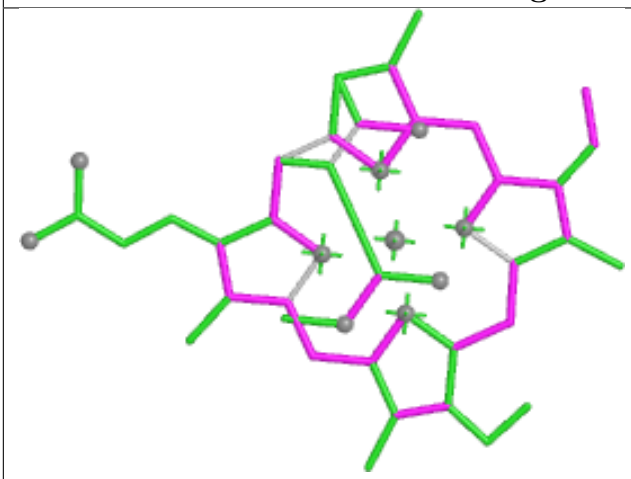

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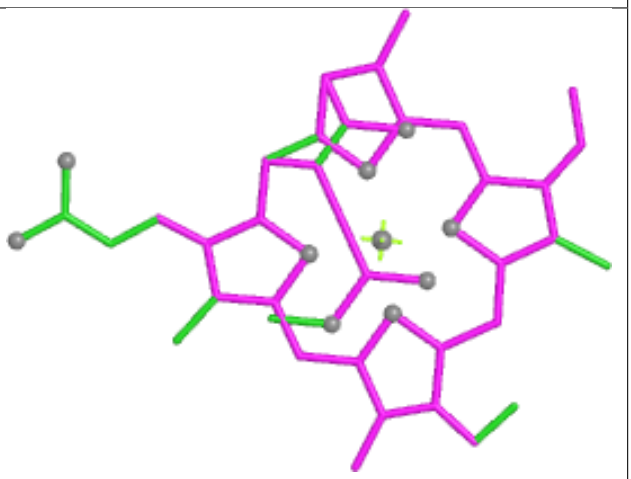

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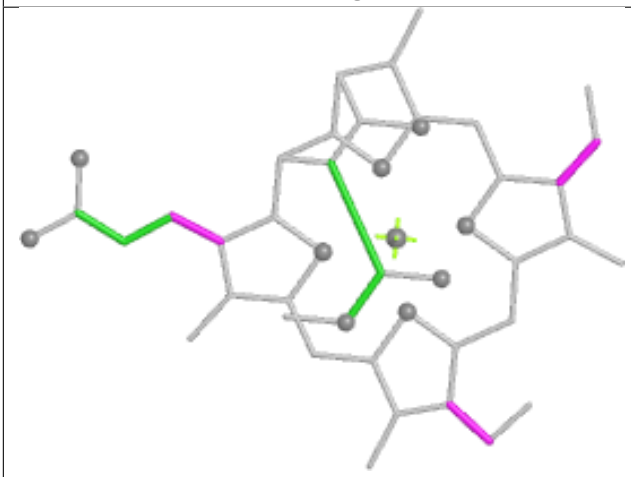

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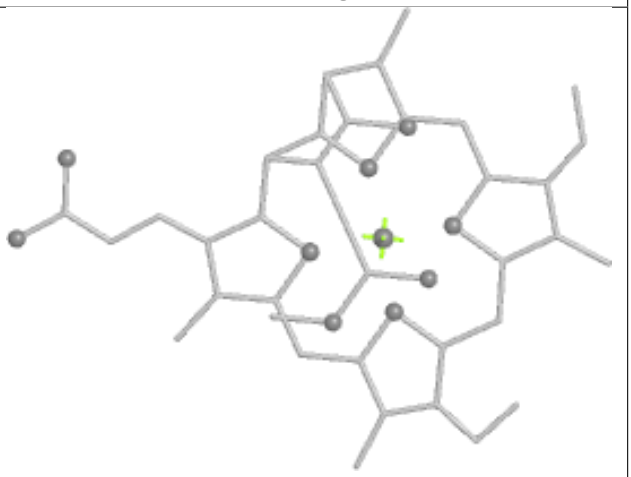

Rings

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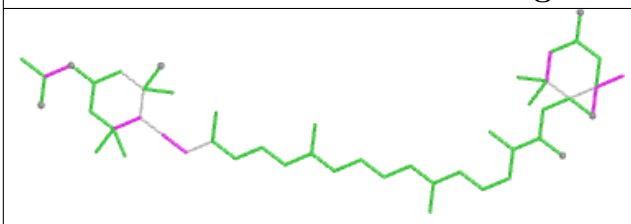

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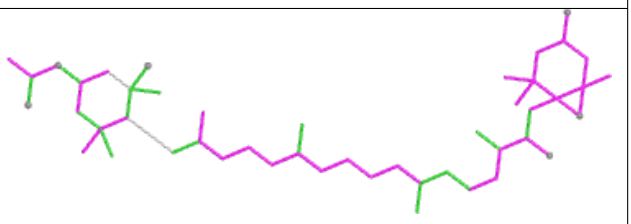

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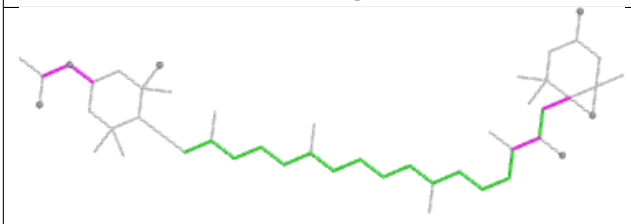

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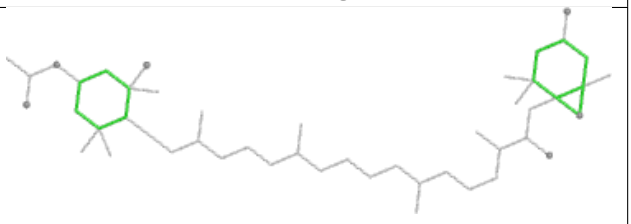
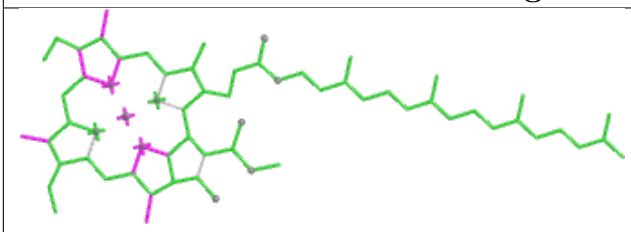


Rings

Ligand CLA C 511



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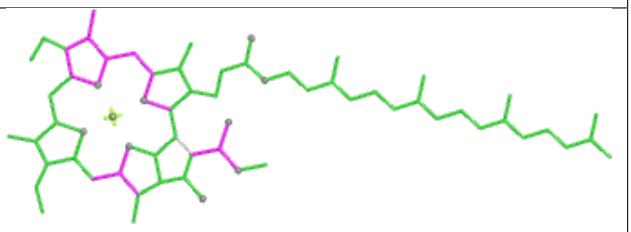

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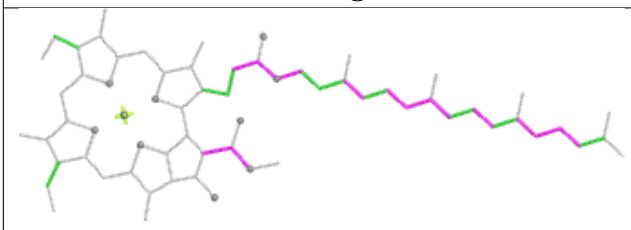

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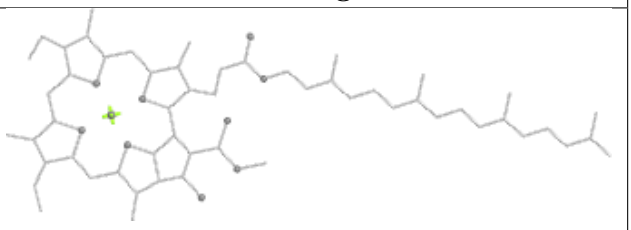

Rings

Ligand A86 17 305



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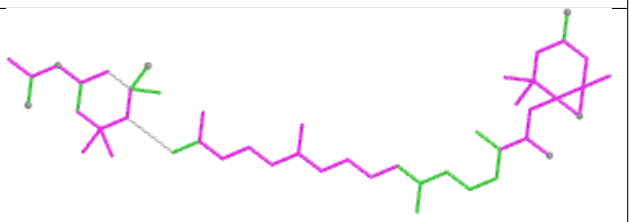

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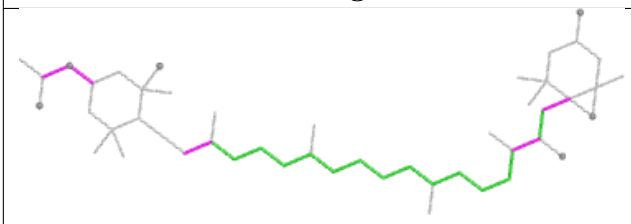

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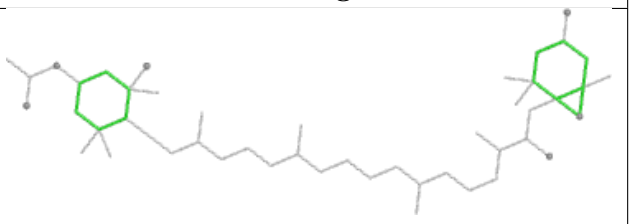

Rings

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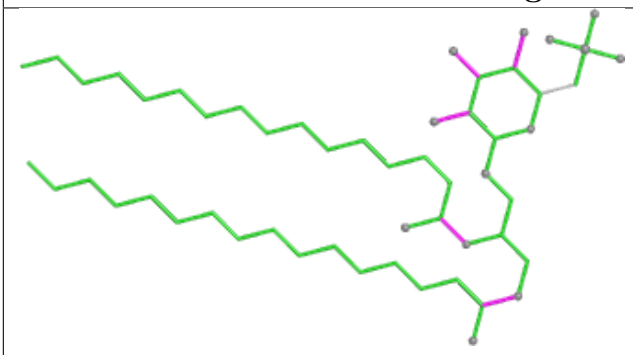

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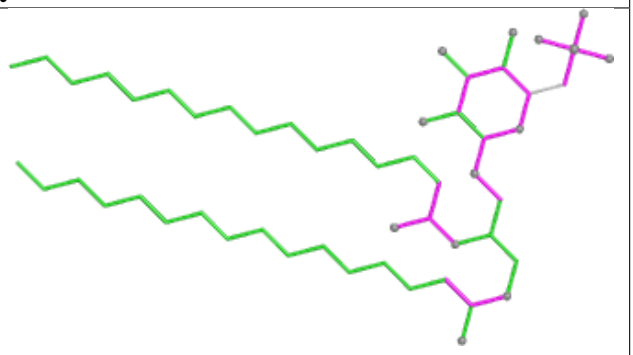

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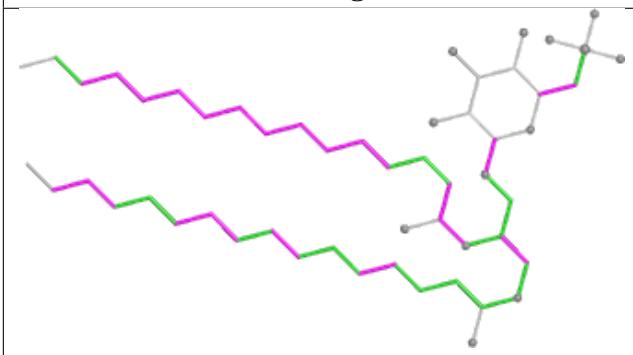

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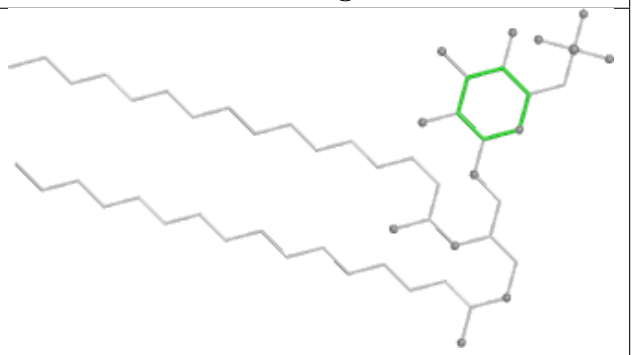
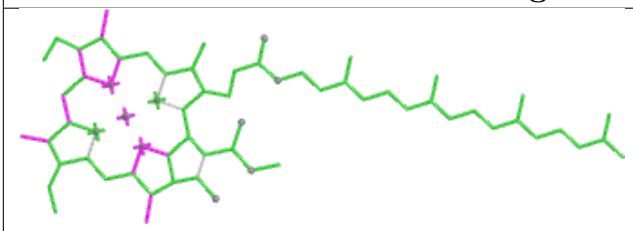


Rings

Ligand CLA c 509



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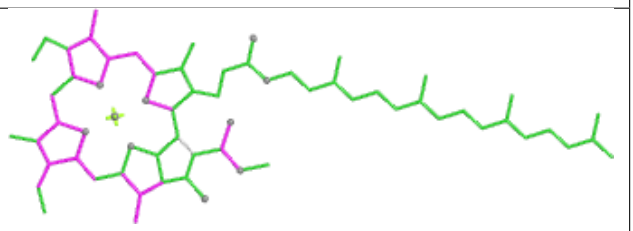

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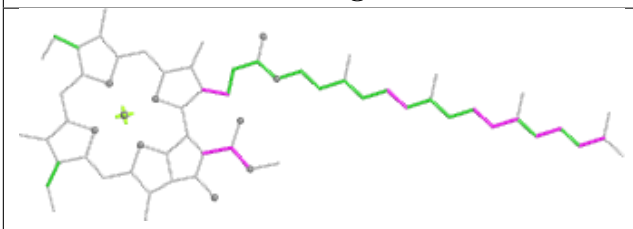

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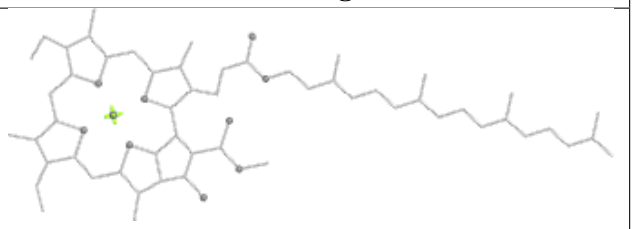
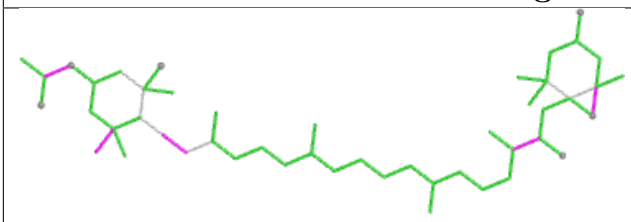


Rings

Ligand A86 5 302



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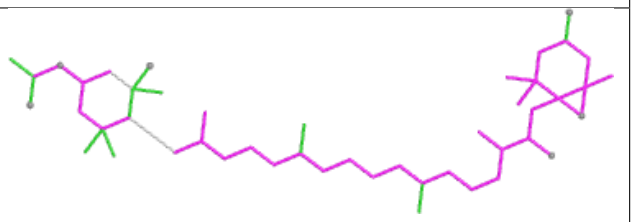

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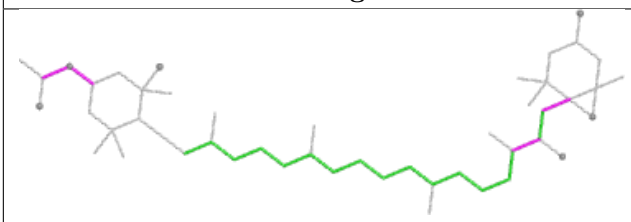

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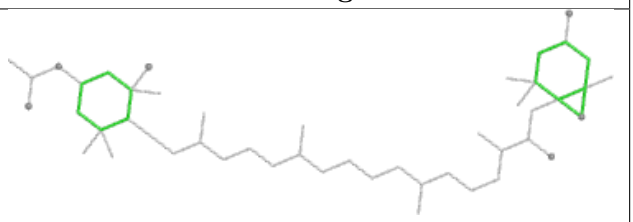

Rings

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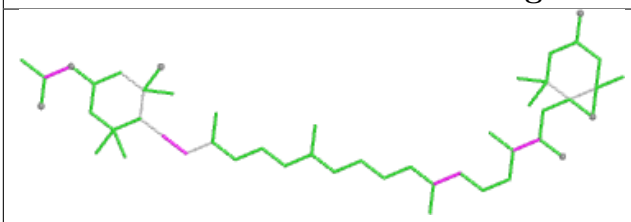

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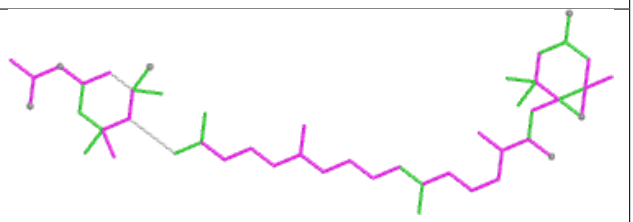

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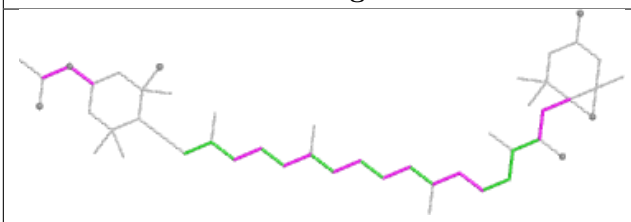

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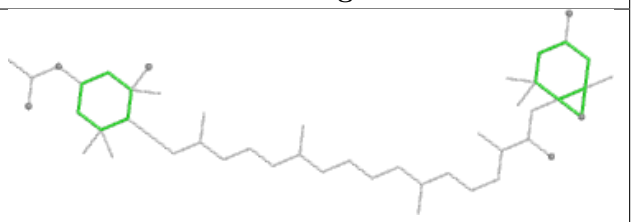

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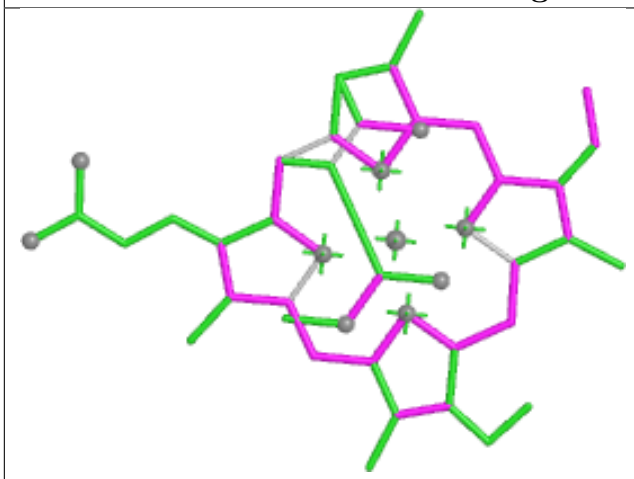

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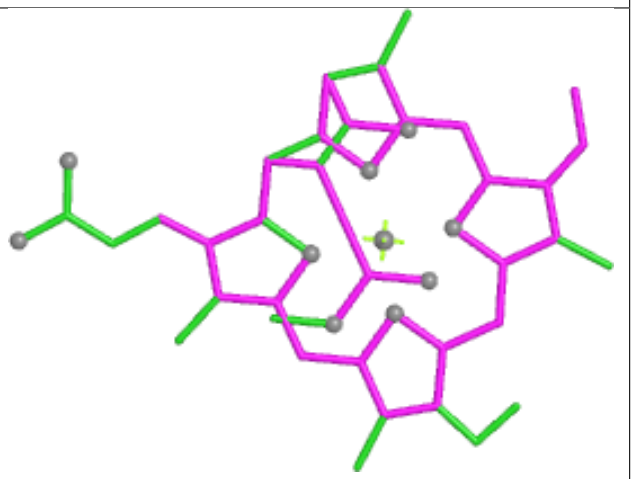

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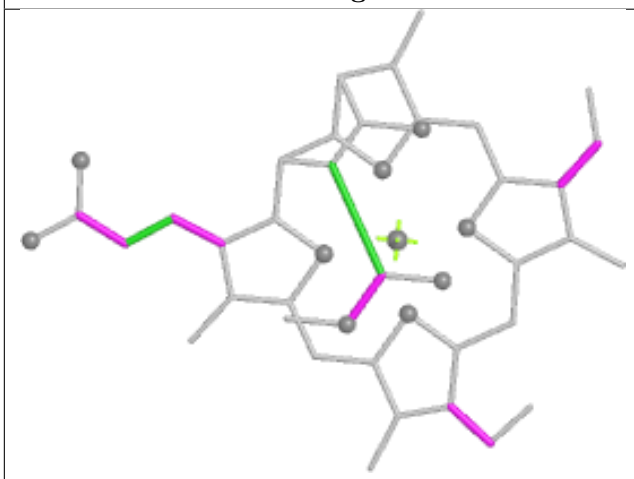

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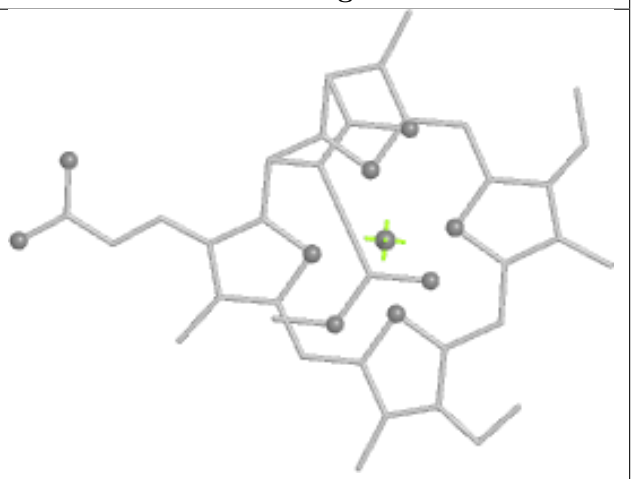
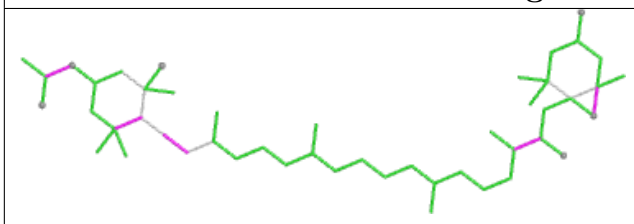


Rings

Ligand A86 14 302



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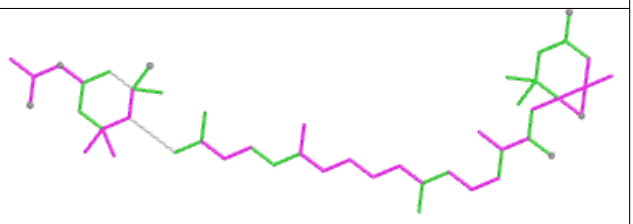

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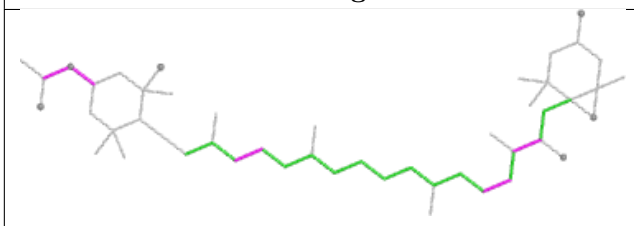

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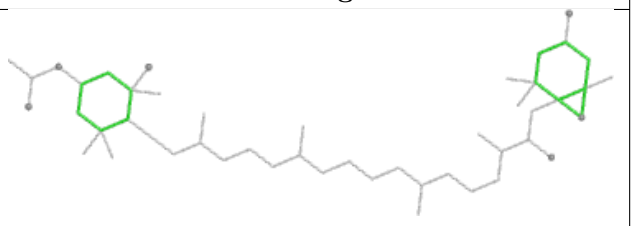

Rings

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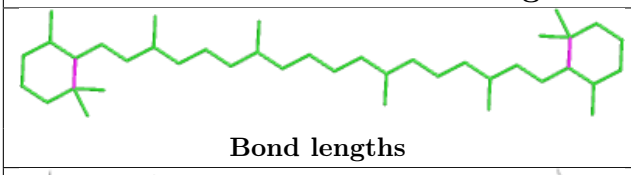

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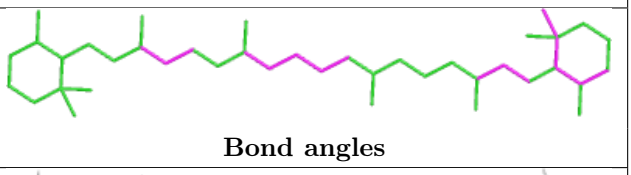

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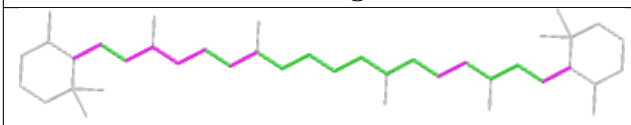

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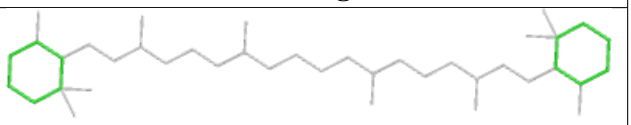

Rings

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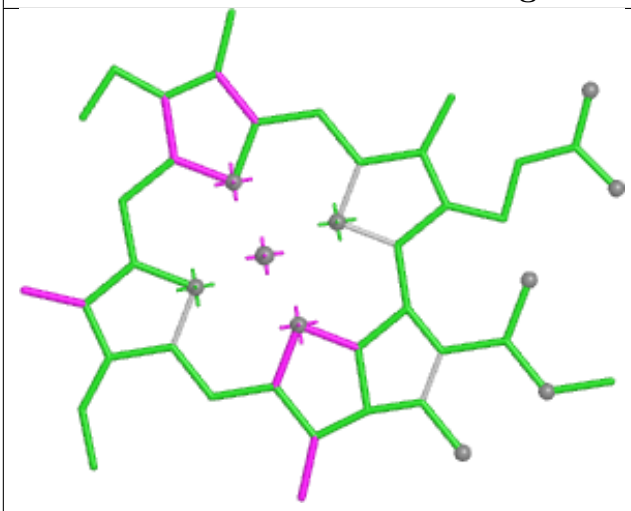

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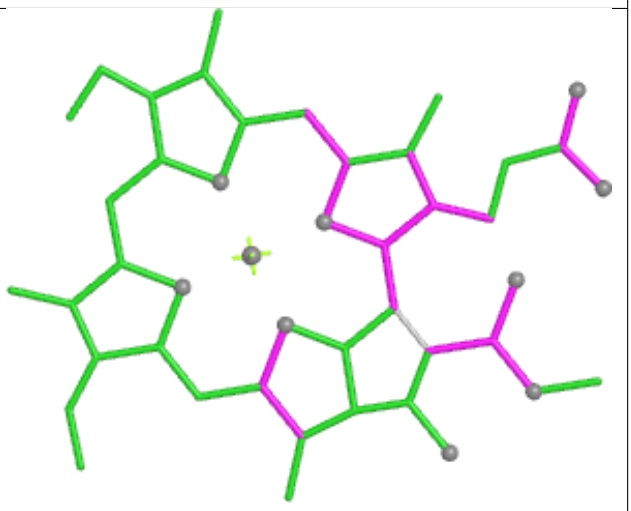

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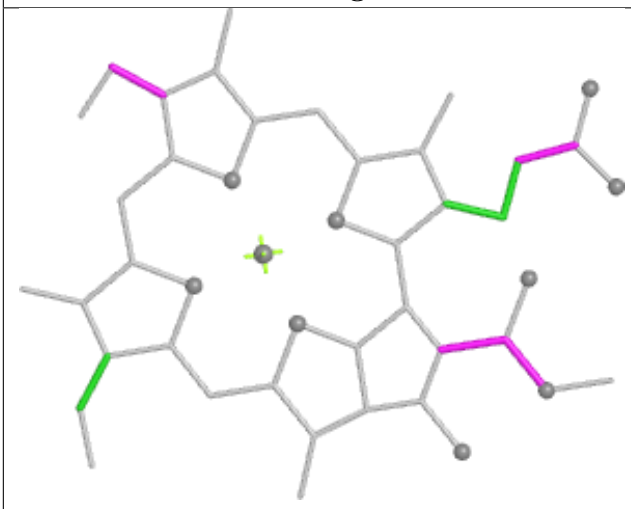

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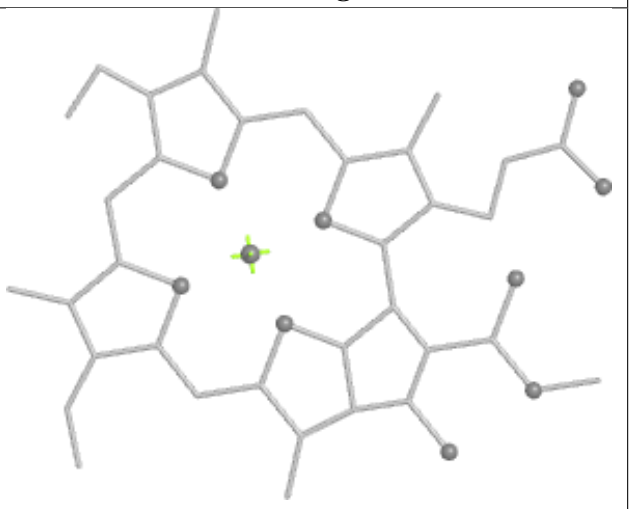
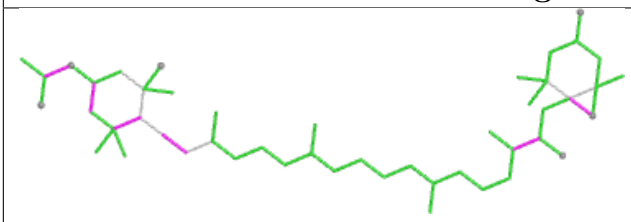


Rings

Ligand A86 8 305



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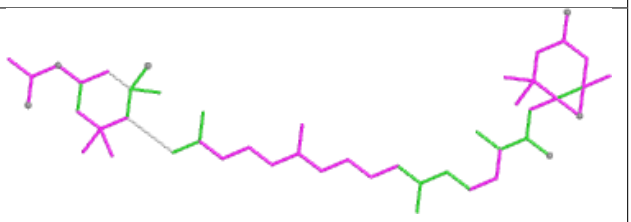

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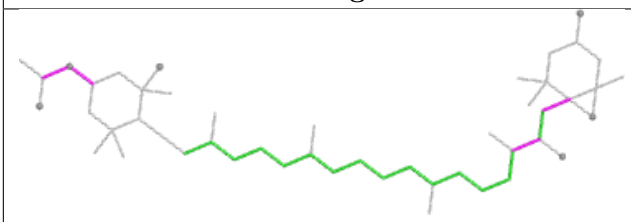

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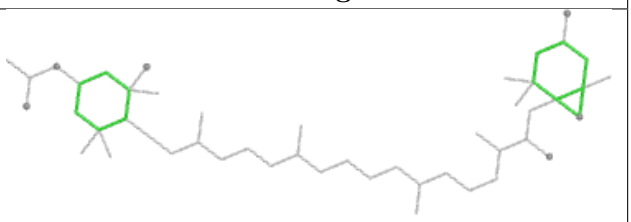
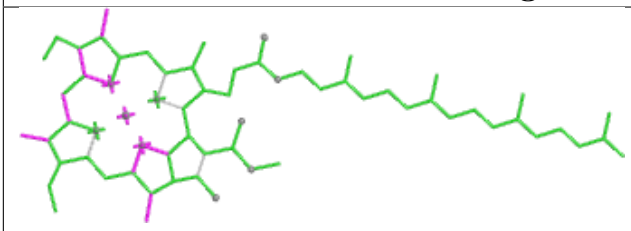


Rings

Ligand CLA 11 313



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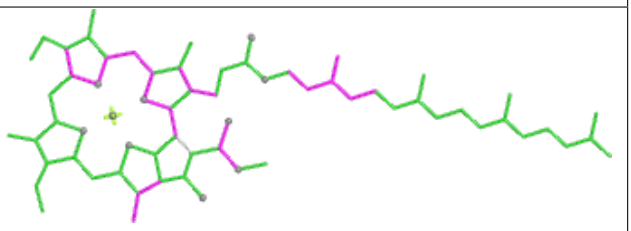

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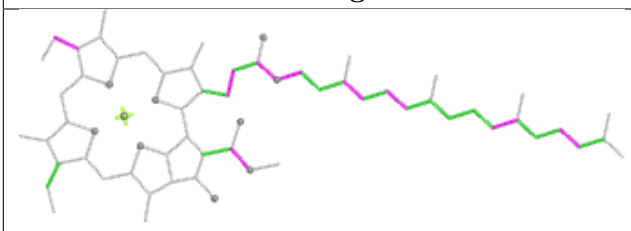

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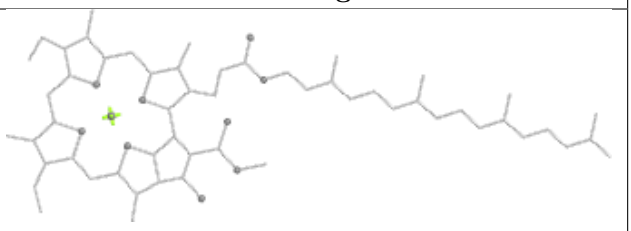
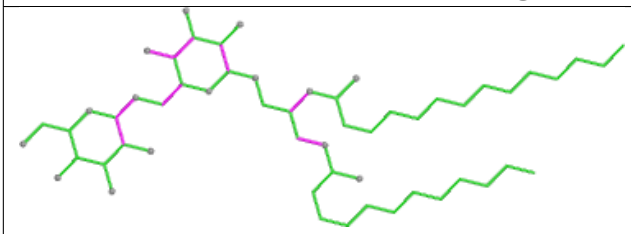


Rings

Ligand DGD W 203



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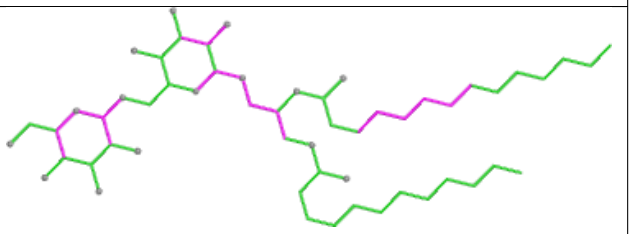
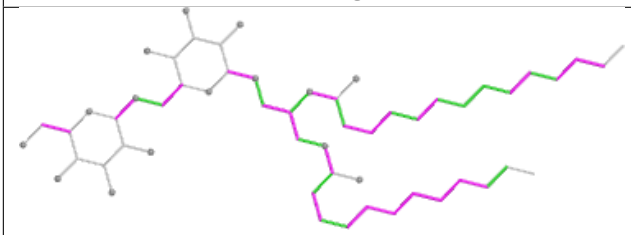


Bond angles



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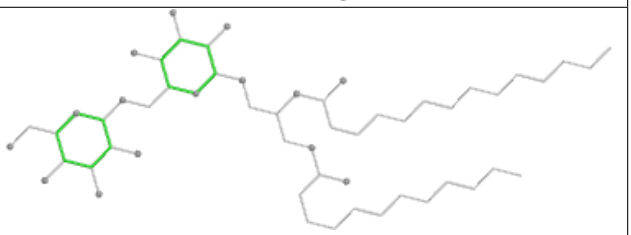
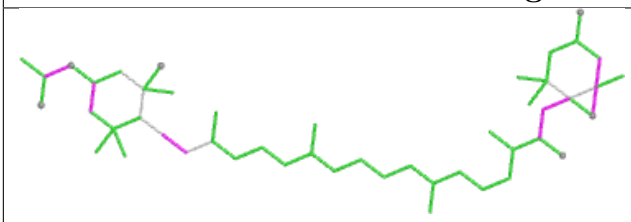


Rings

Ligand A86 16 305



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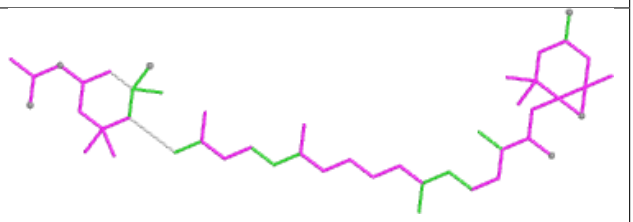

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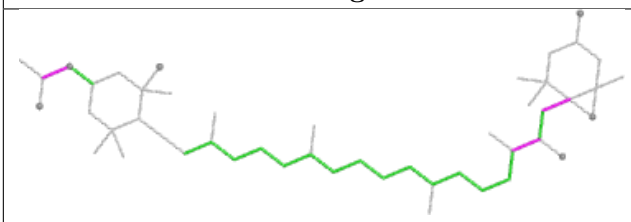

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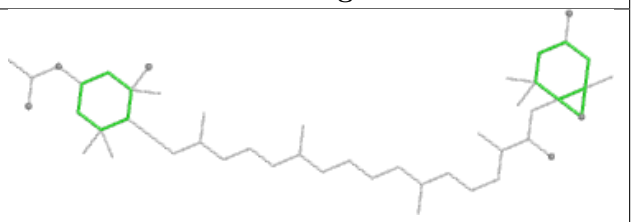
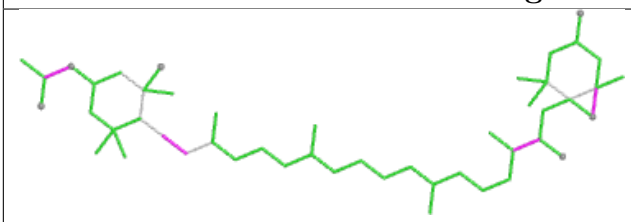


Rings

Ligand A86 13 305



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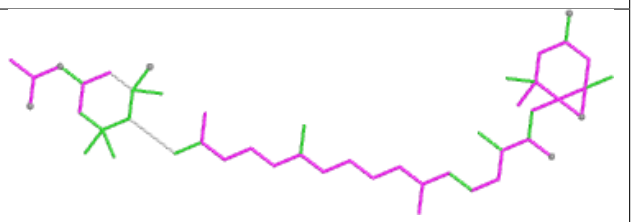

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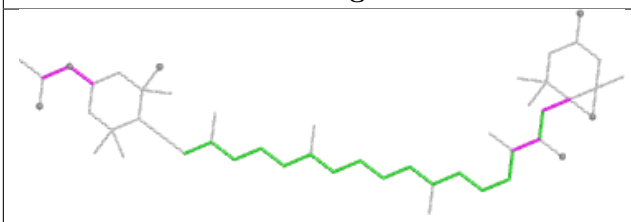

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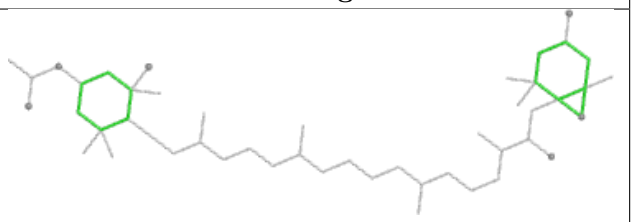
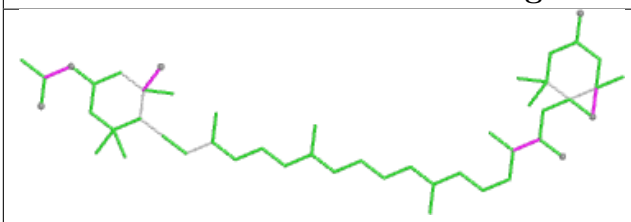


Rings

Ligand A86 12 303



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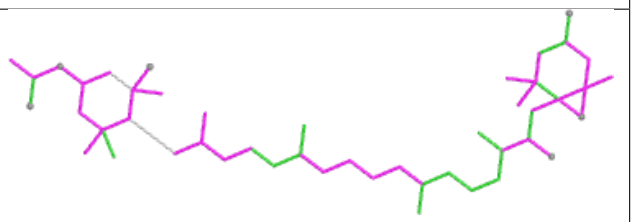

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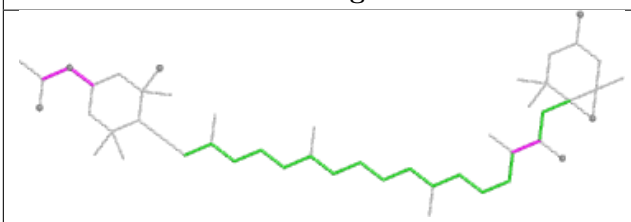

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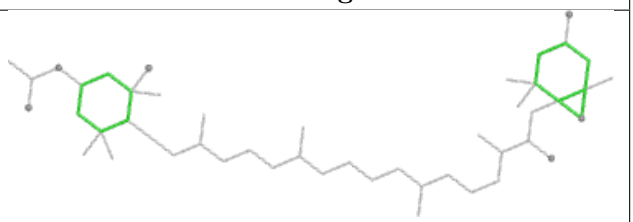

Rings

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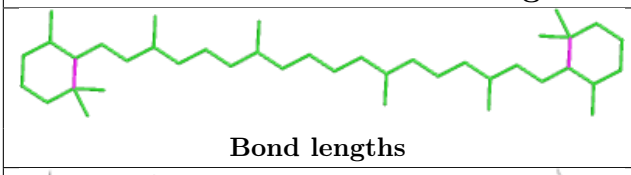

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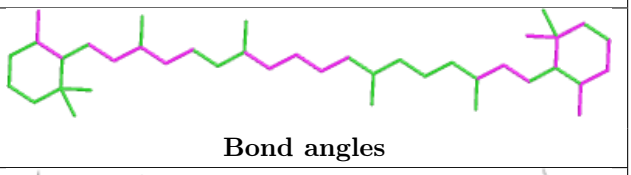

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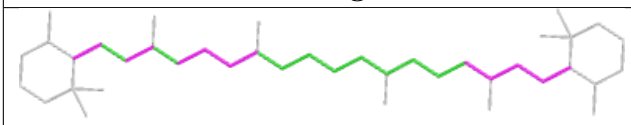

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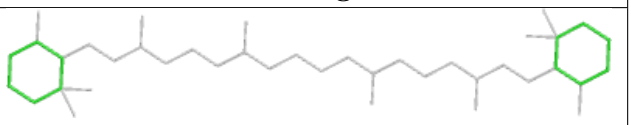

Rings

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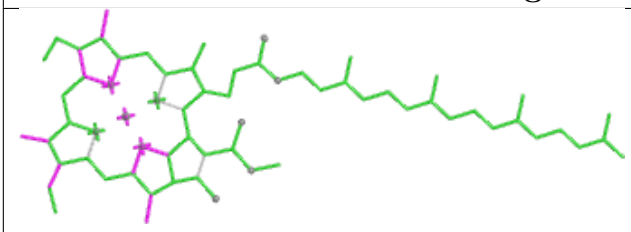

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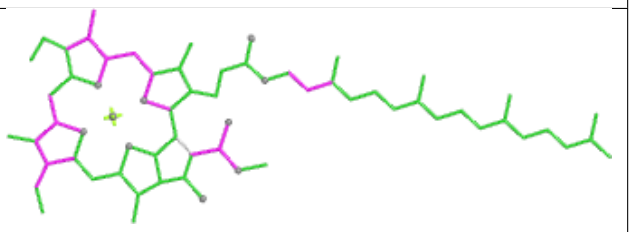

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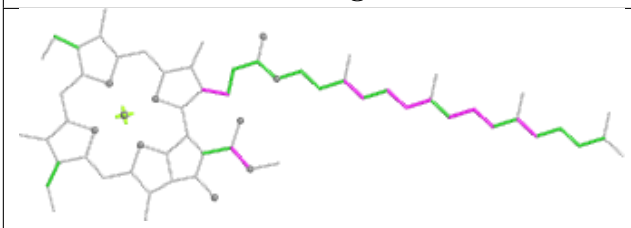

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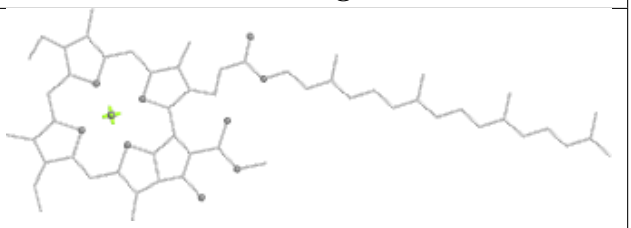
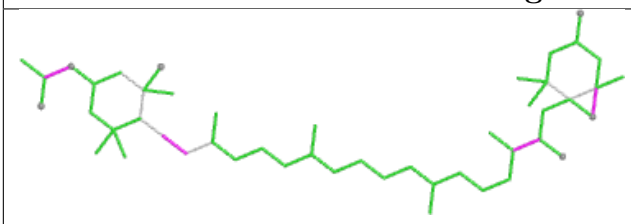


Rings

Ligand A86 13 302



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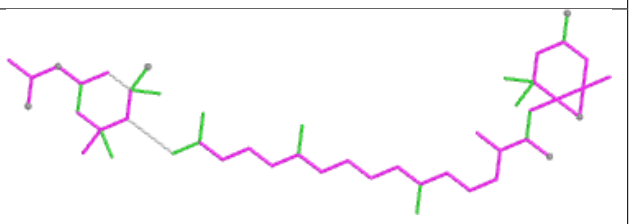

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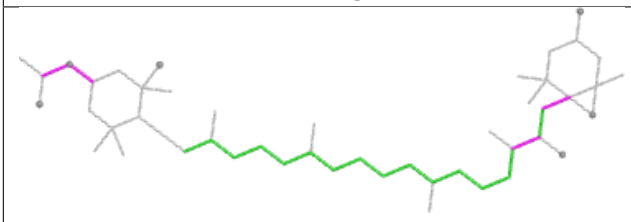

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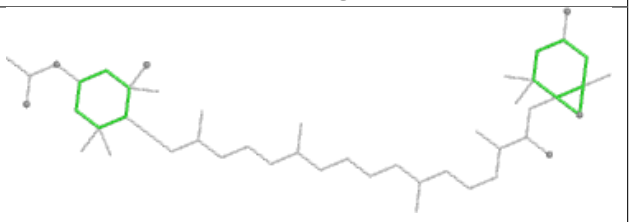

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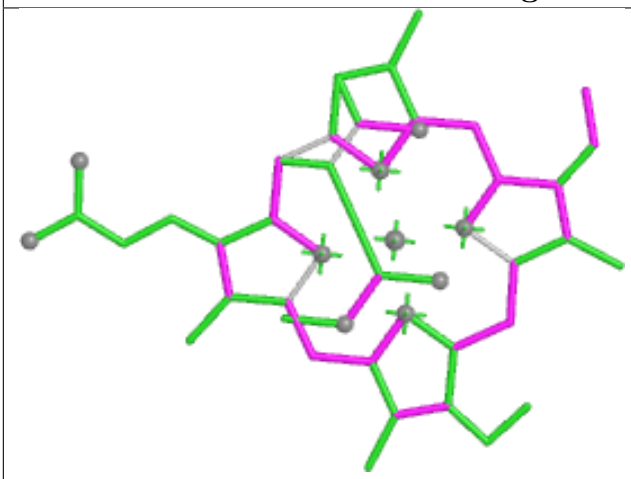

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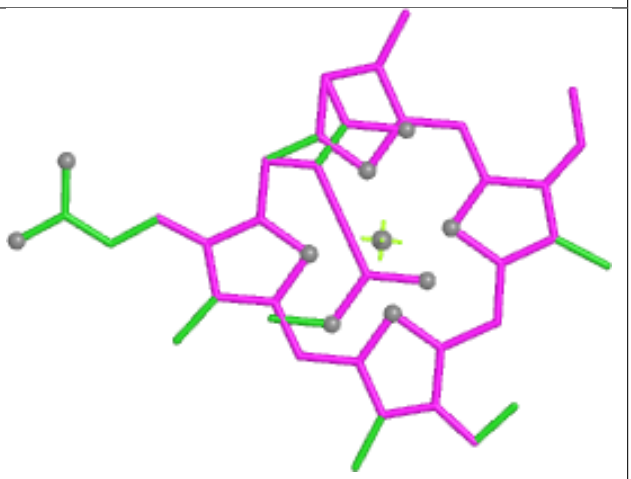

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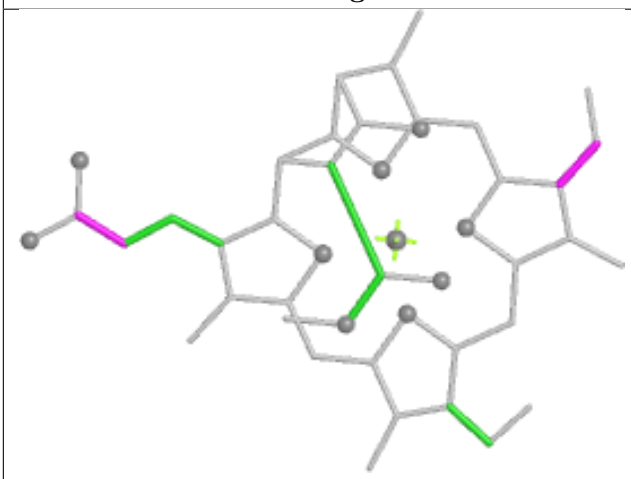

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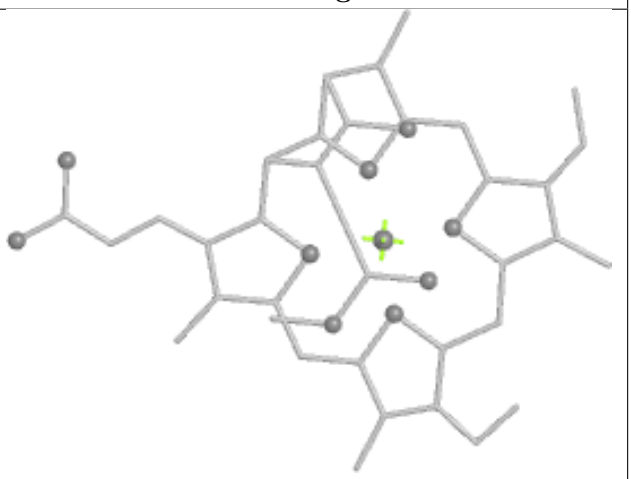

Rings

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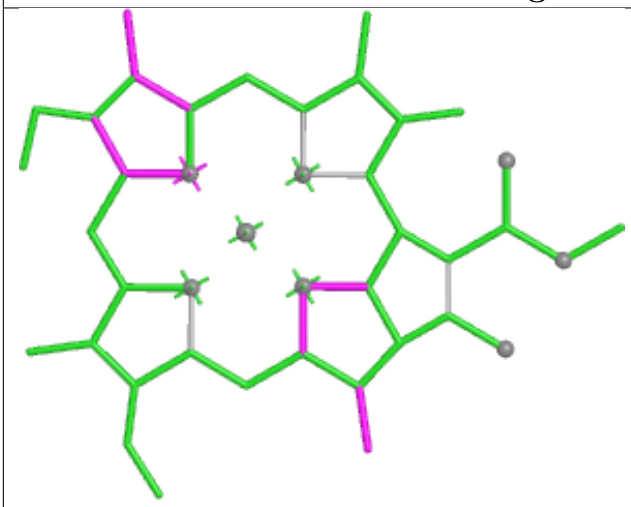

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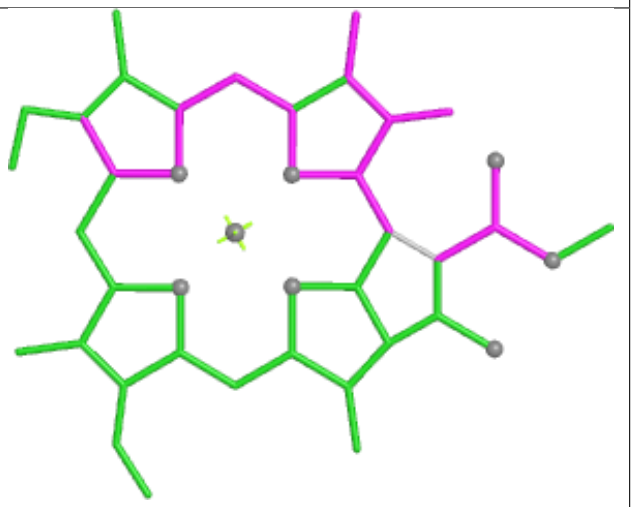

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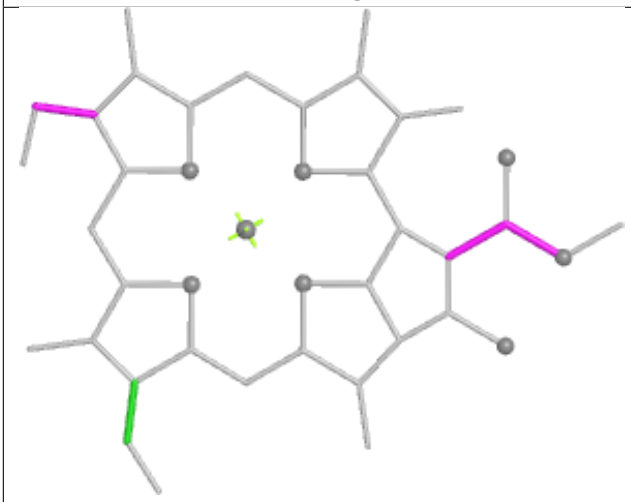

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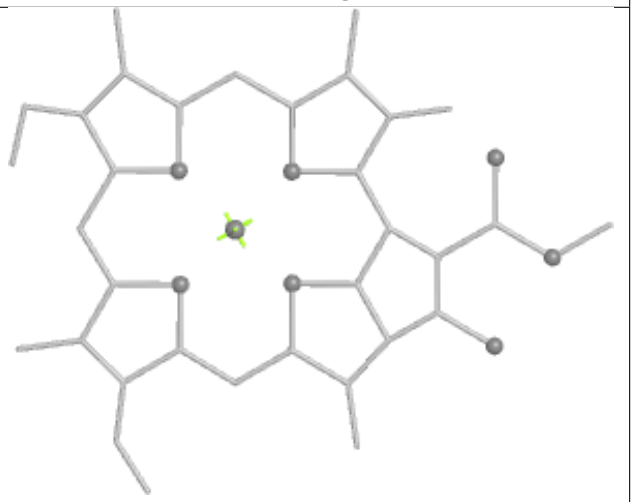

Rings

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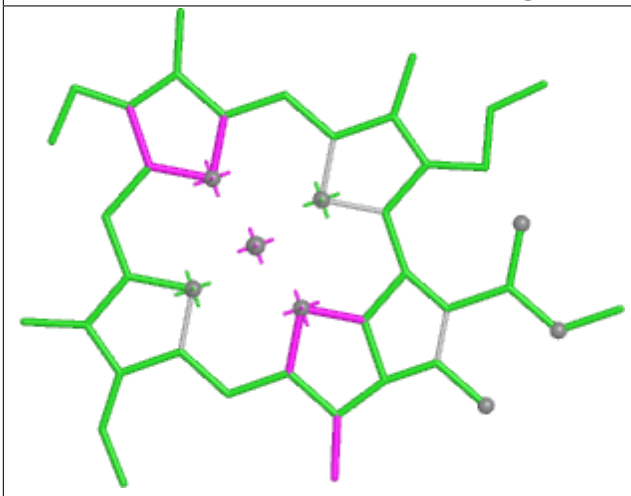

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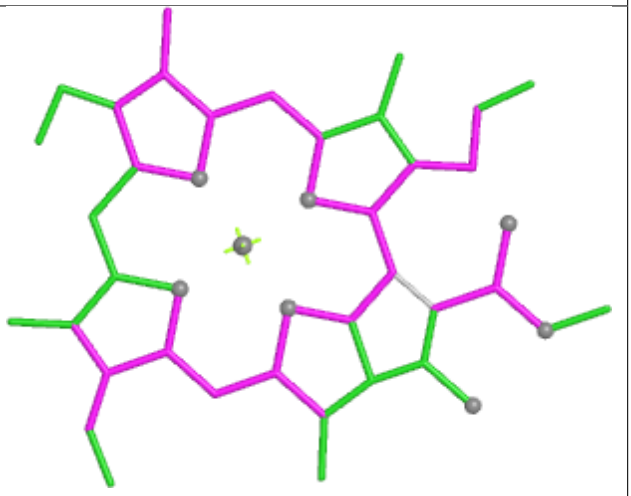

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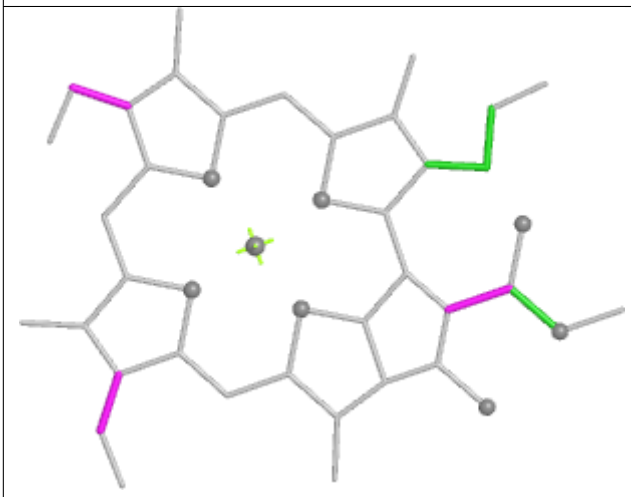

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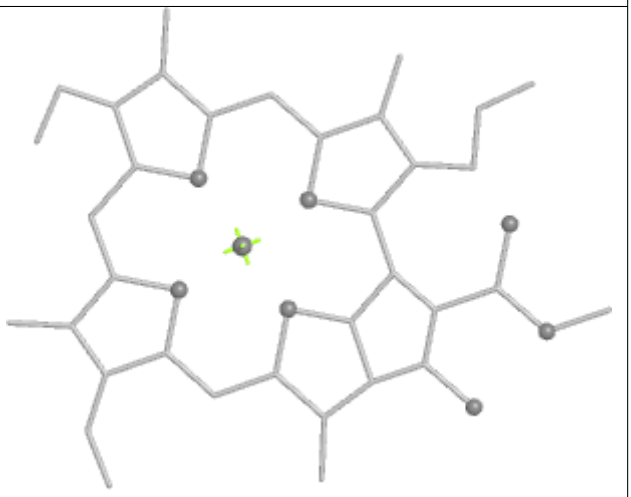

Rings

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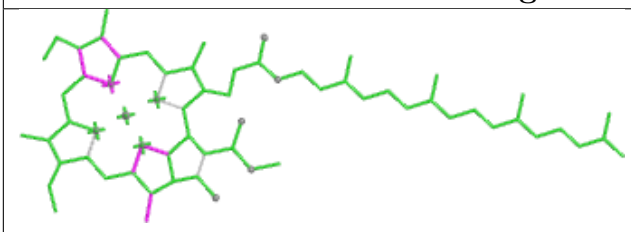

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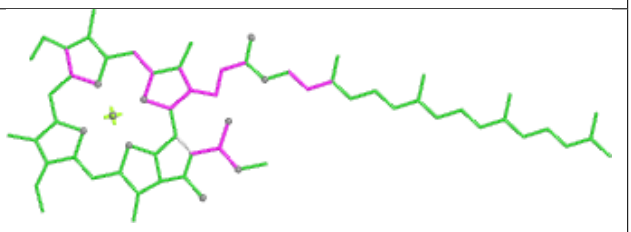

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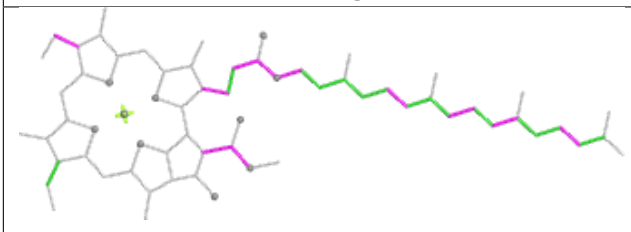

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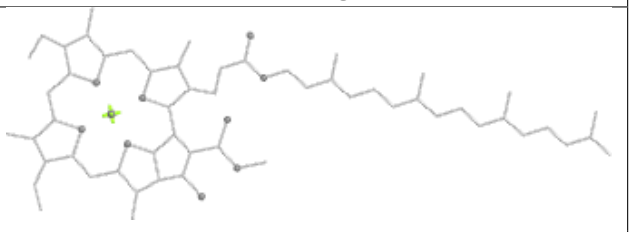

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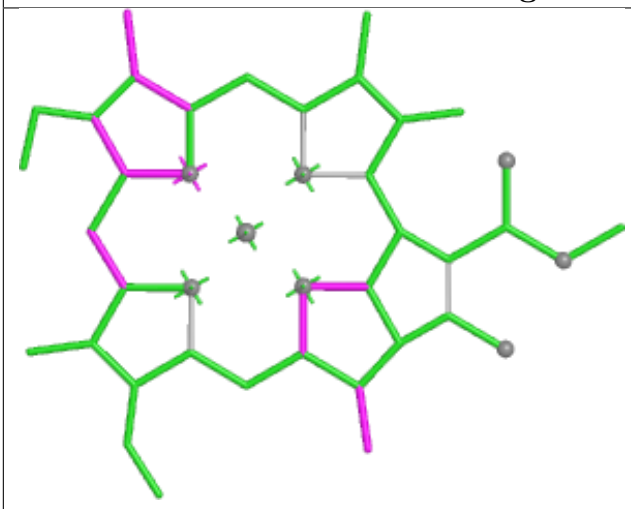

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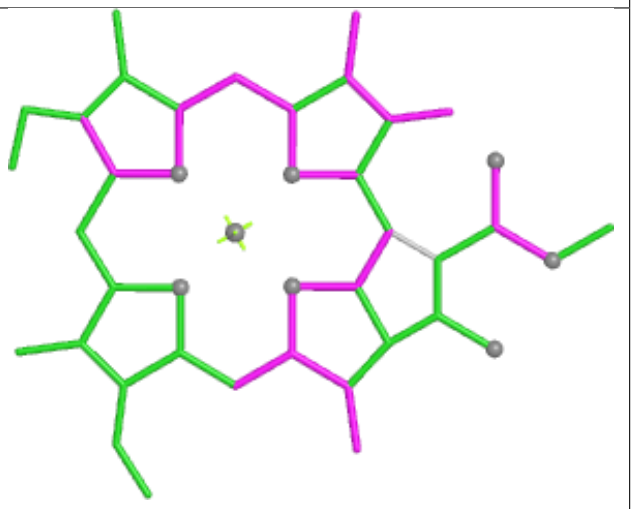

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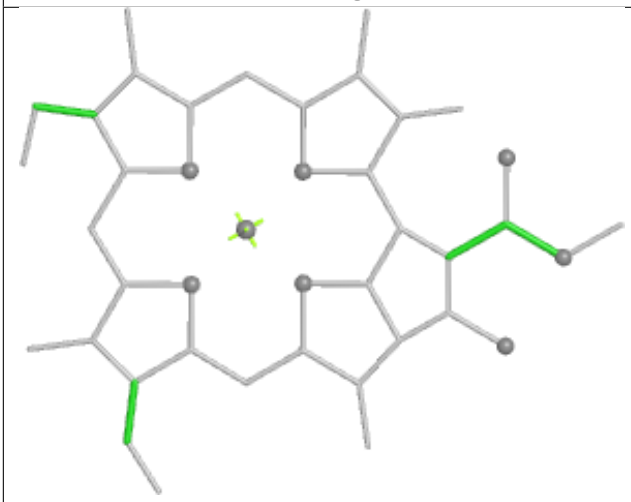

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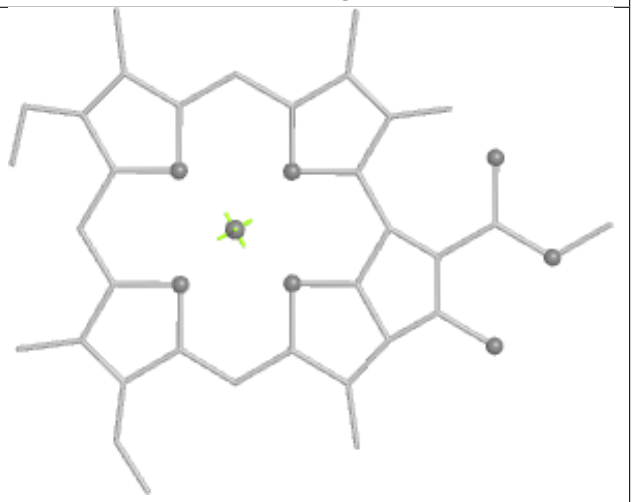
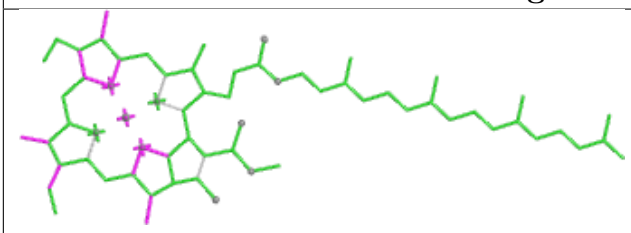


Rings

Ligand CLA b 607



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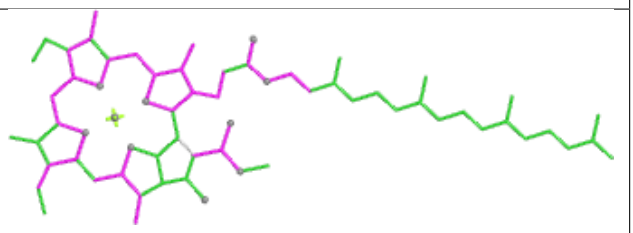

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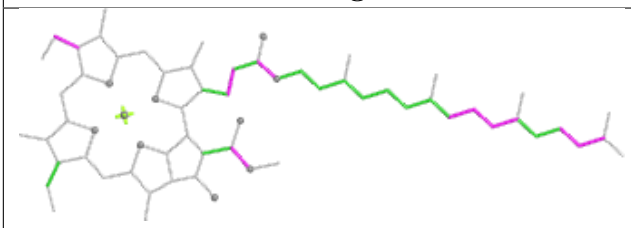

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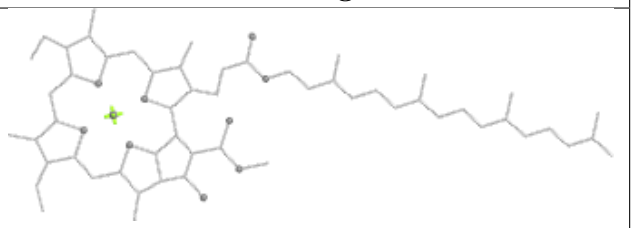

Rings

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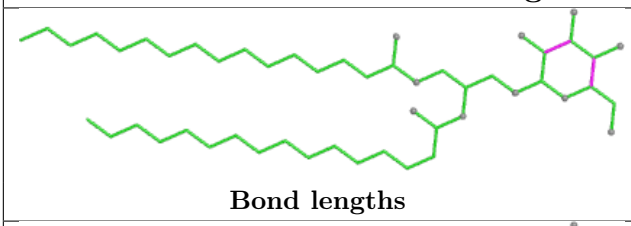

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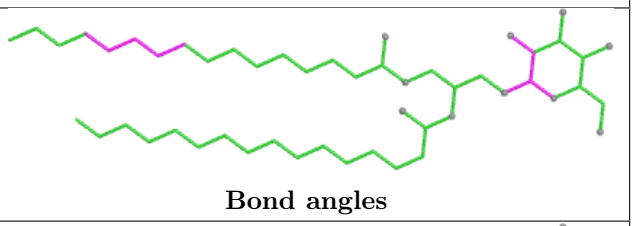

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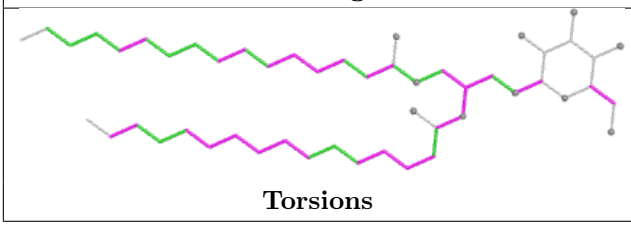

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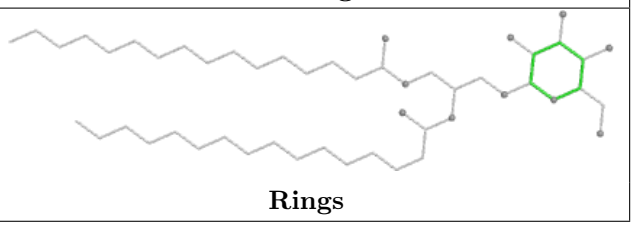
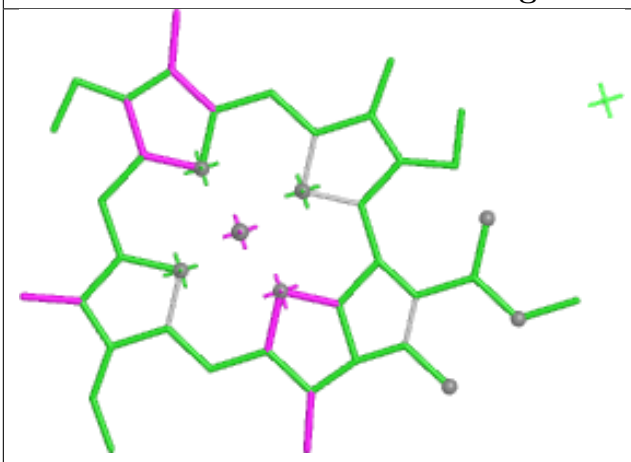


Rings

Ligand CLA 10 313



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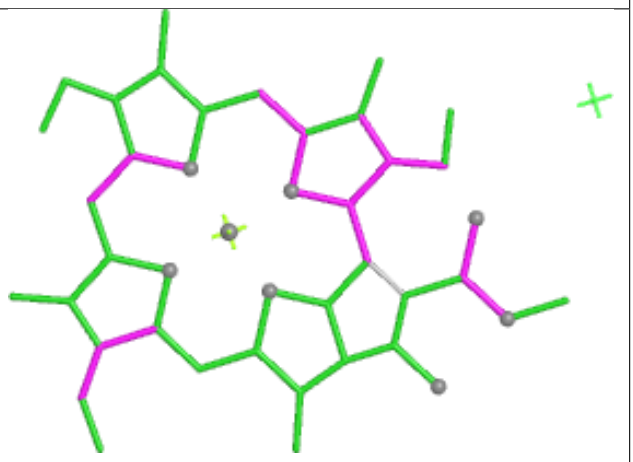

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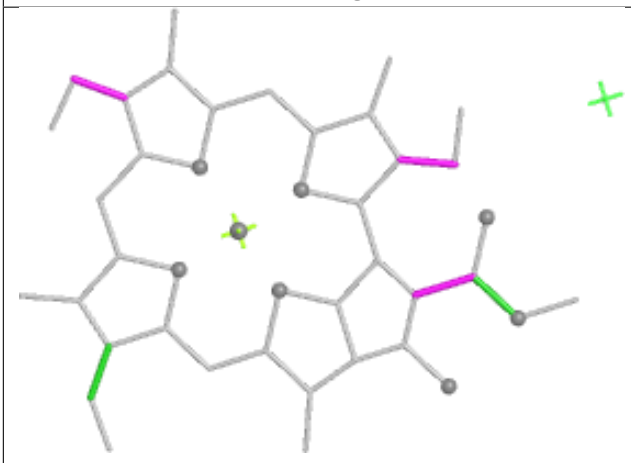
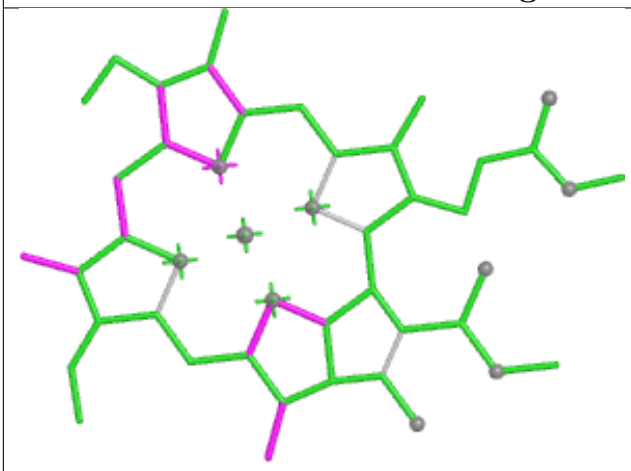


Torsions



Rings

Ligand CLA 10 316



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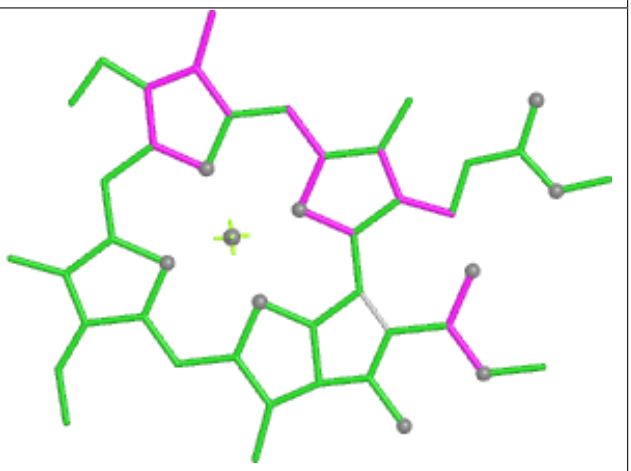

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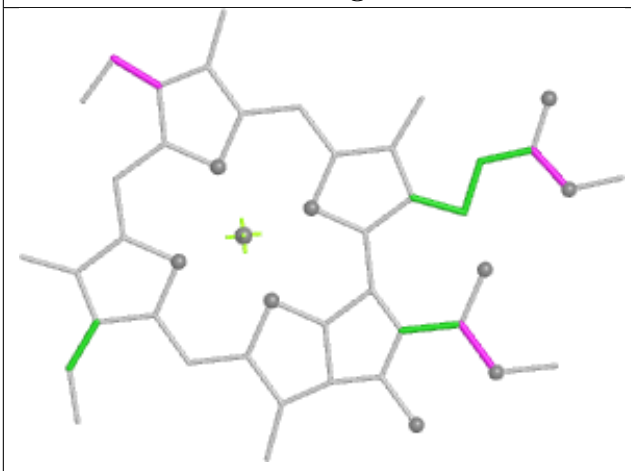

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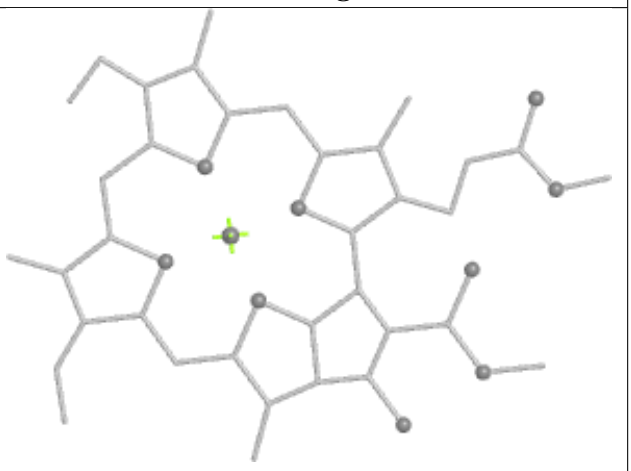
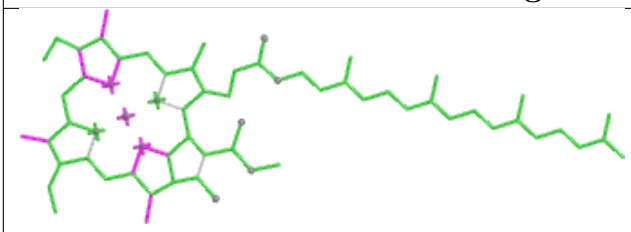


Rings

Ligand CLA B 607



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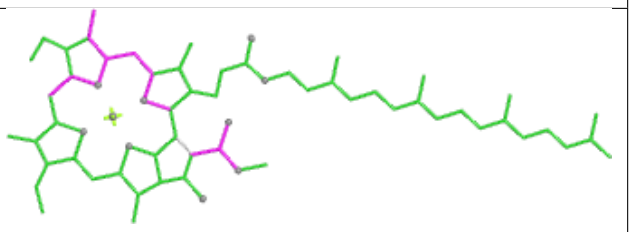

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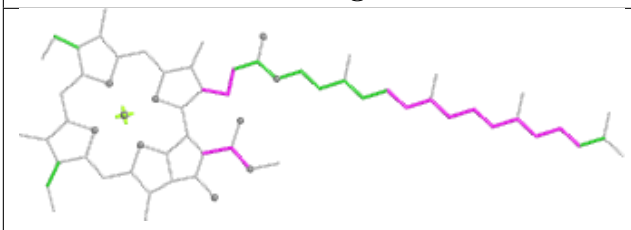

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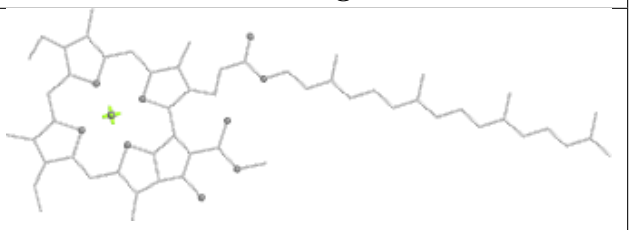
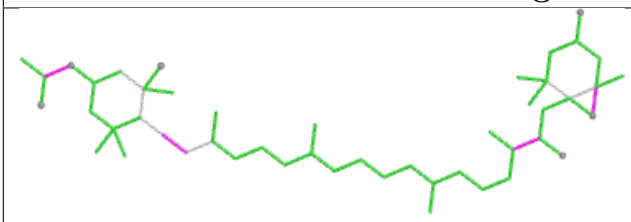


Rings

Ligand A86 p 613



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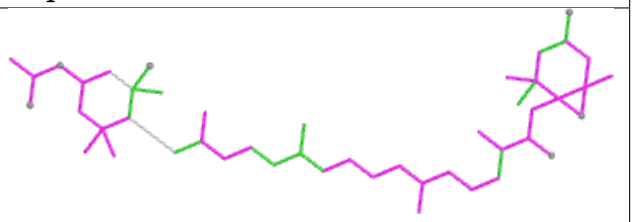
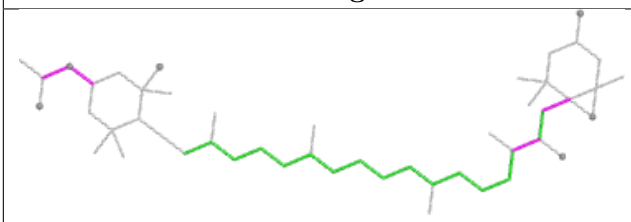


Bond angles



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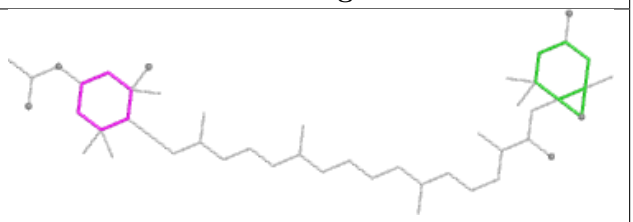
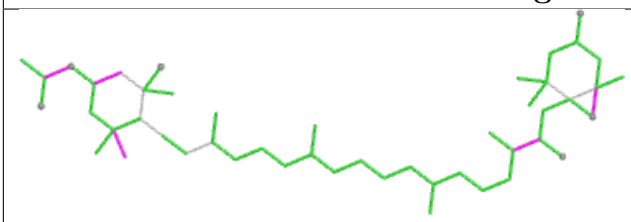


Rings

Ligand A86 1 320



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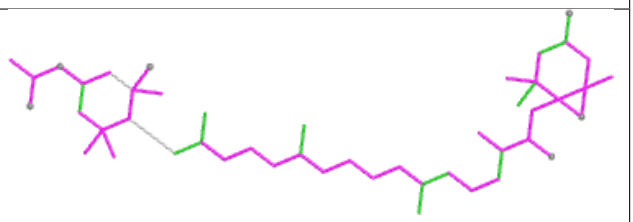

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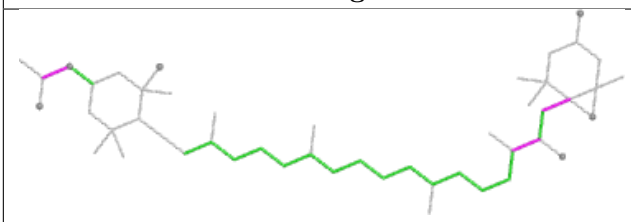

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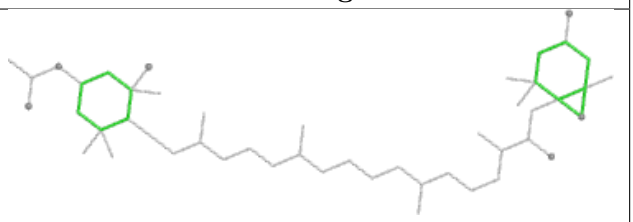
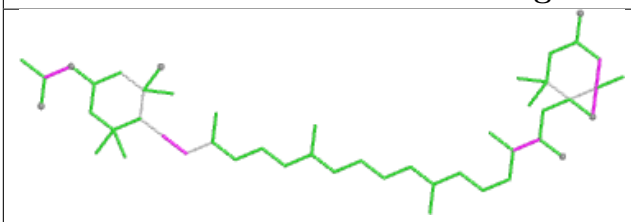


Rings

Ligand A86 6 303



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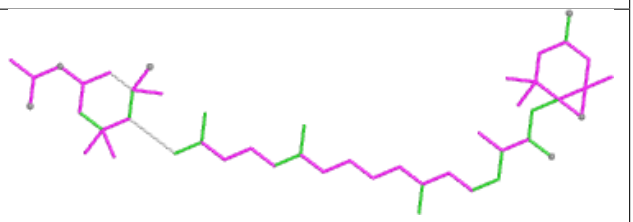

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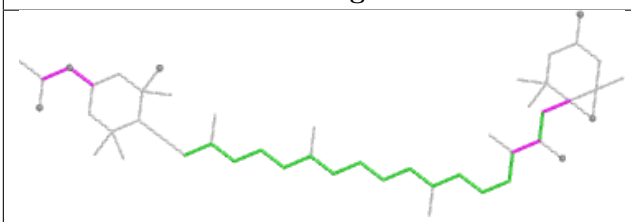

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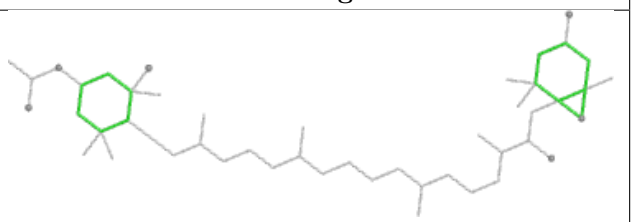
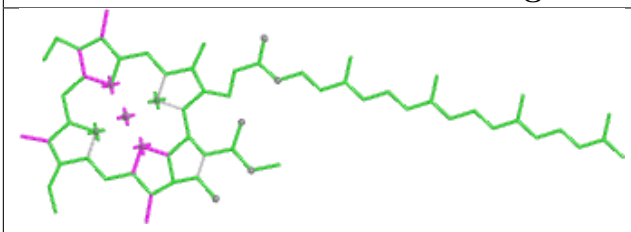


Rings

Ligand CLA B 609



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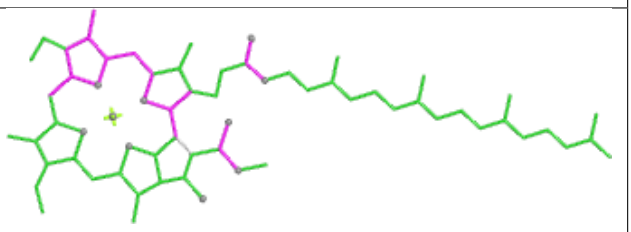

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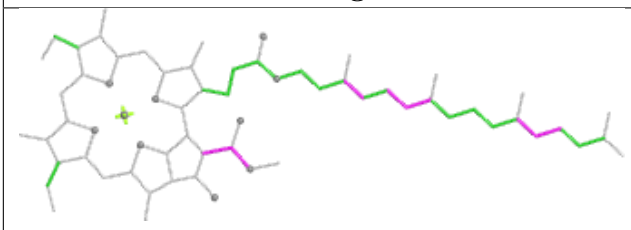

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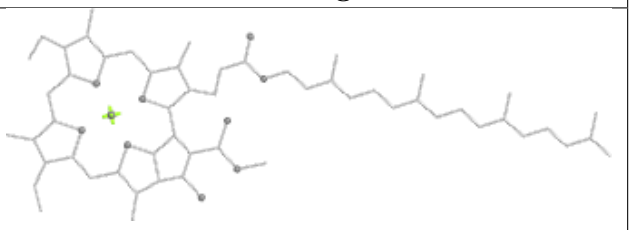
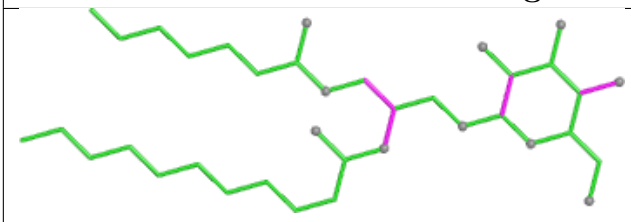


Rings

Ligand LMG 5 315



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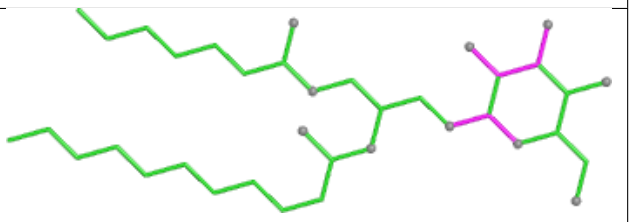

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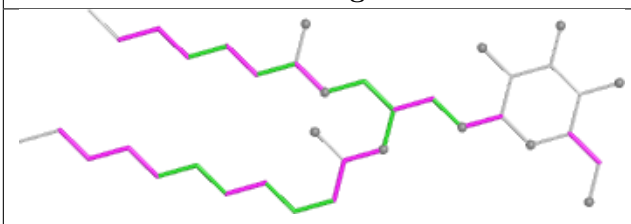

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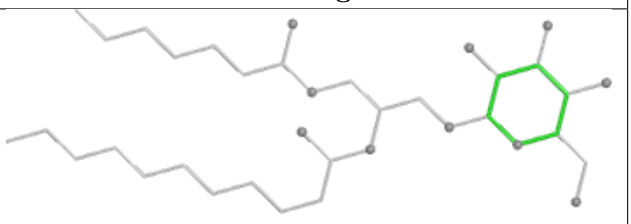
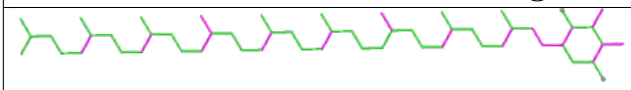


Rings

Ligand PL9 D 407



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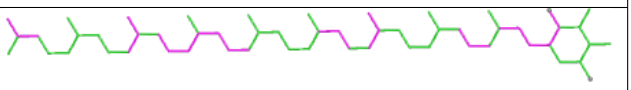

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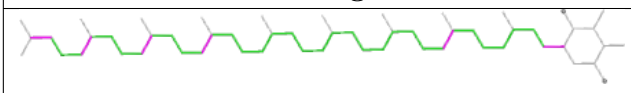

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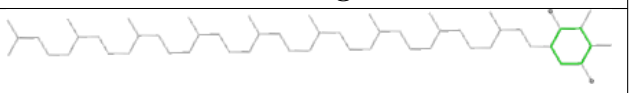
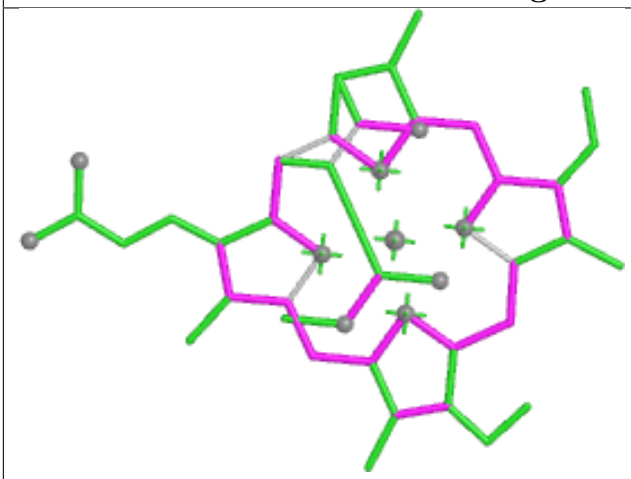


Rings

Ligand KC1 6 315



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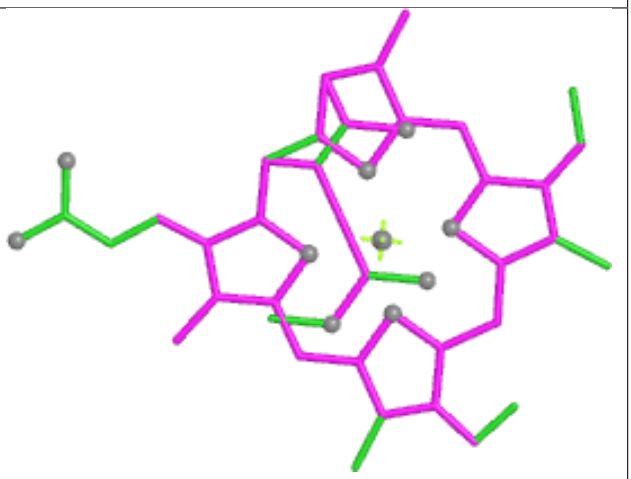

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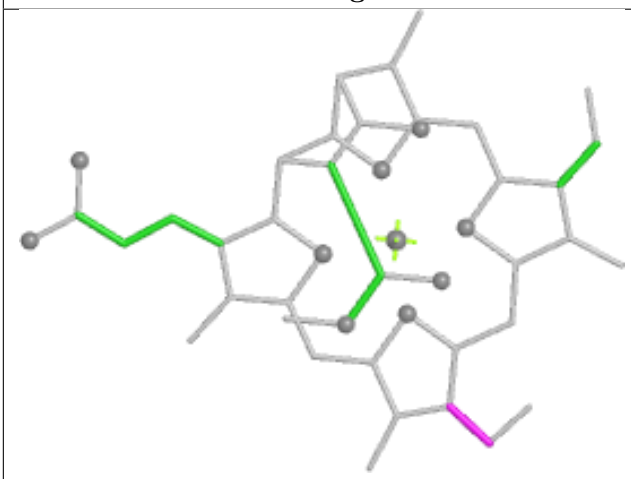

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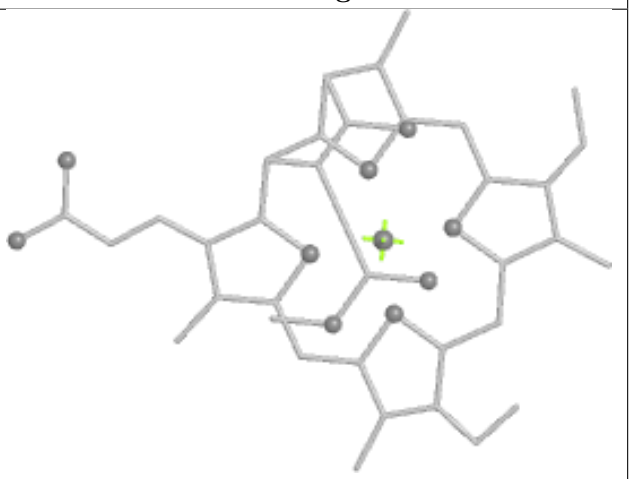
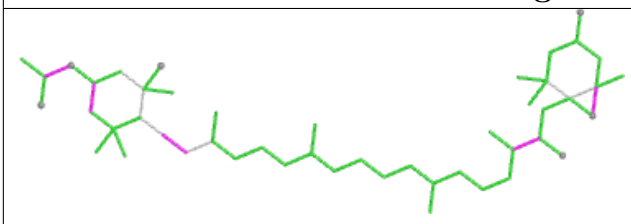


Rings

Ligand A86 6 302



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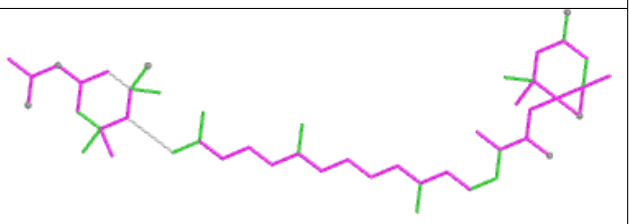
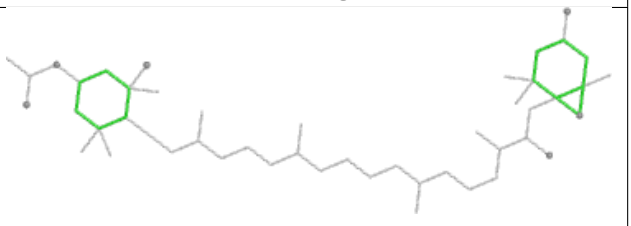


Bond angles

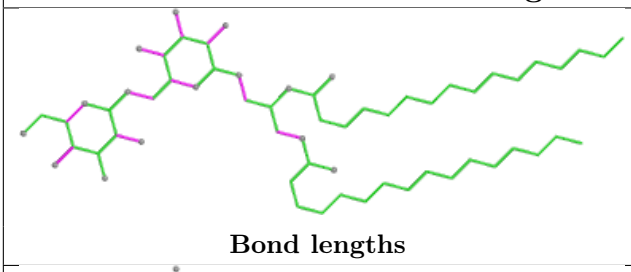


Torsions



Rings

Ligand DGD c 519



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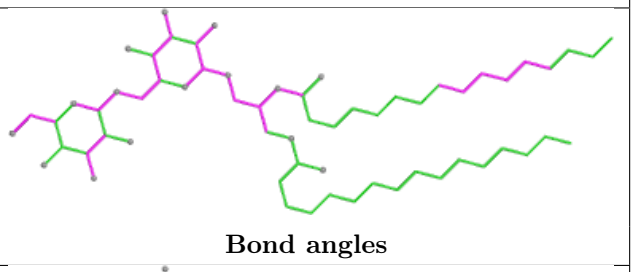

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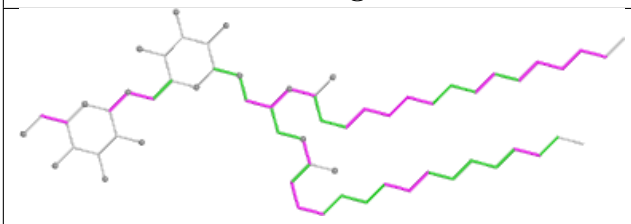

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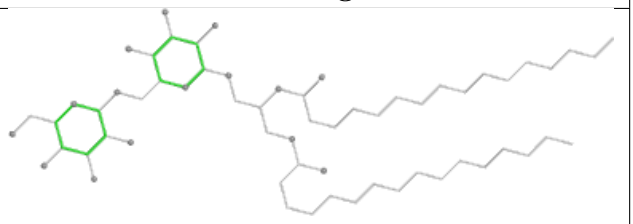
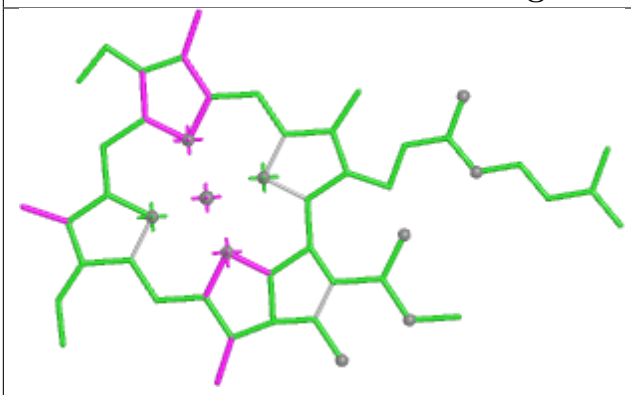


Rings

Ligand CLA p 603



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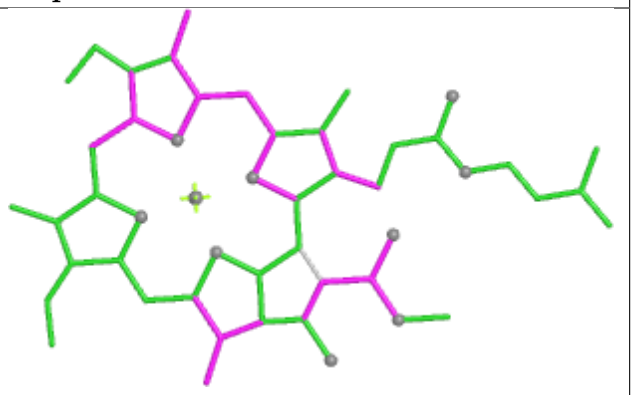

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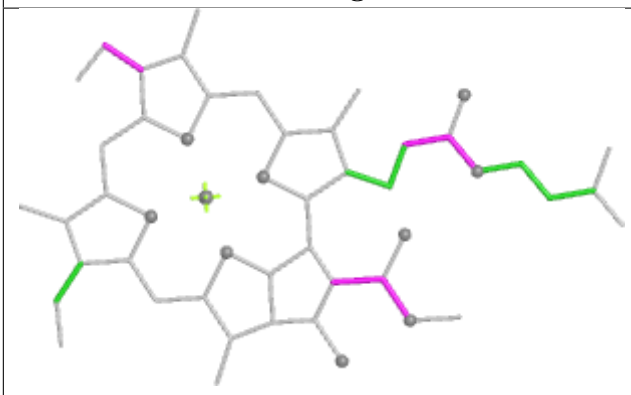

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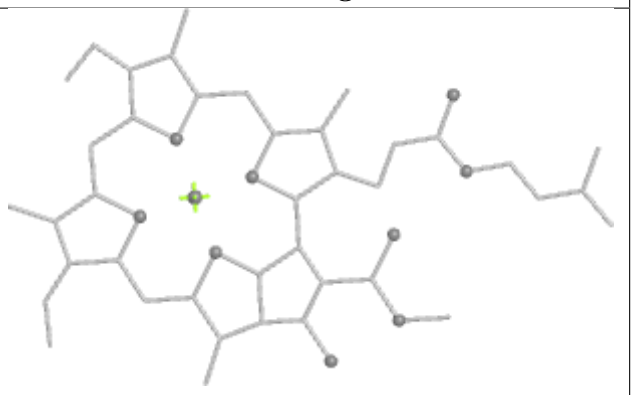
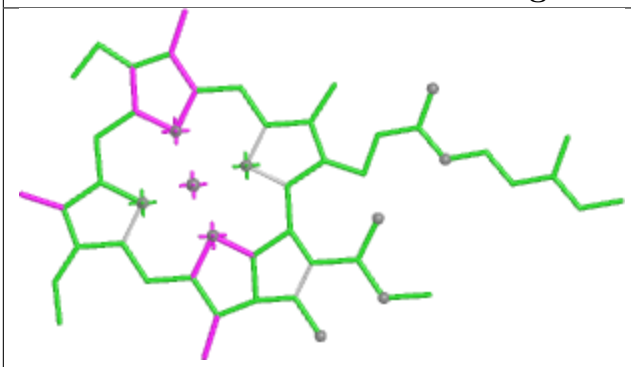


Rings

Ligand CLA z 101



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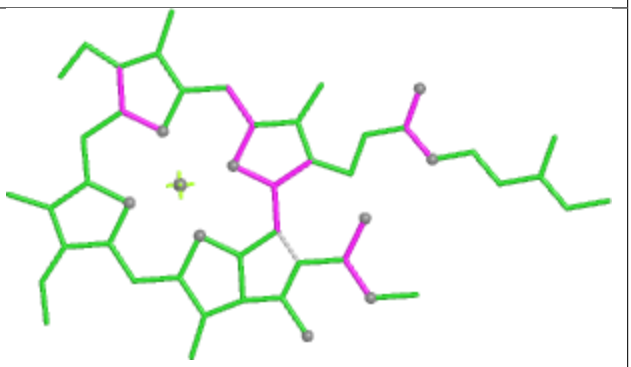

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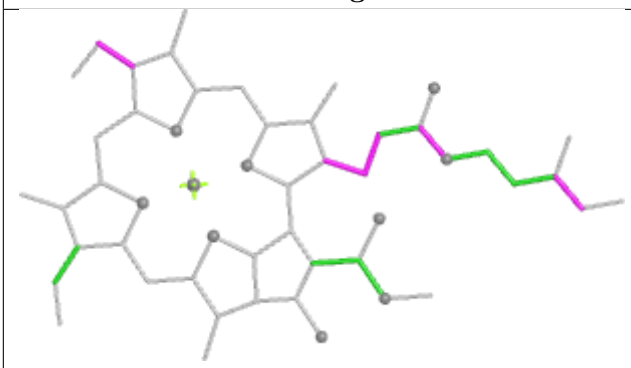

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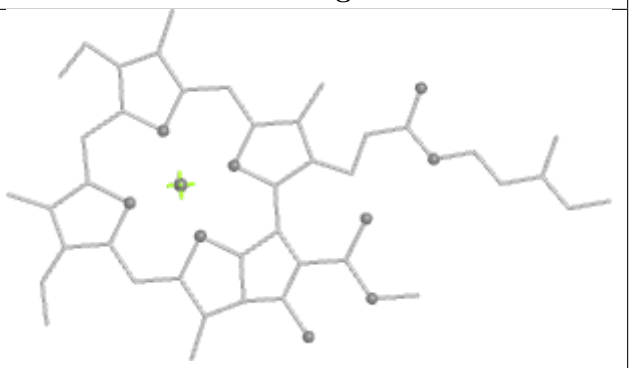
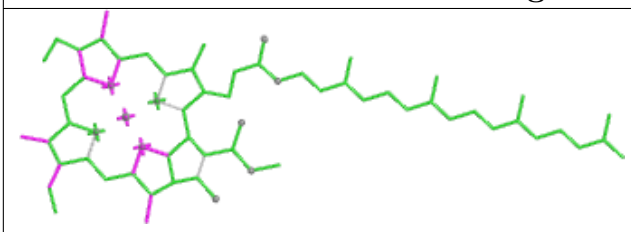


Rings

Ligand CLA b 612



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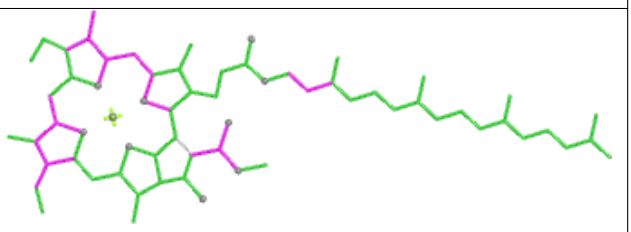
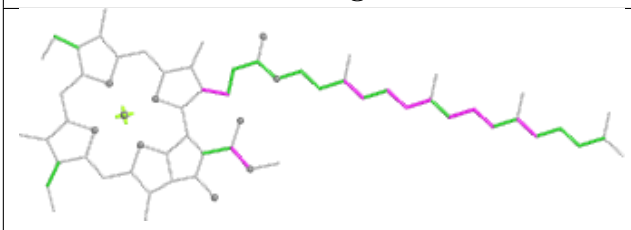


Bond angles



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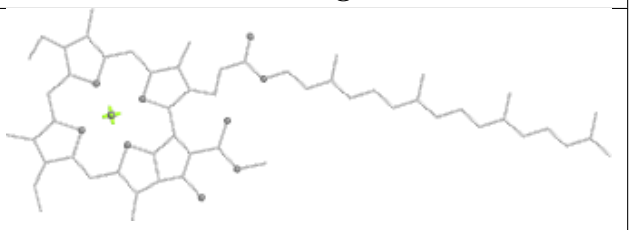
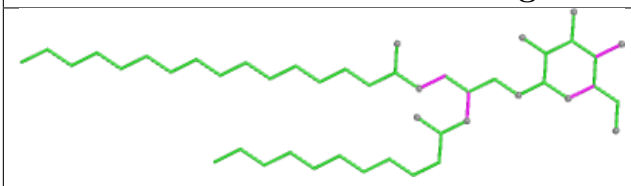
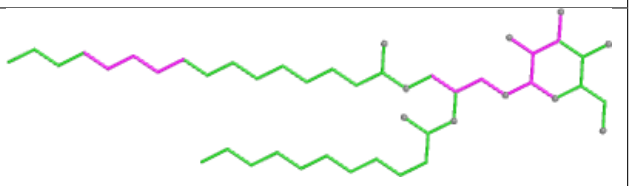
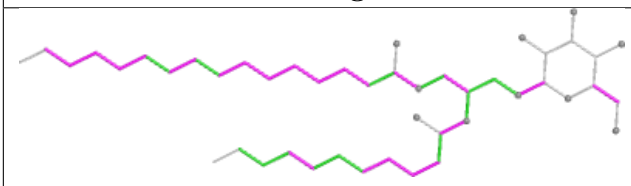
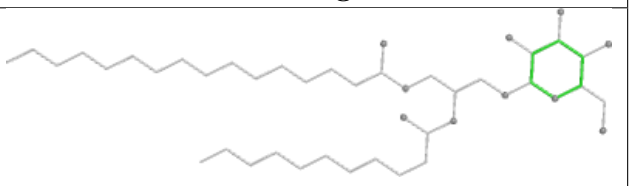
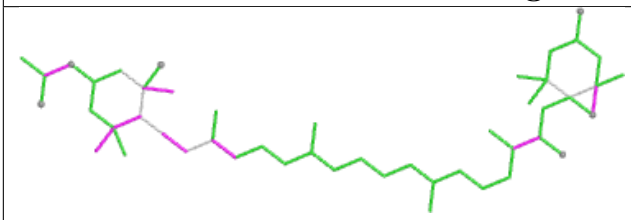
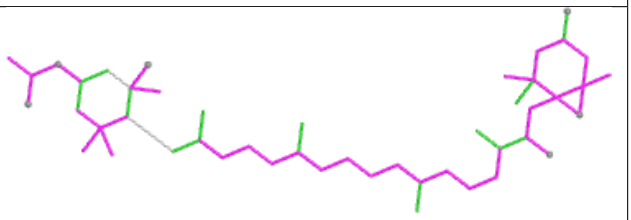
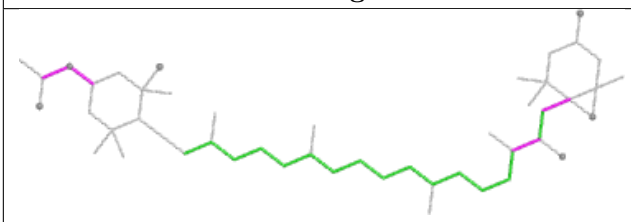
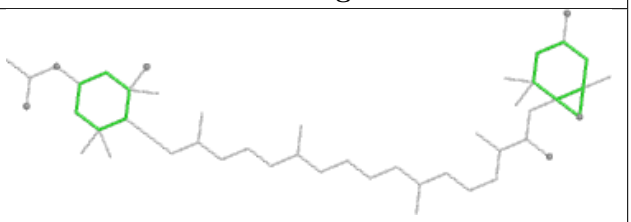
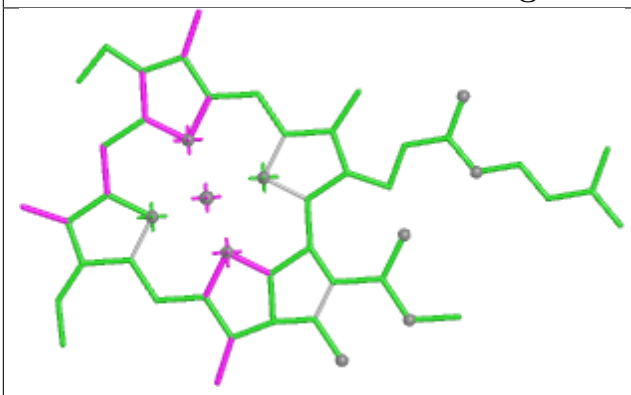


Rings

Ligand LMG K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 17 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 17 313



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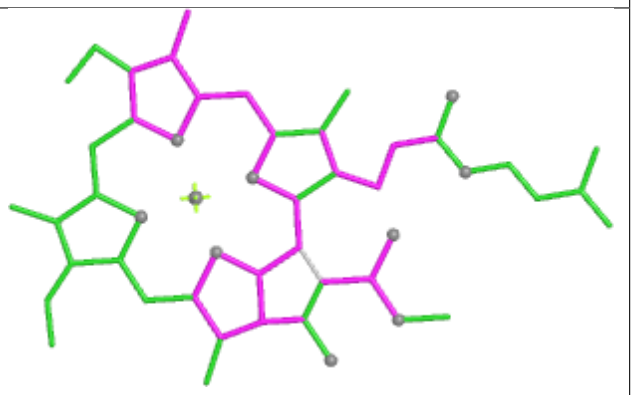
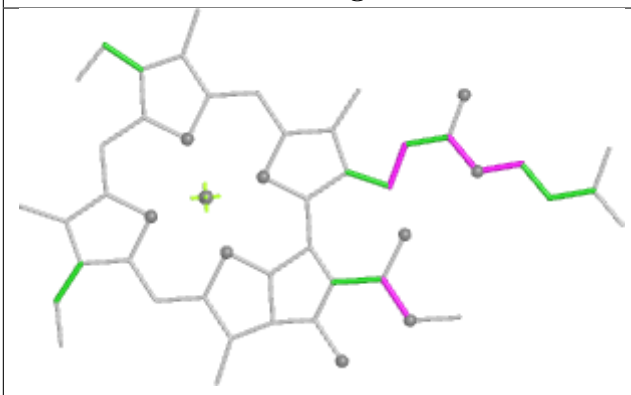


Bond angles



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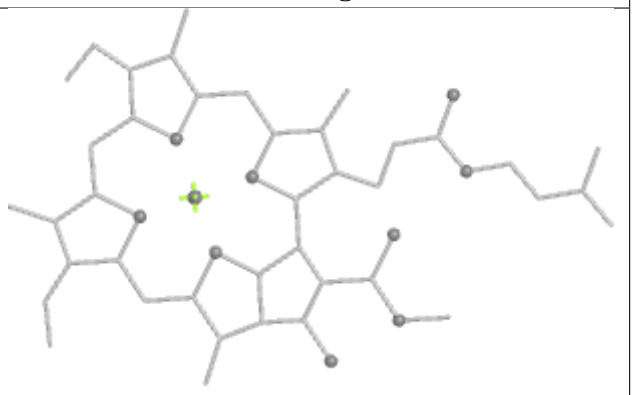
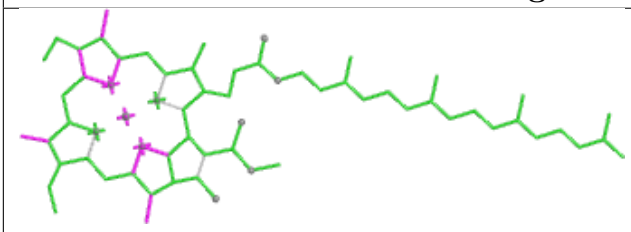


Rings

Ligand CLA a 403



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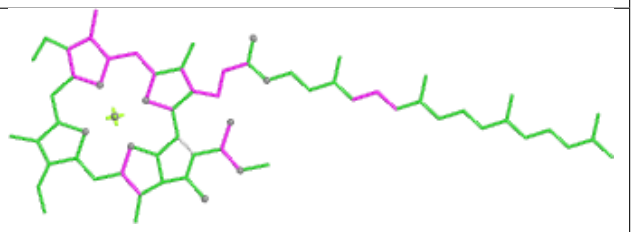
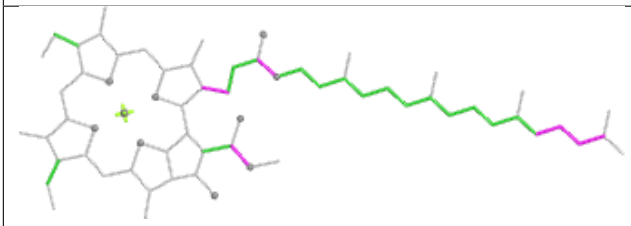


Bond angles



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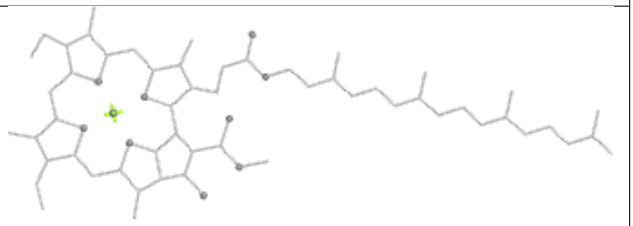
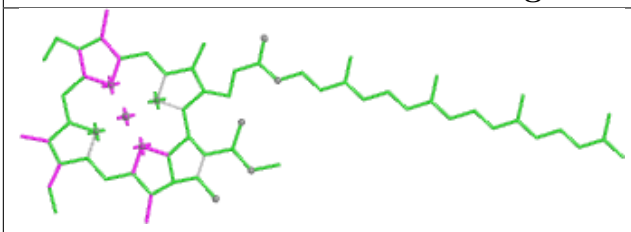
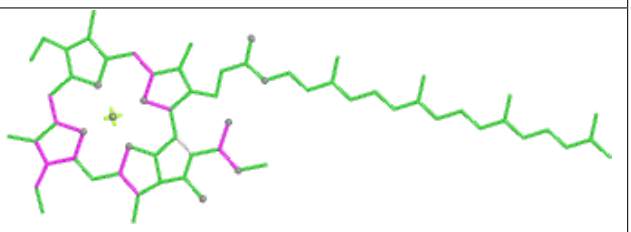


Rings

Ligand CLA C 505



Bond lengths



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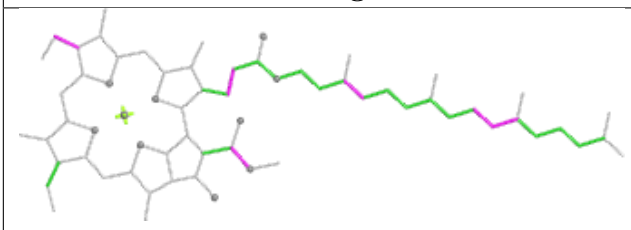
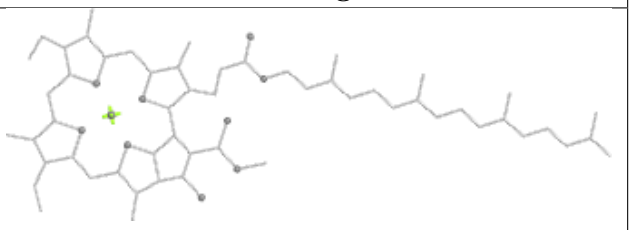
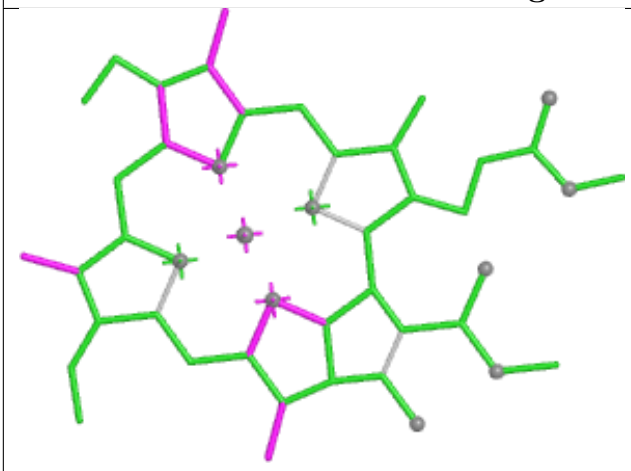


Torsions



Rings

Ligand CLA 8 312



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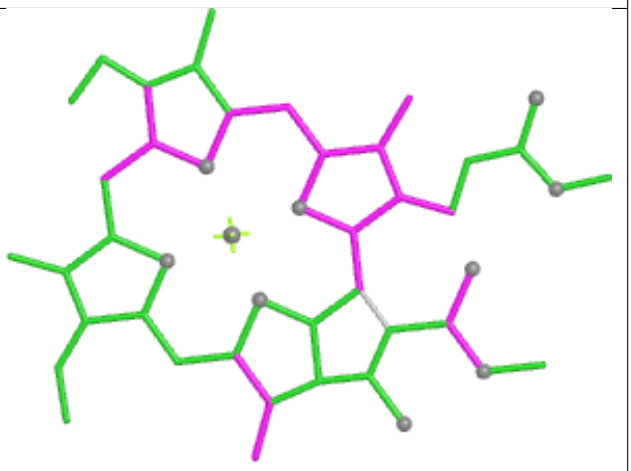

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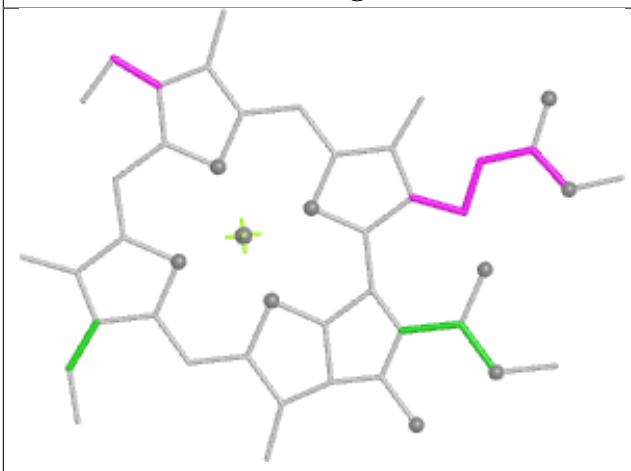
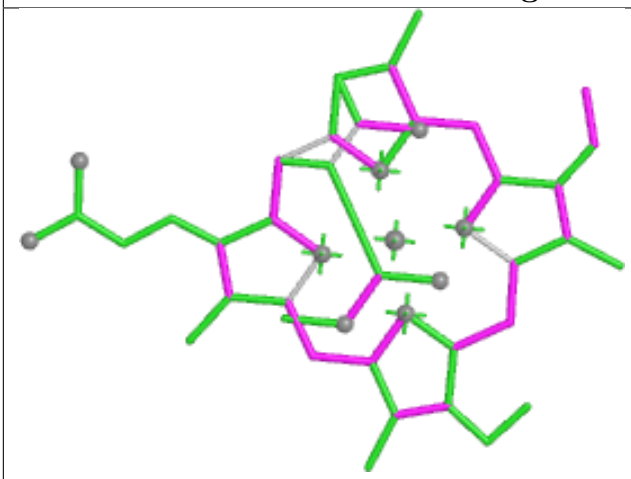


Torsions



Rings

Ligand KC2 12 309



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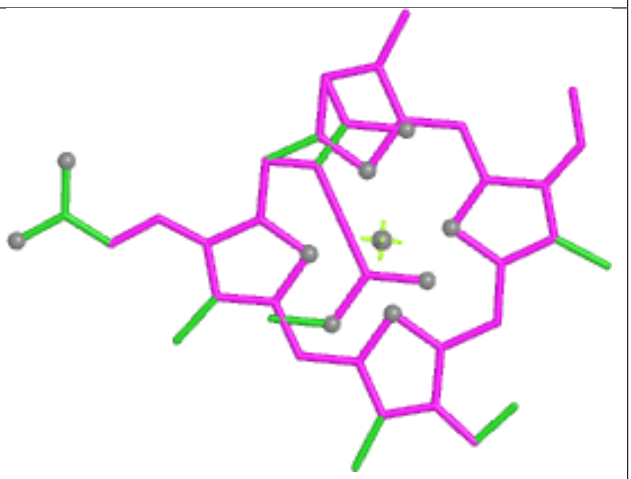

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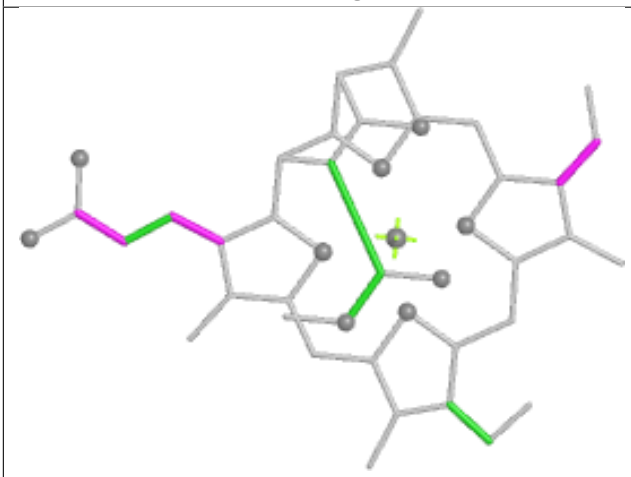

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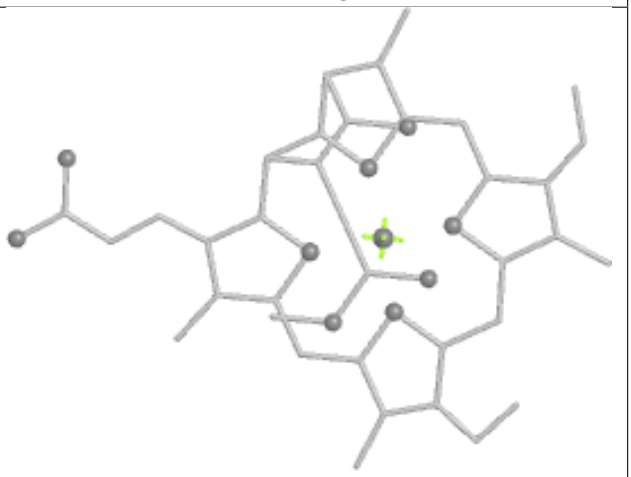
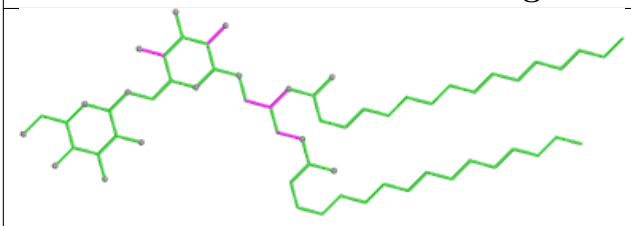


Rings

Ligand DGD h 102



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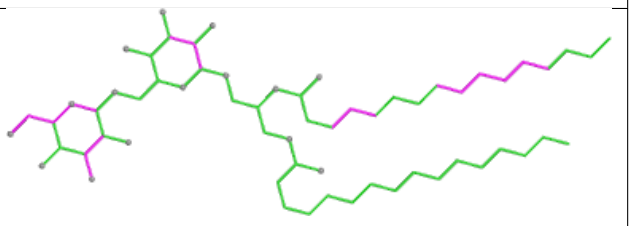

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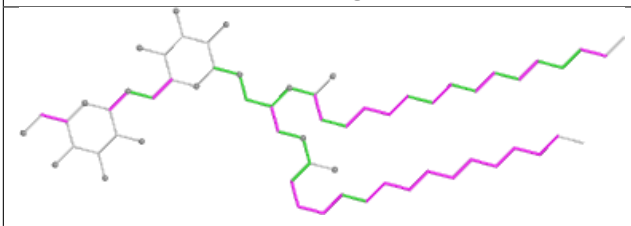

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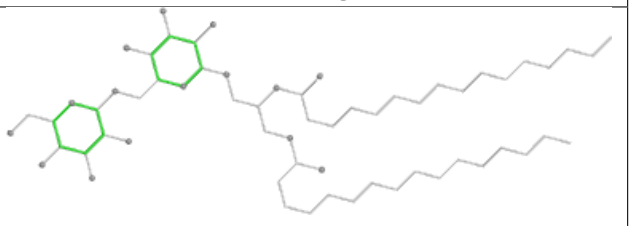

Rings

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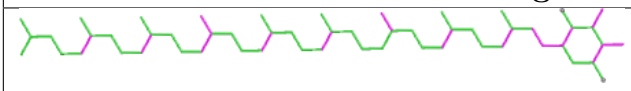	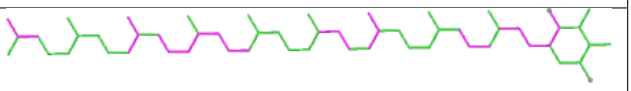
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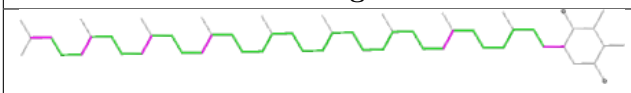	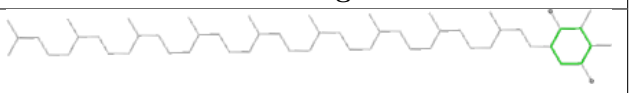
Torsions	Rings

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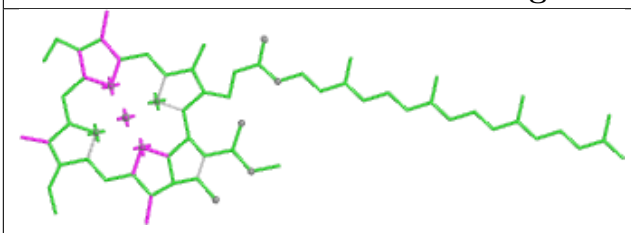	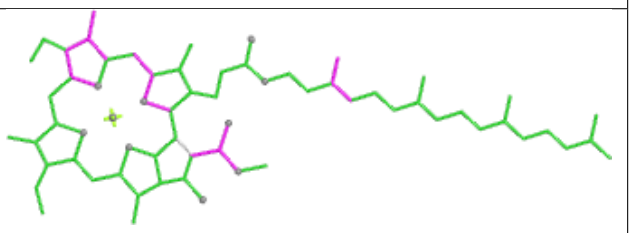
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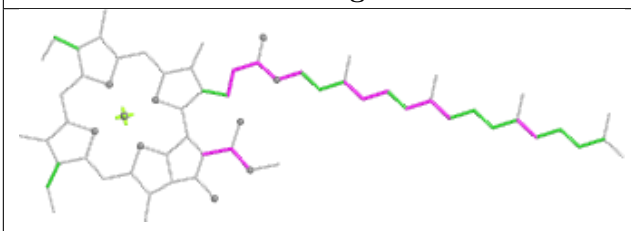
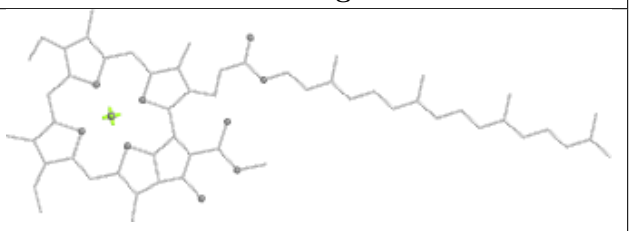
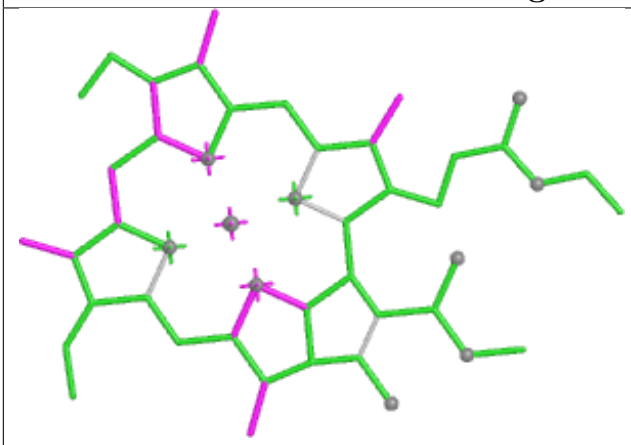
	
Torsions	Rings

Ligand CLA 5 312



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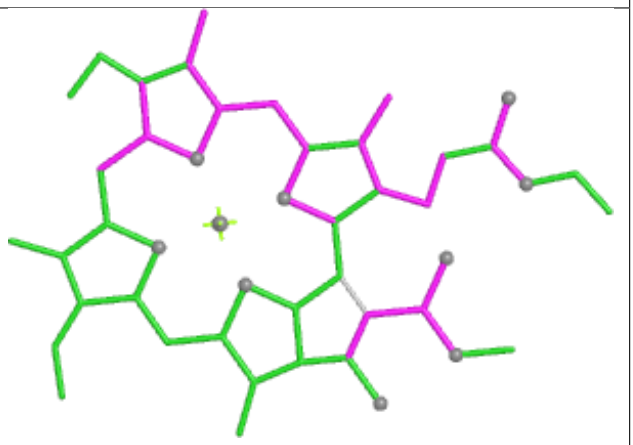
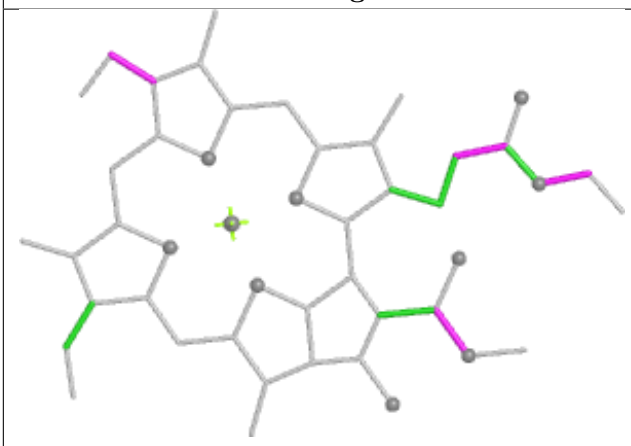


Bond angles



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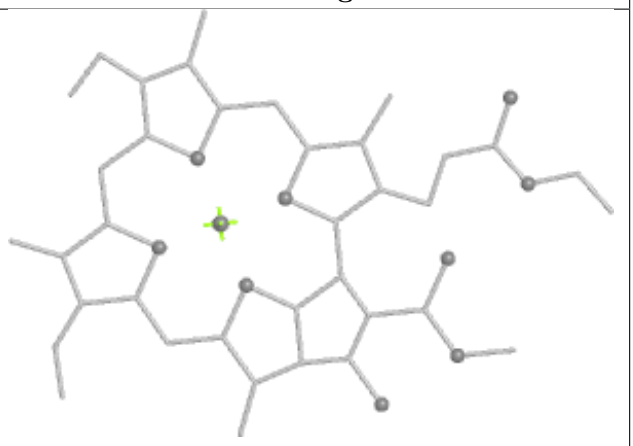
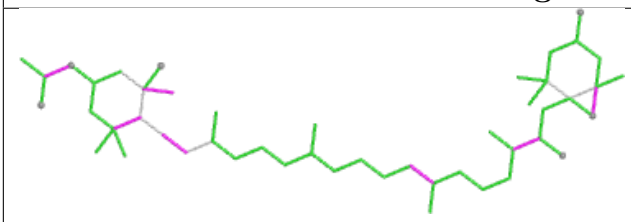


Rings

Ligand A86 0 303



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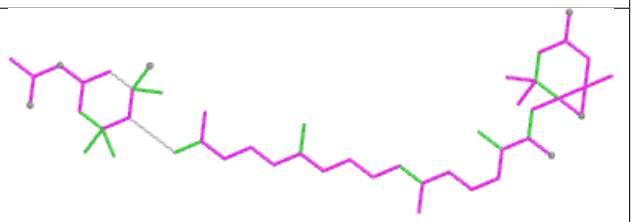

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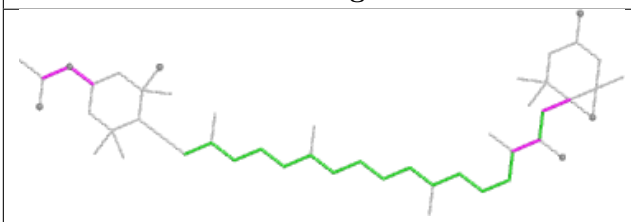

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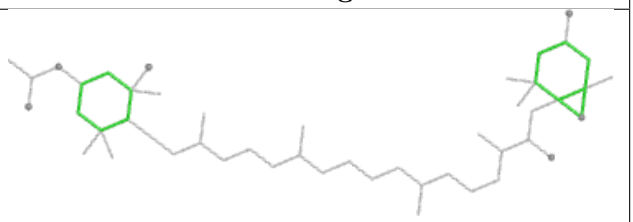
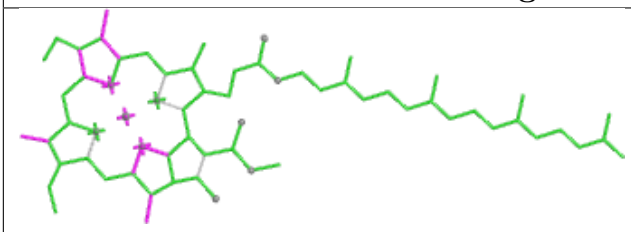


Rings

Ligand CLA W 202



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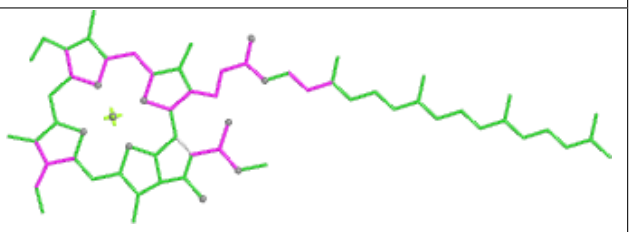
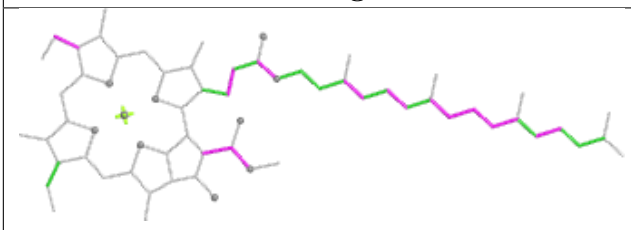


Bond angles



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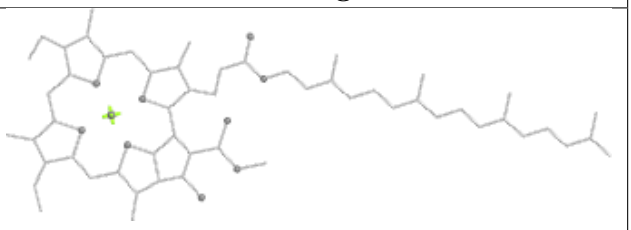
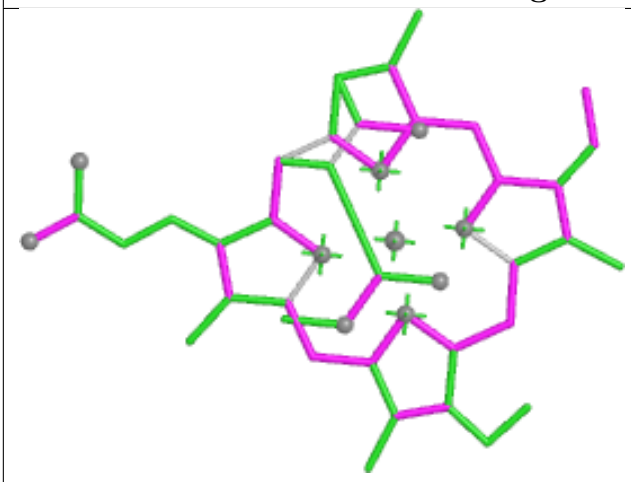


Rings

Ligand KC2 5 310



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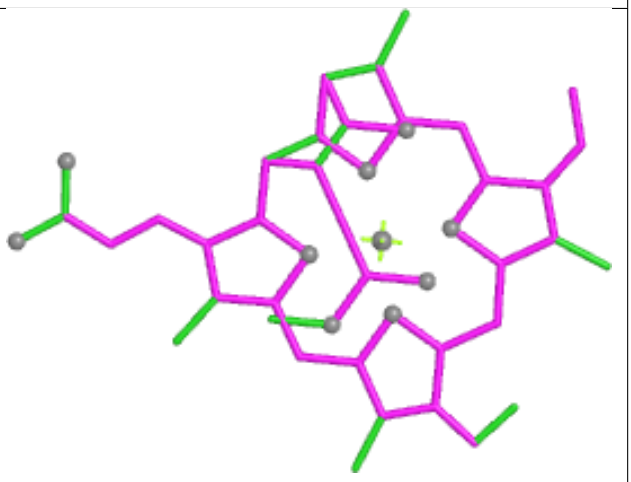

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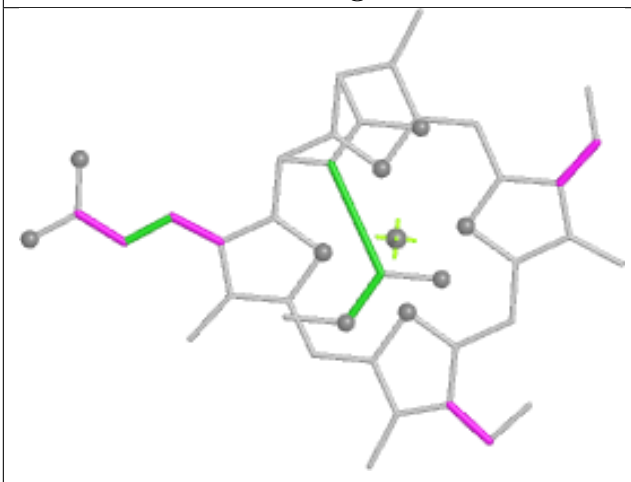

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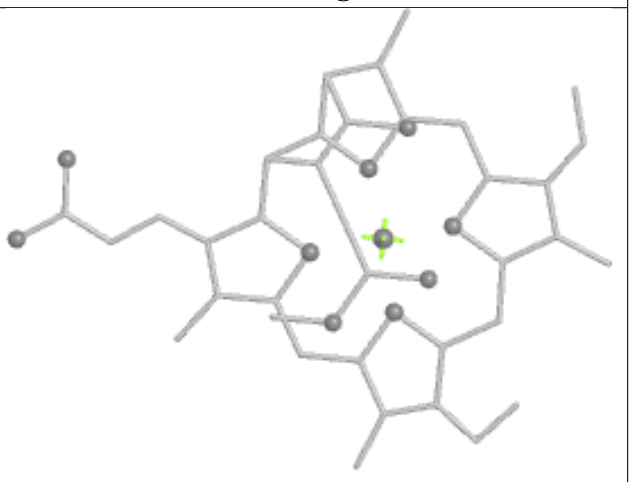
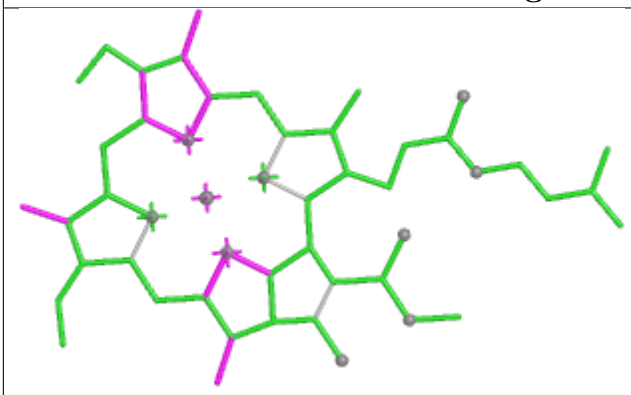


Rings

Ligand CLA P 603



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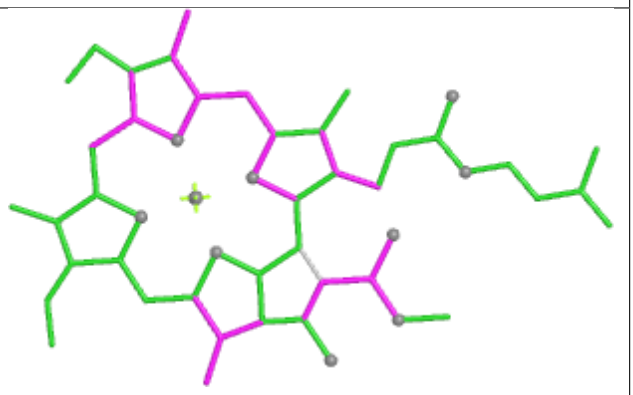

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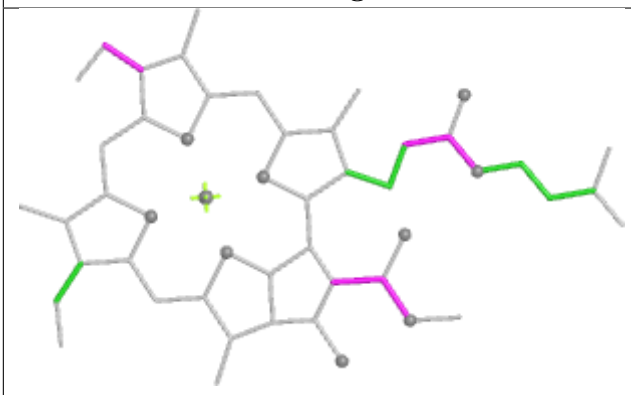

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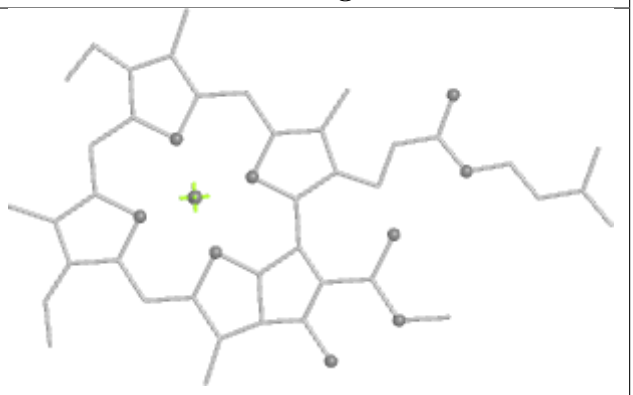
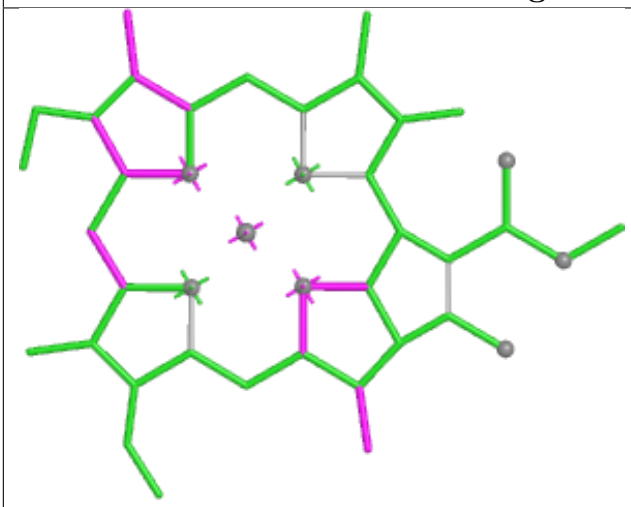


Rings

Ligand CLA 7 308



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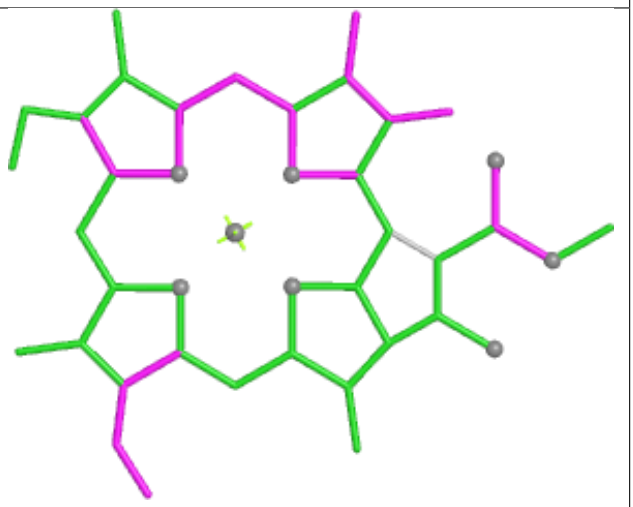

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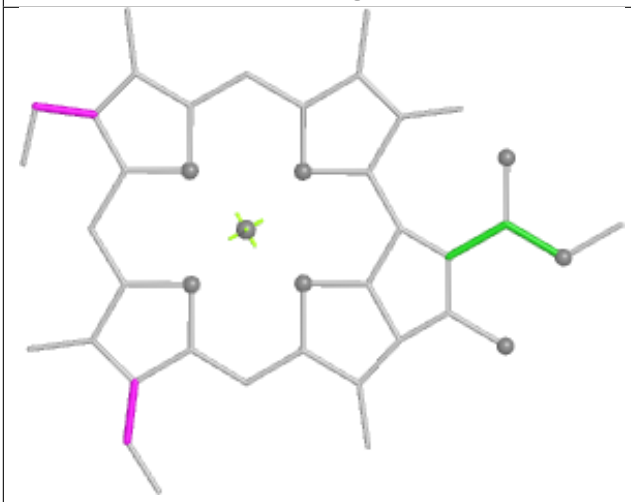

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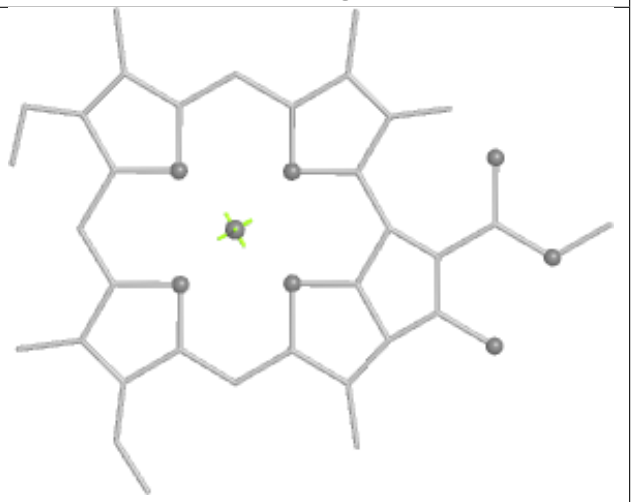
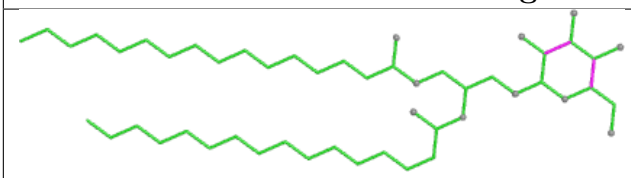


Rings

Ligand LMG C 522



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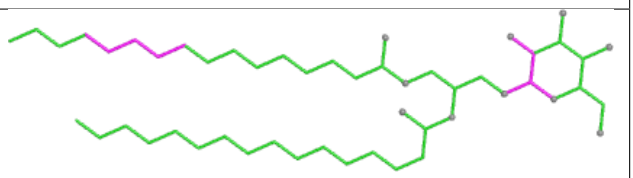
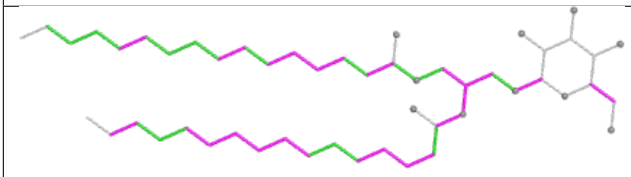


Bond angles



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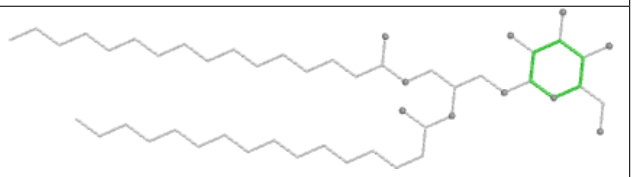
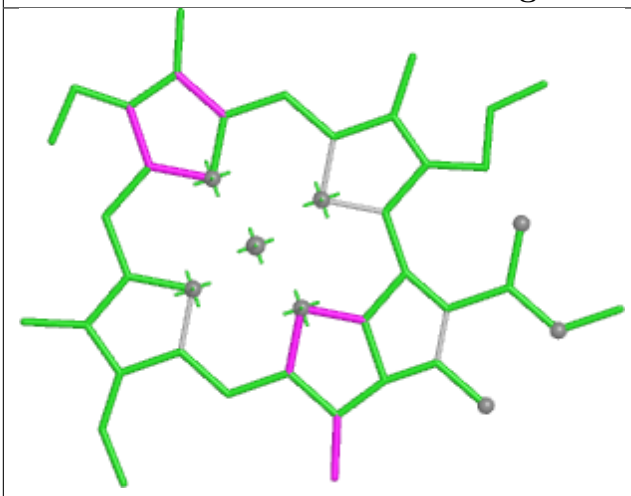


Rings

Ligand CLA 16 315



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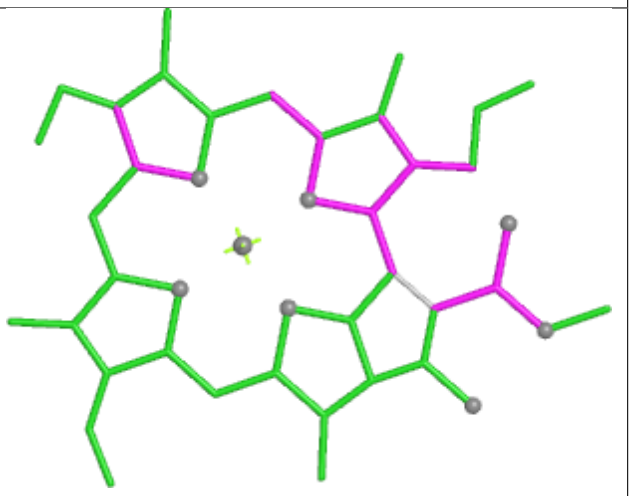
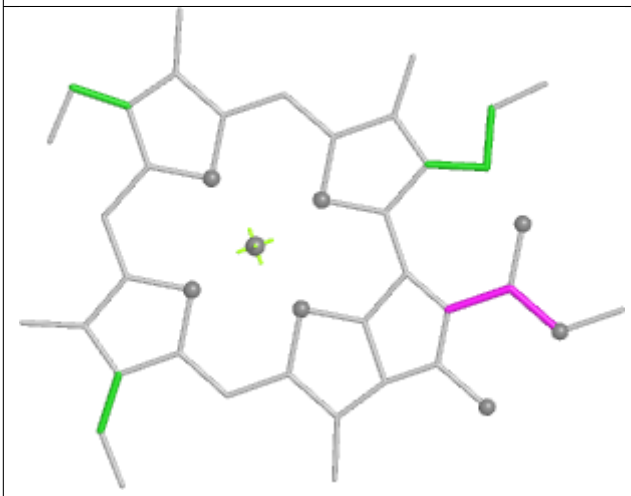


Bond angles



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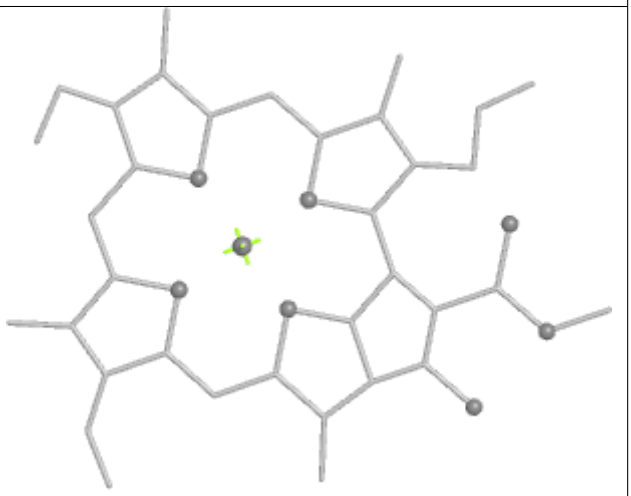
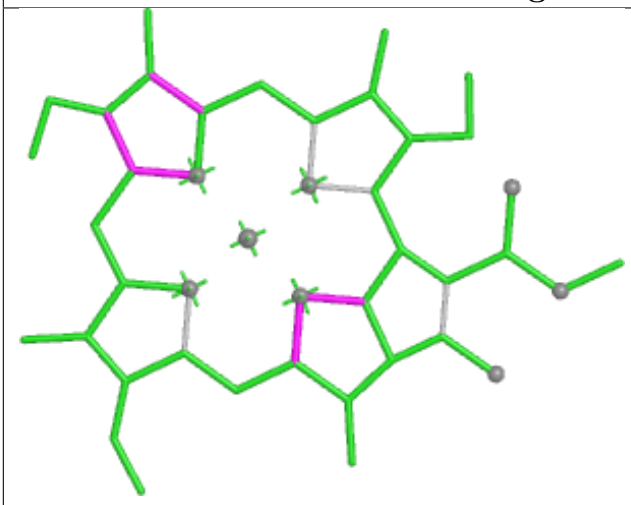


Rings

Ligand CLA 2 306



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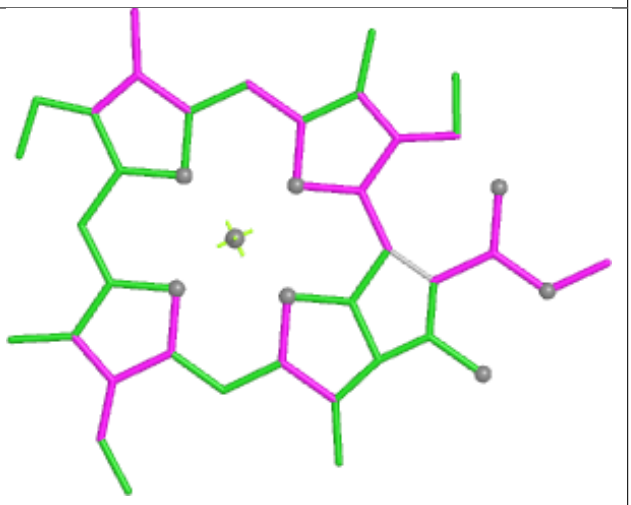
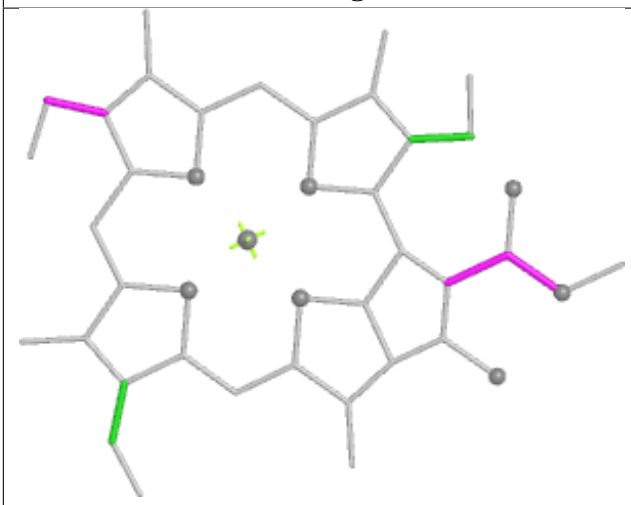


Bond angles

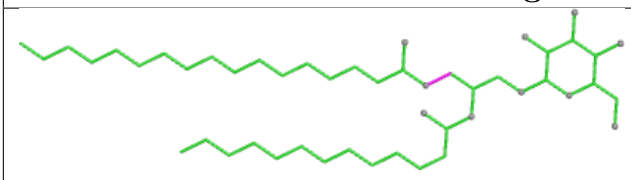


Torsions

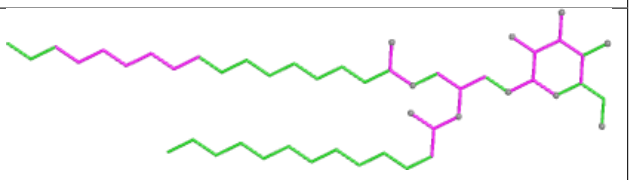


Rings

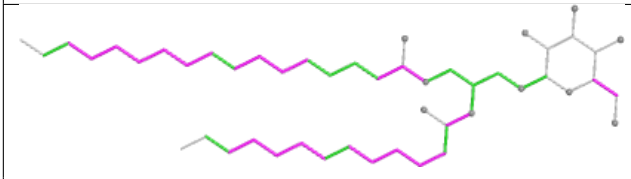
Ligand LMG 4 316



Bond lengths



Bond angles



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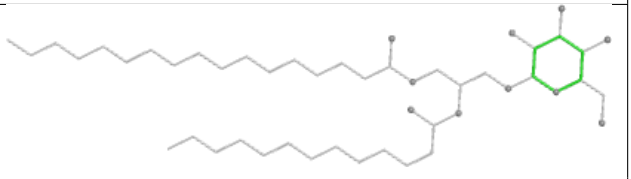
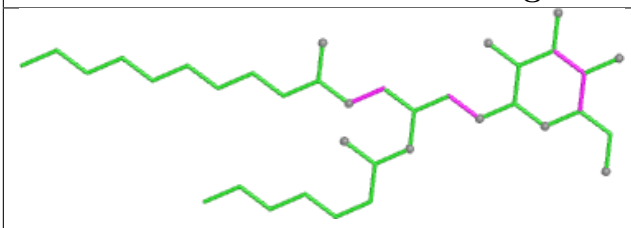


Rings

Ligand LMG 5 316



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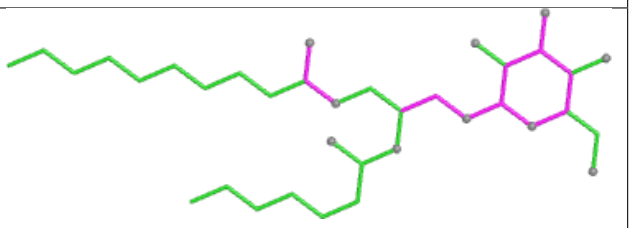

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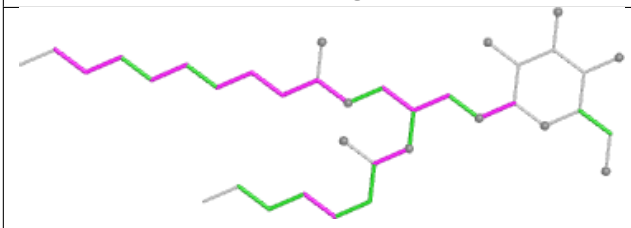

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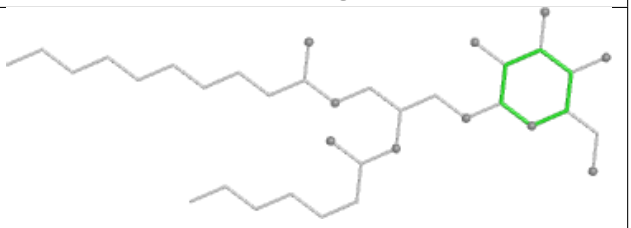
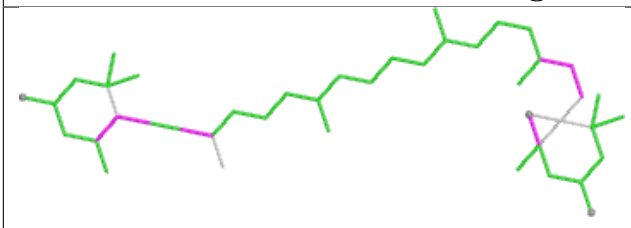


Rings

Ligand DD6 p 612



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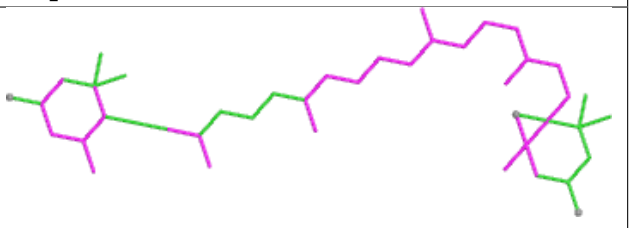

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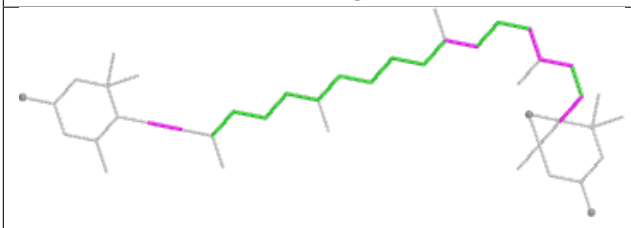

Torsions



Rings

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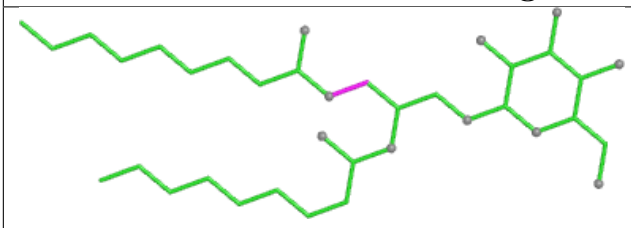

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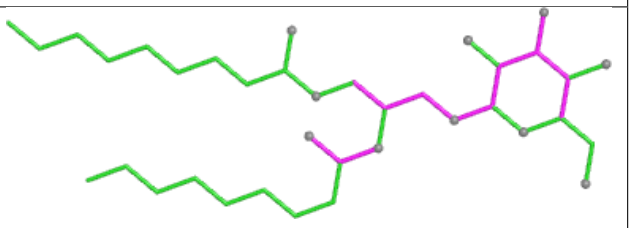

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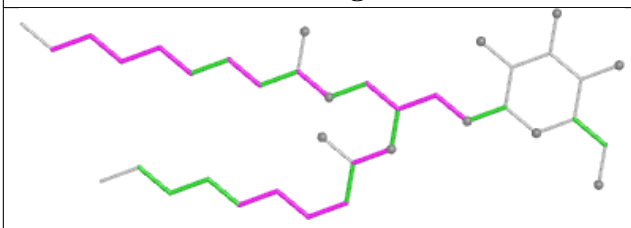

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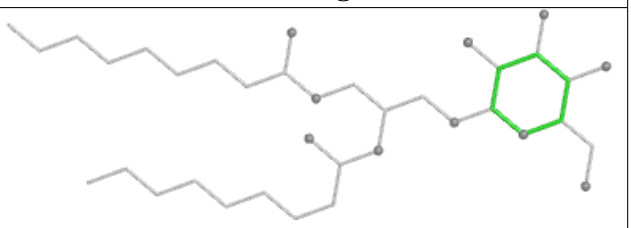
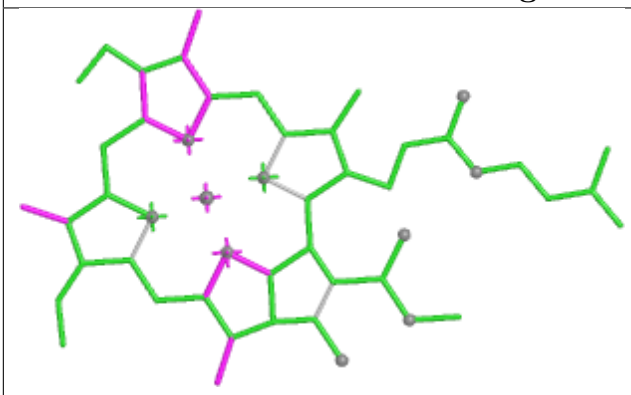


Rings

Ligand CLA 18 306



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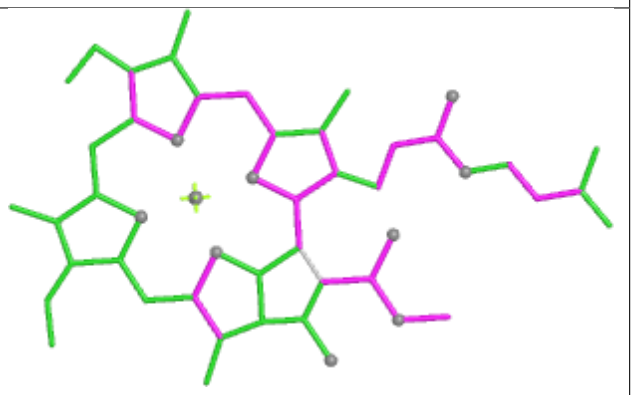

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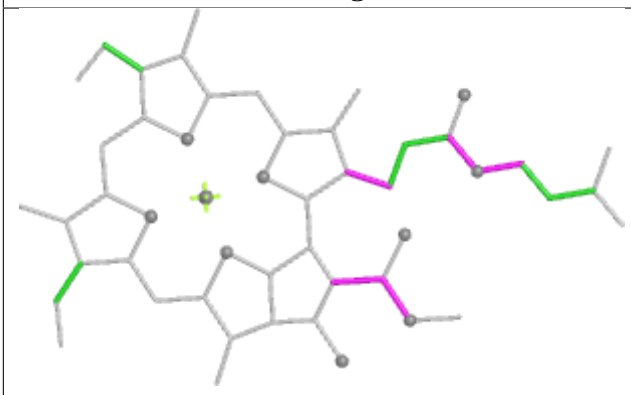

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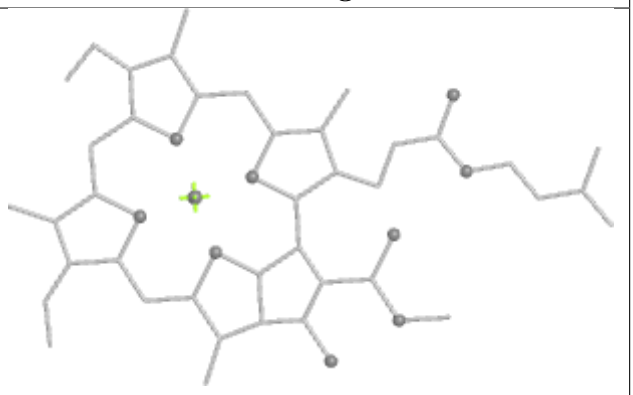

Rings

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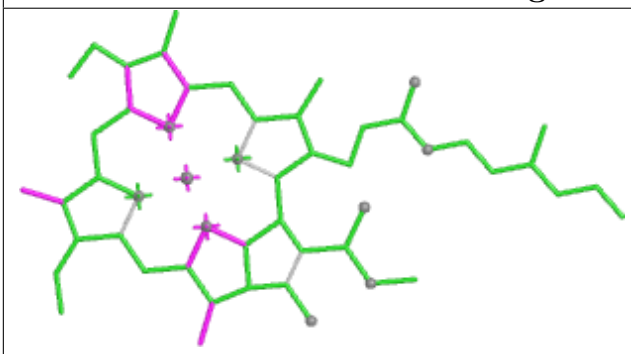

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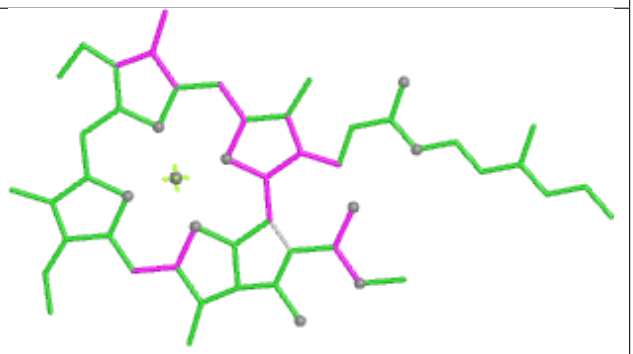

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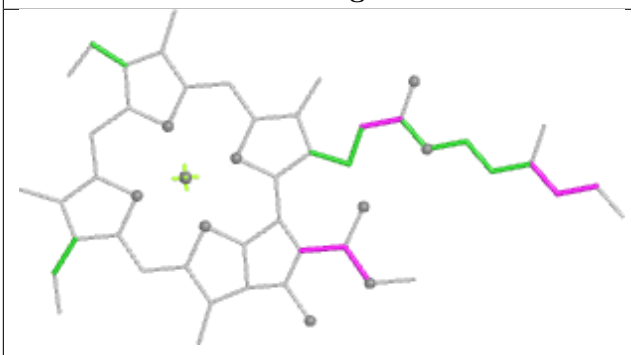

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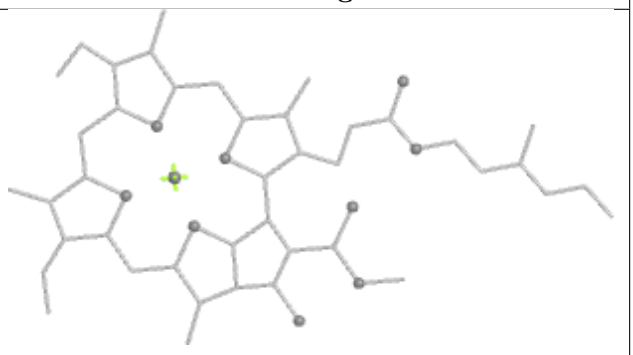

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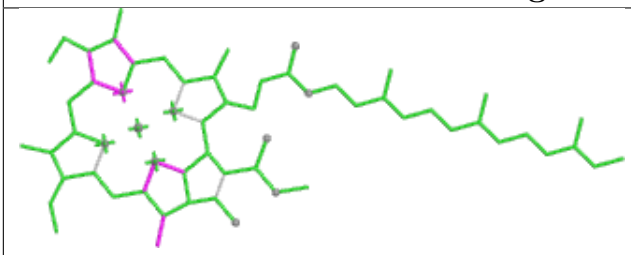

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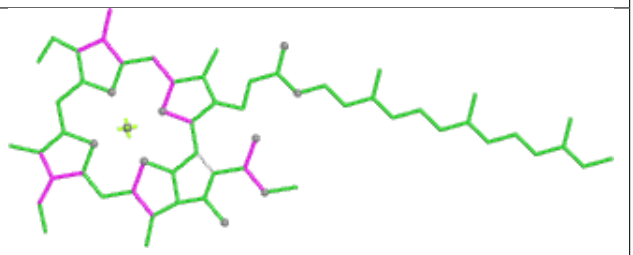

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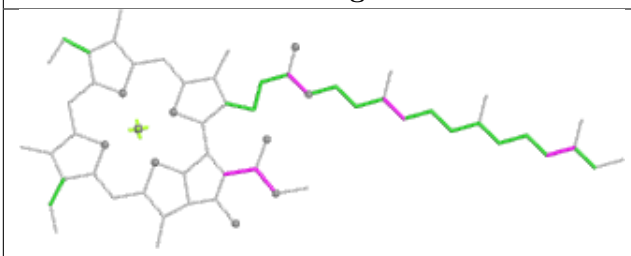

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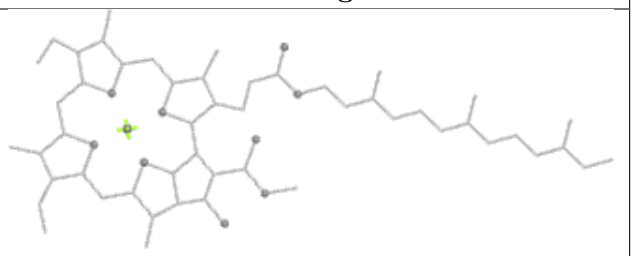

Rings

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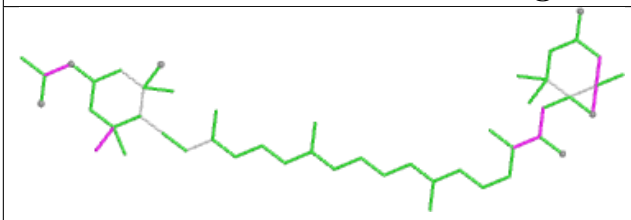

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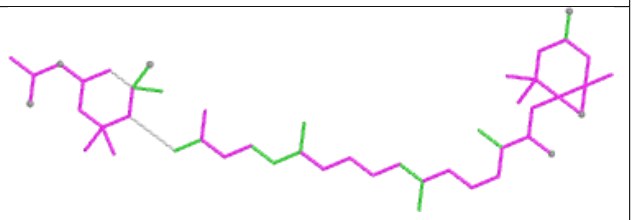

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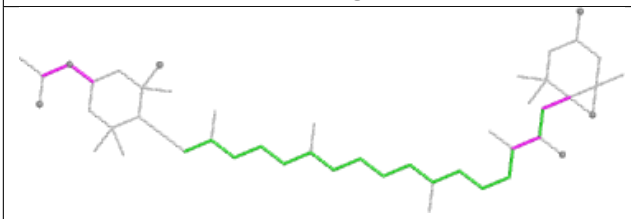

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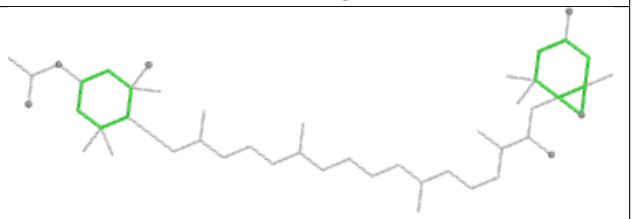

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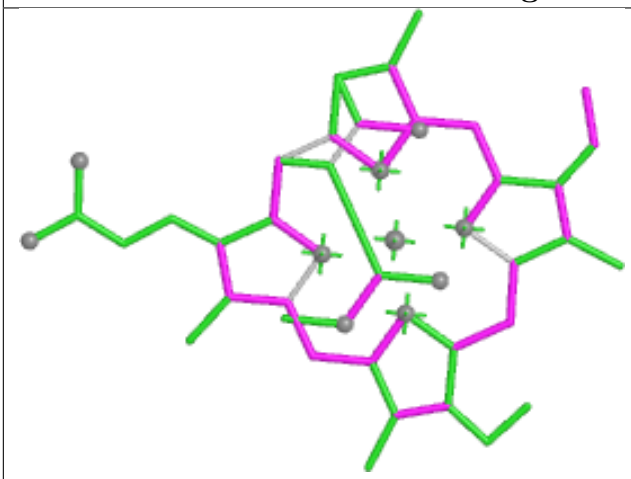

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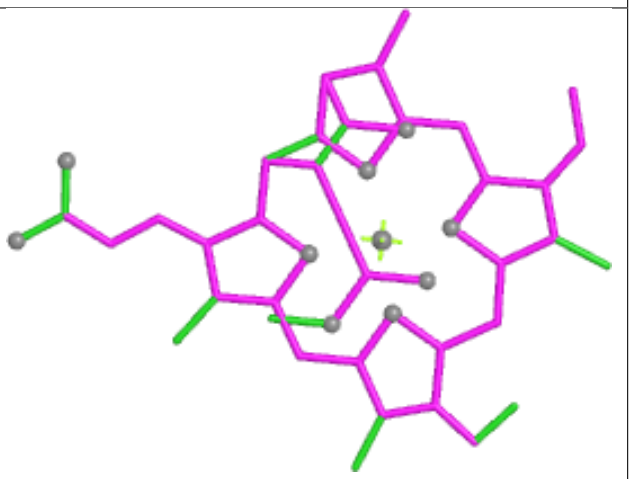

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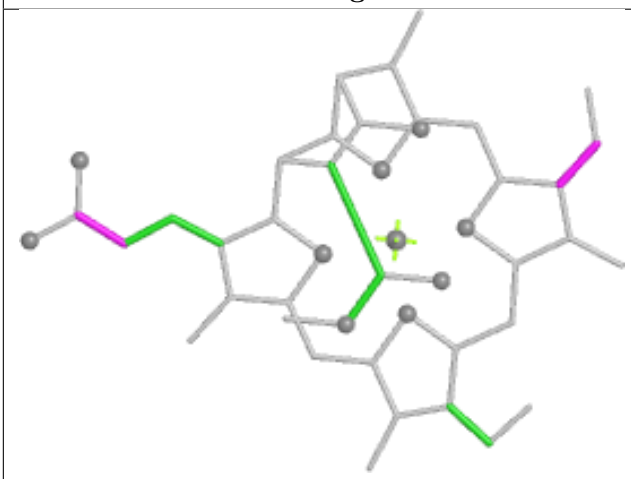

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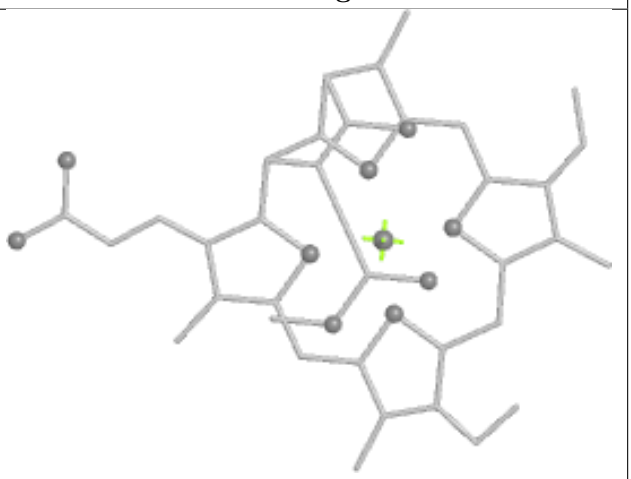

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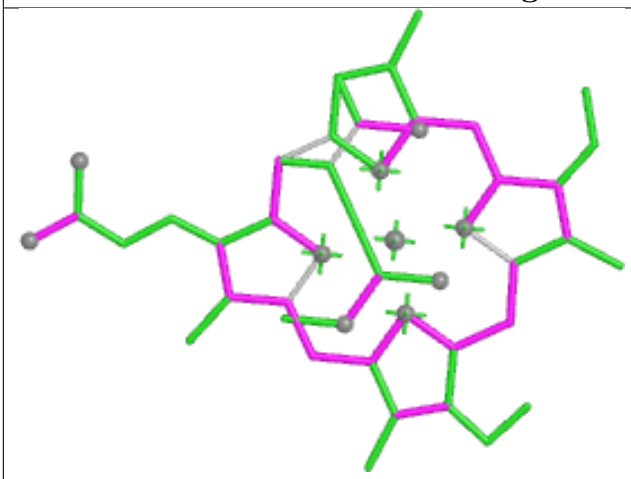

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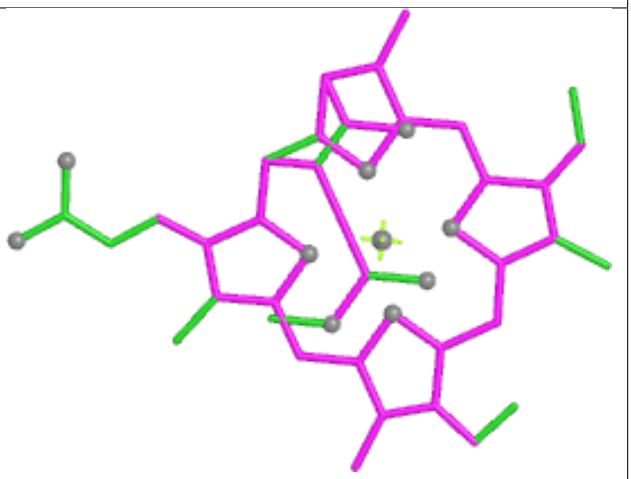

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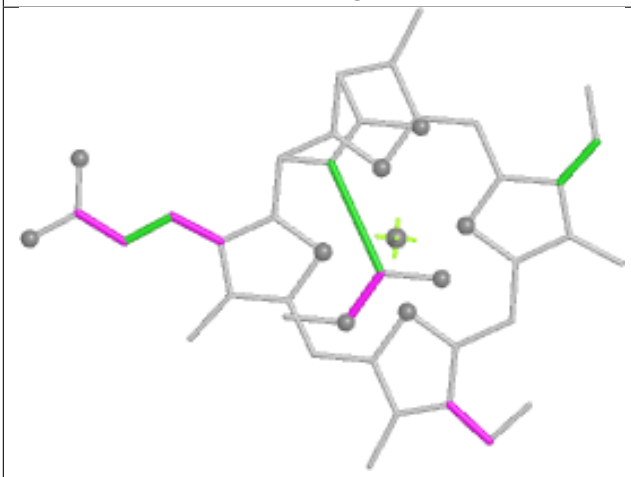

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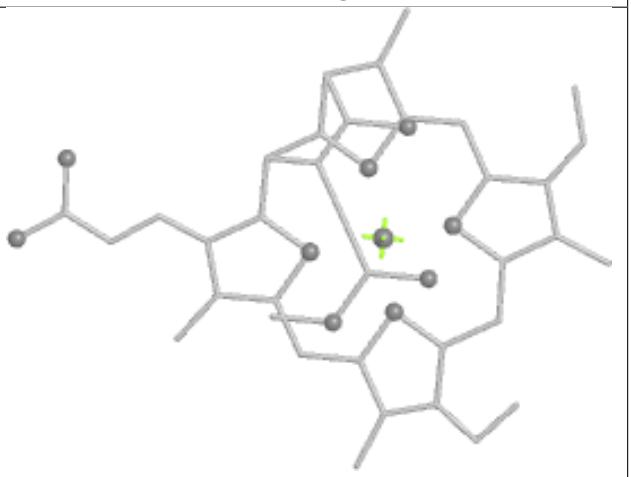

Rings

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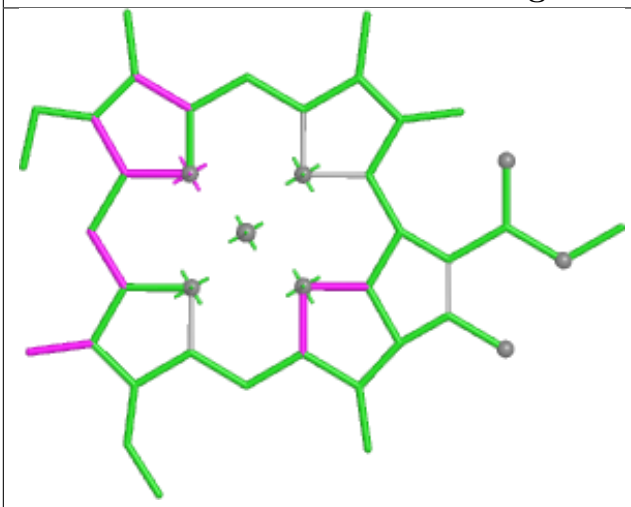

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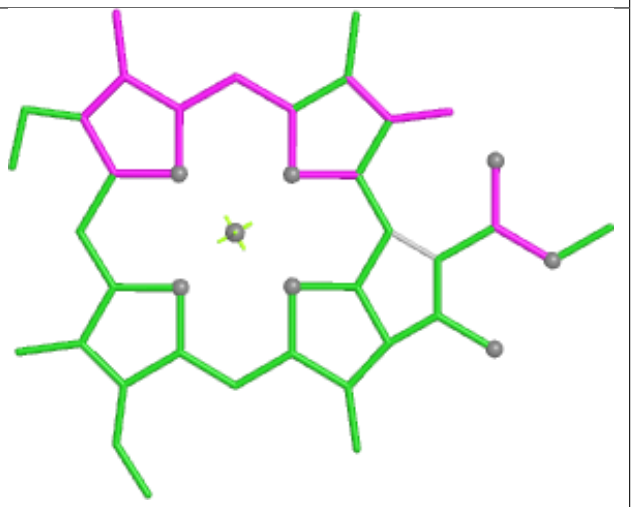

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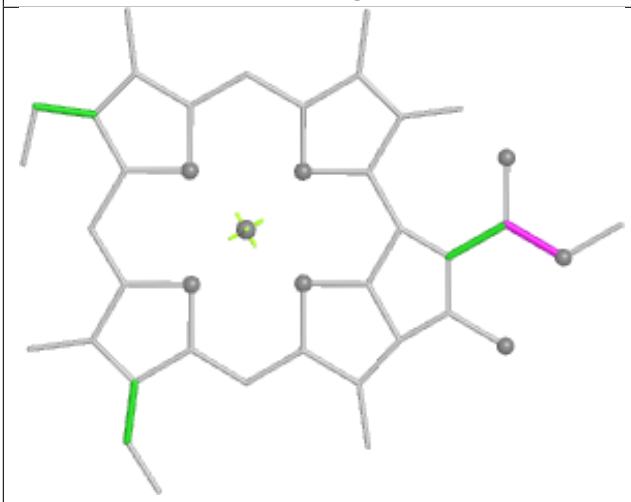

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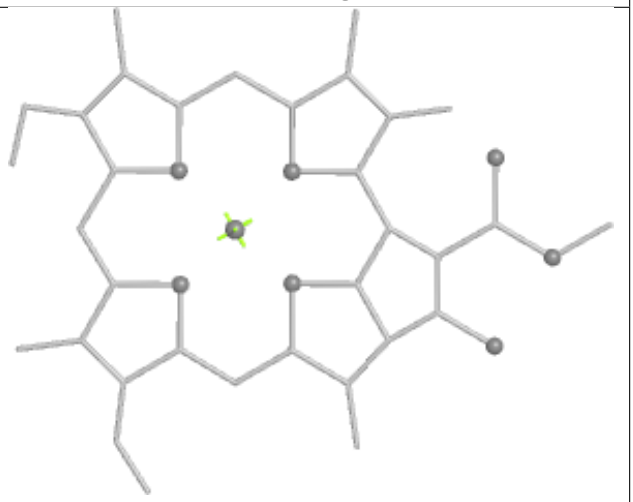
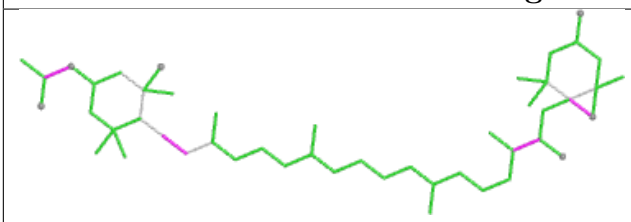


Rings

Ligand A86 19 304



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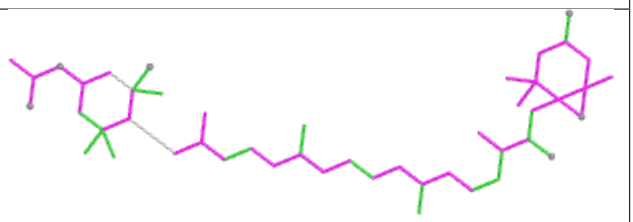

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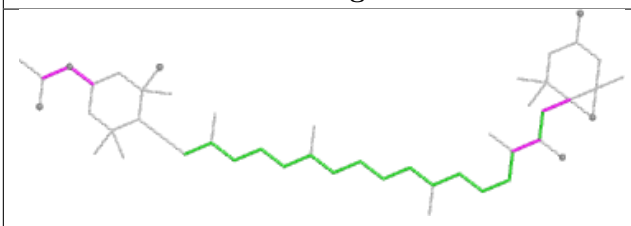

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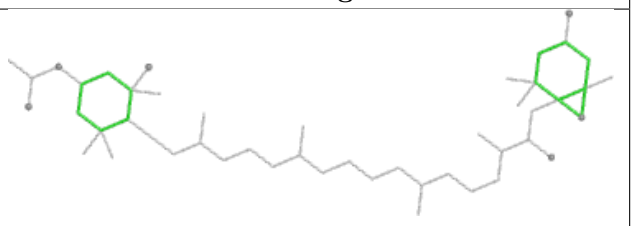
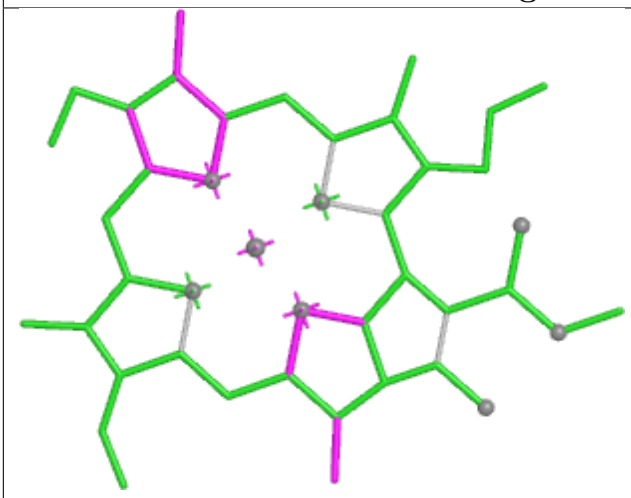


Rings

Ligand CLA 18 314



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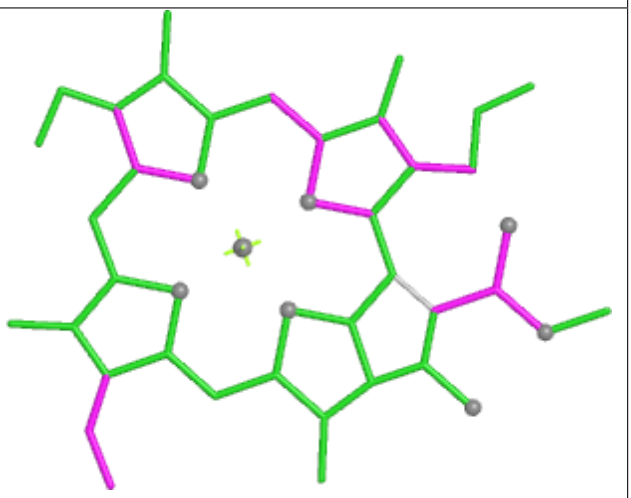

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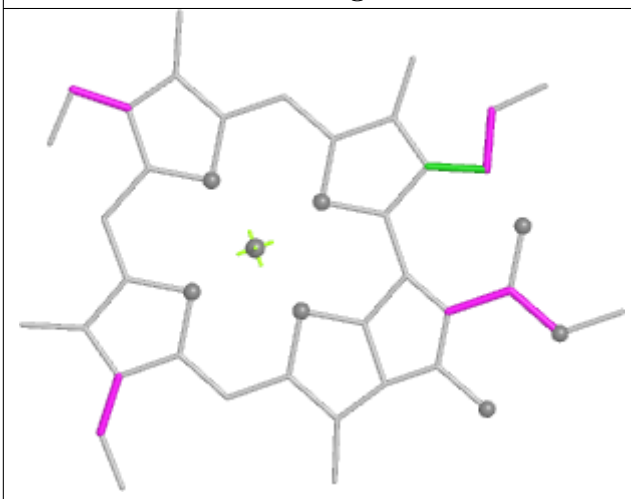

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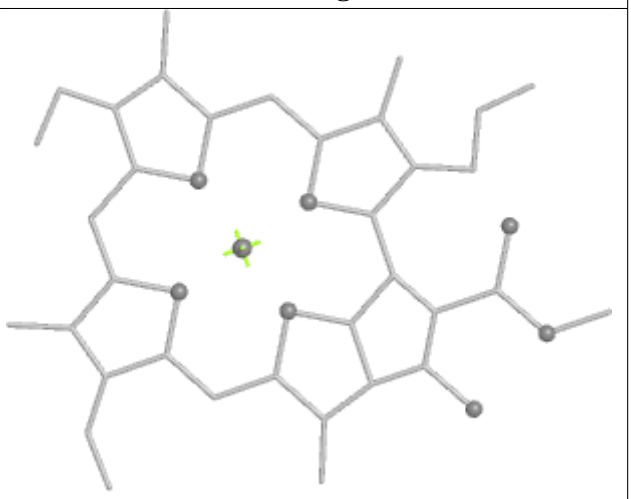
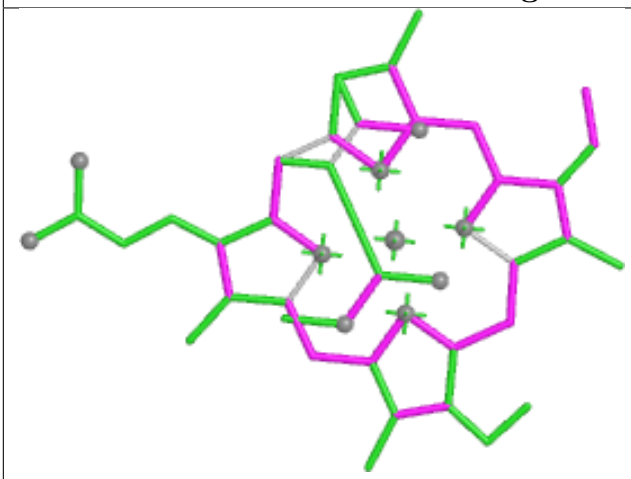


Rings

Ligand KC2 17 311



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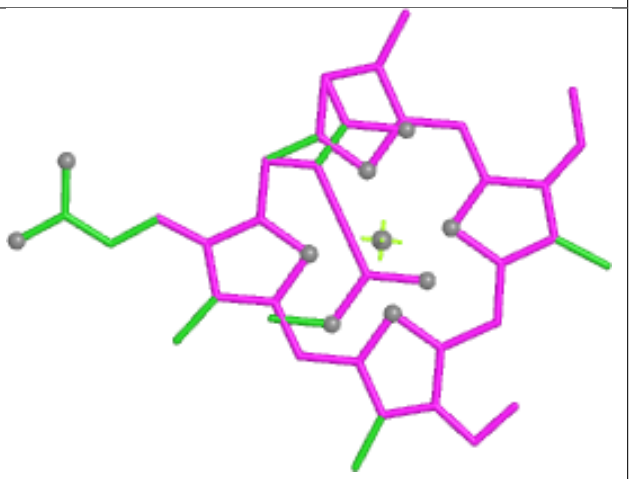

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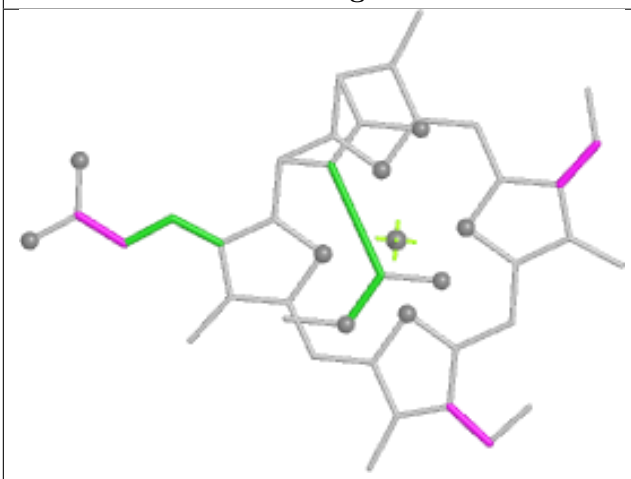

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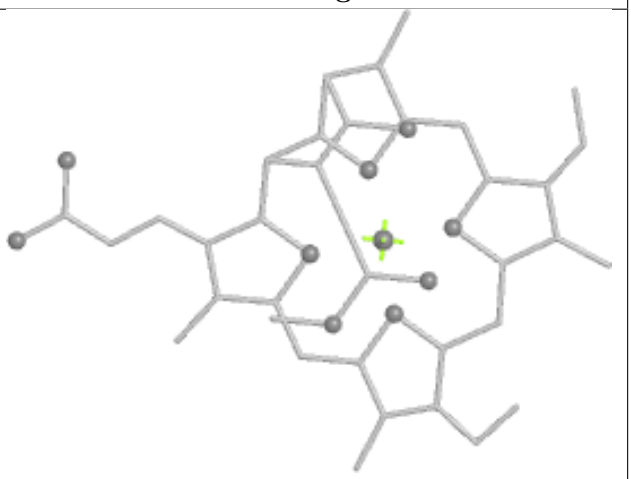
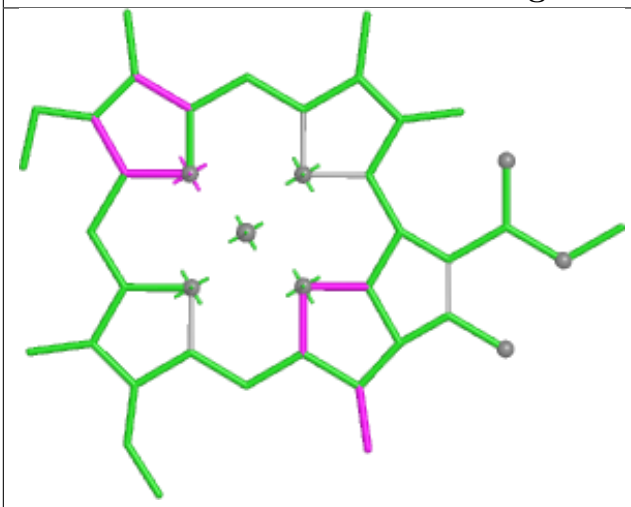


Rings

Ligand CLA 1 315



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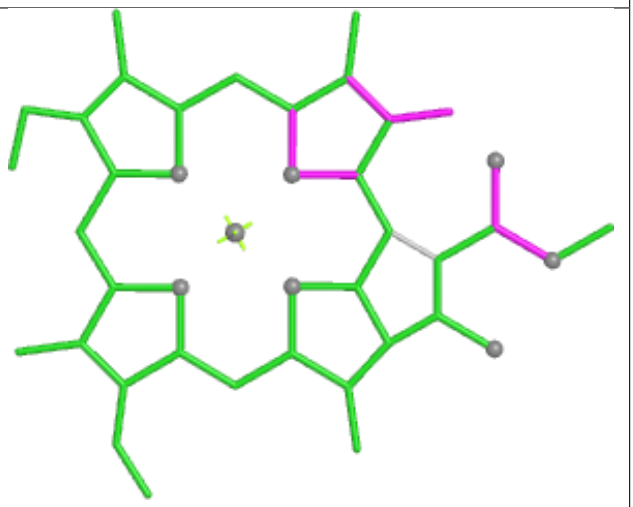
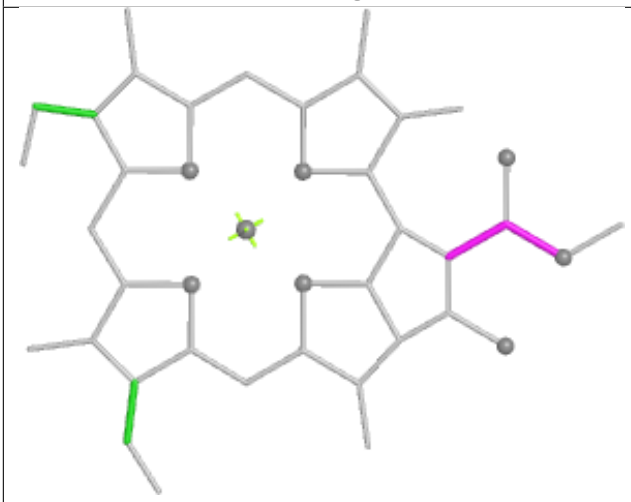


Bond angles



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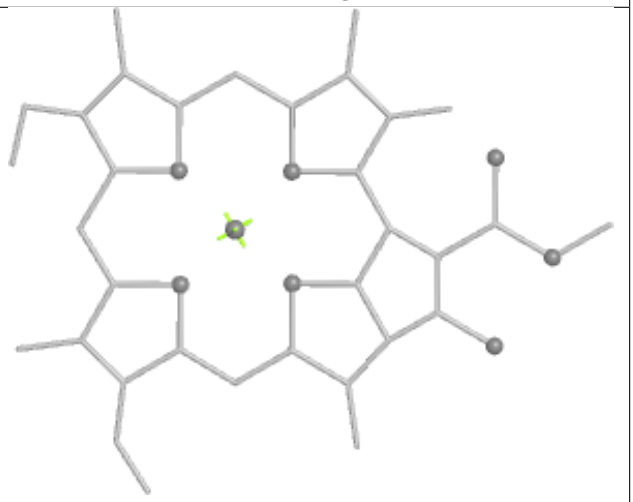
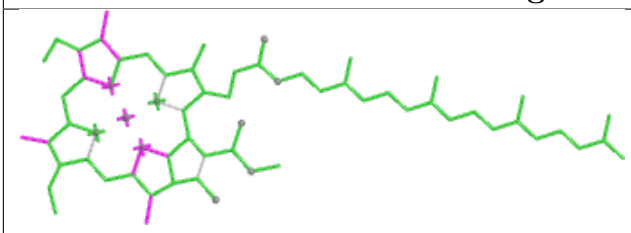


Rings

Ligand CLA b 602



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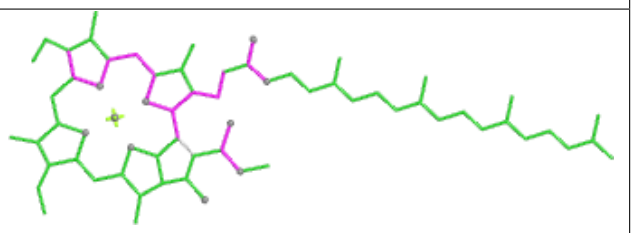

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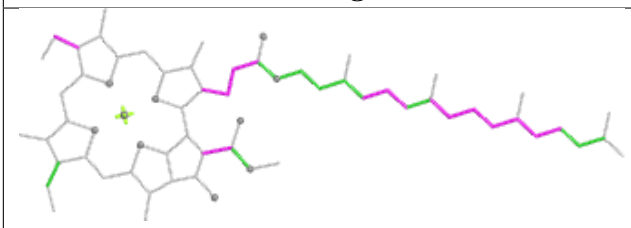
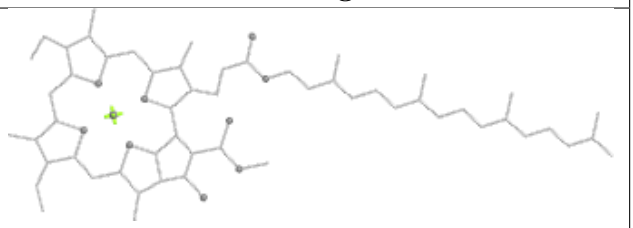
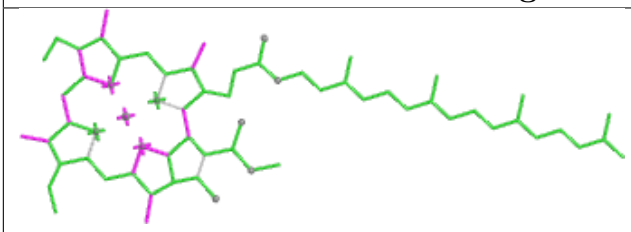


Torsions



Rings

Ligand CLA 13 313



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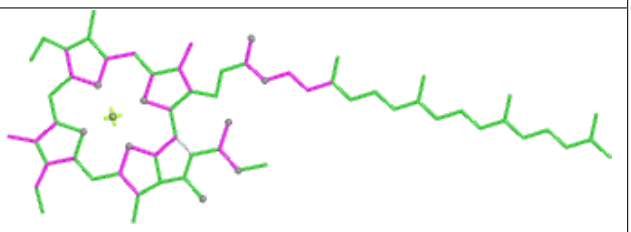

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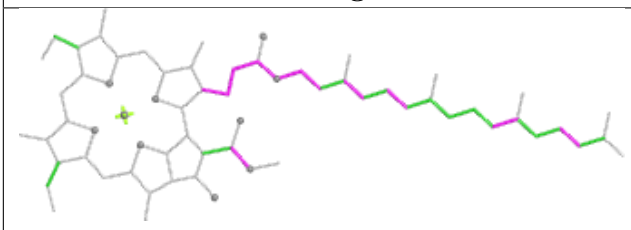

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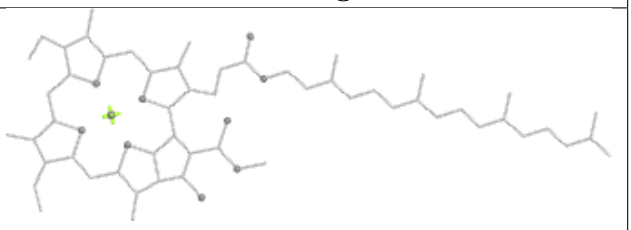


Rings

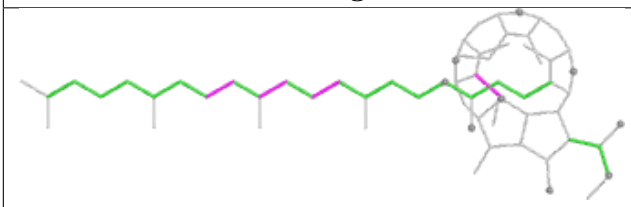
Ligand PHO D 403



Bond lengths



Bond angles



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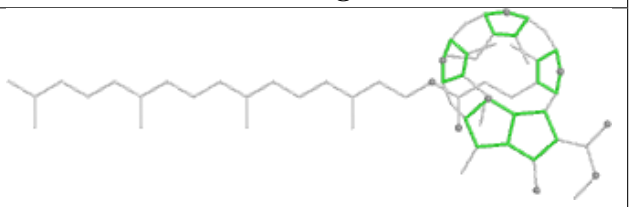
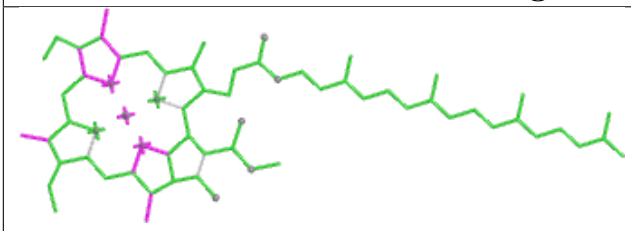


Rings

Ligand CLA c 510



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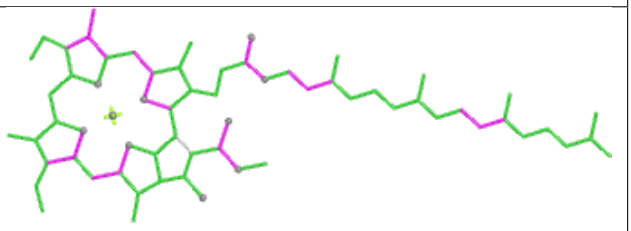

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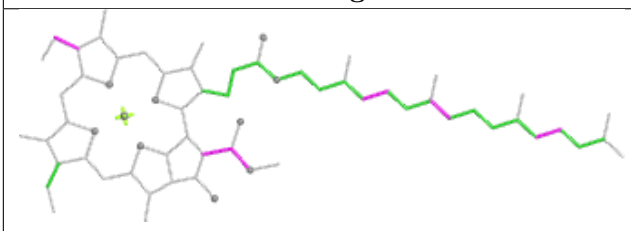

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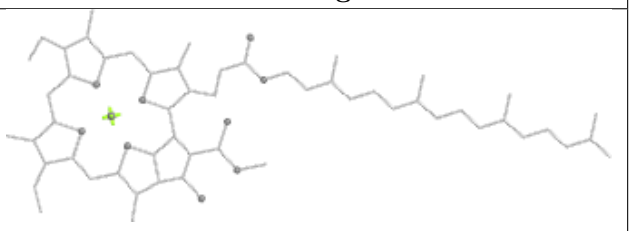
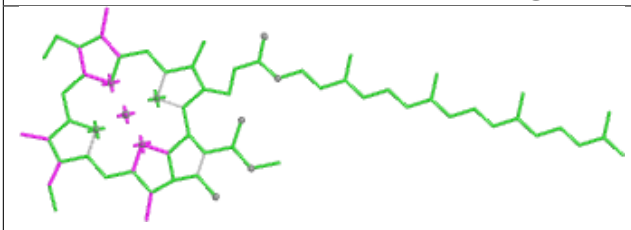


Rings

Ligand CLA b 606



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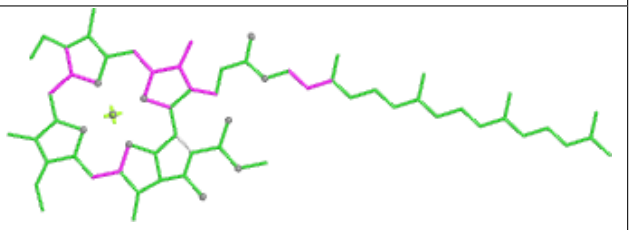

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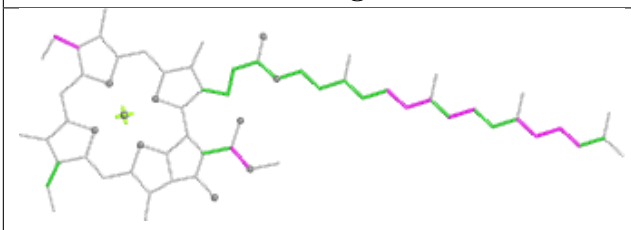

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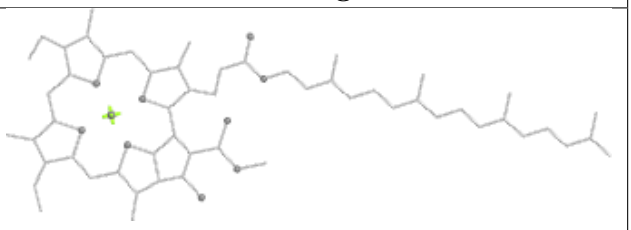
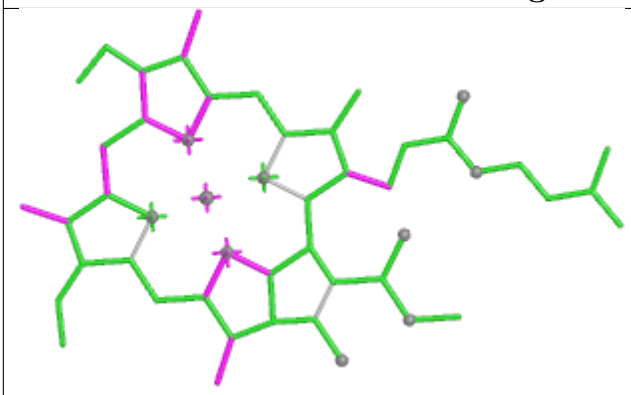


Rings

Ligand CLA 7 313



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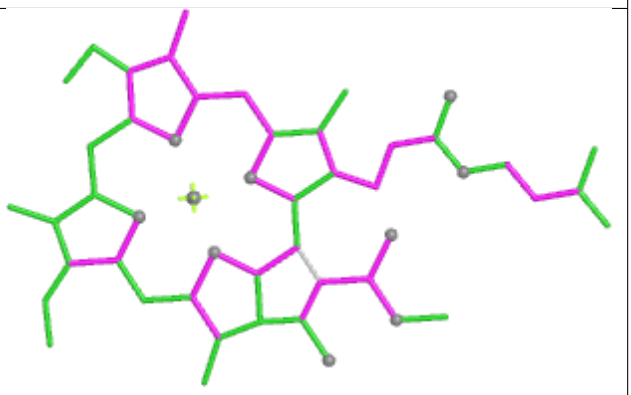

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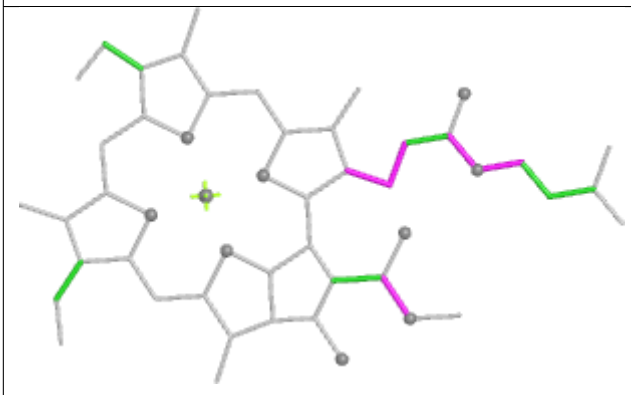

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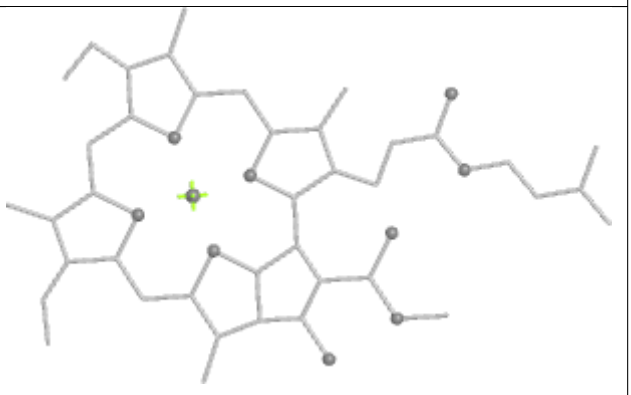
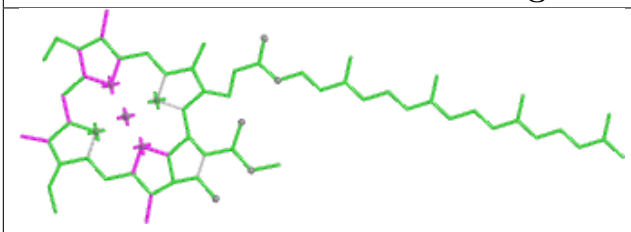


Rings

Ligand CLA 3 313



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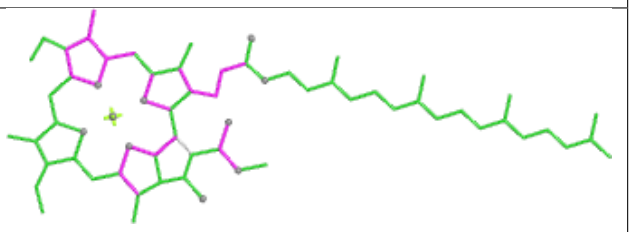

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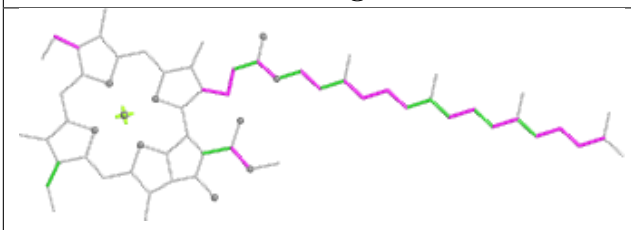

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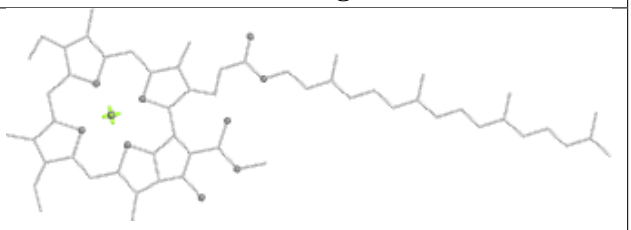
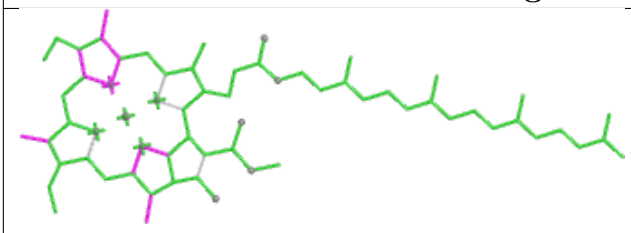


Rings

Ligand CLA B 615



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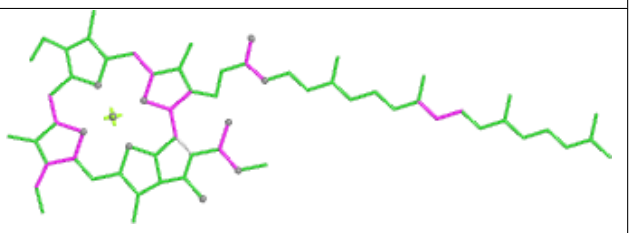

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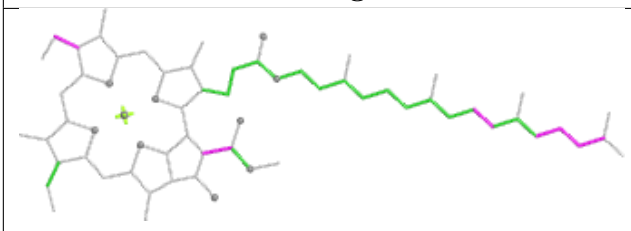

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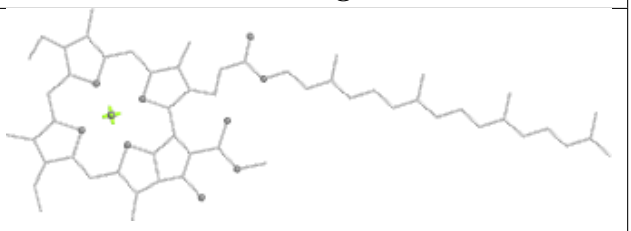
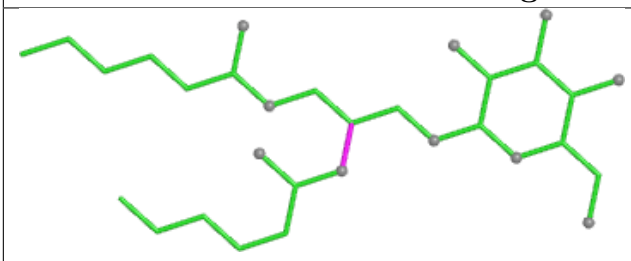


Rings

Ligand LMG P 614



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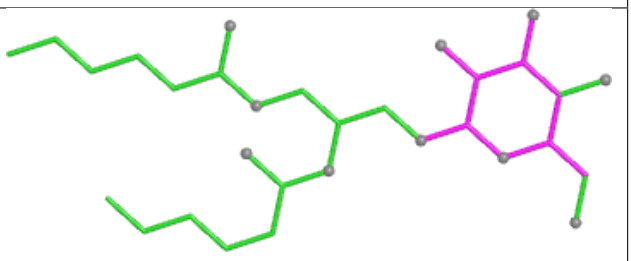

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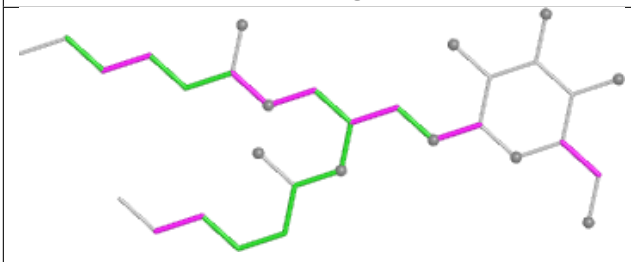

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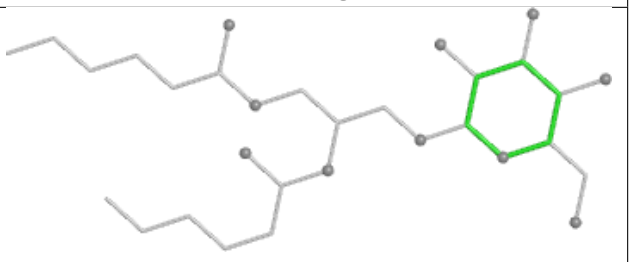
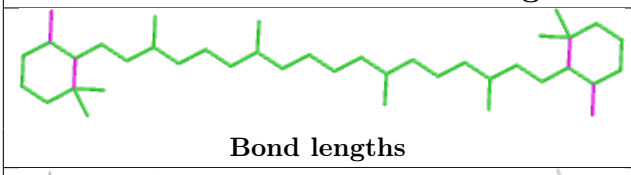


Rings

Ligand BCR Y 101



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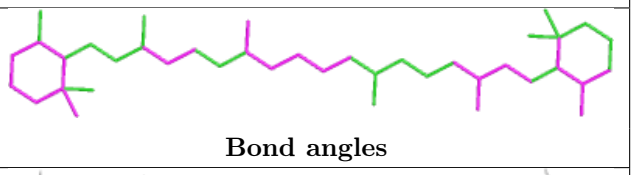

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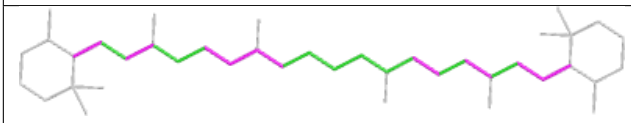

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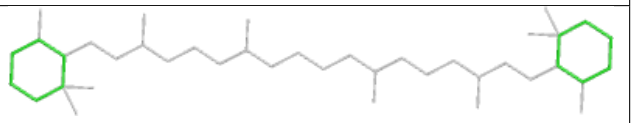
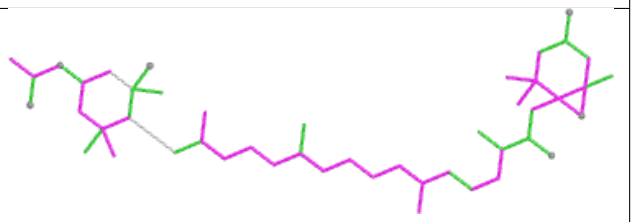


Rings

Ligand A86 13 303



Bond lengths



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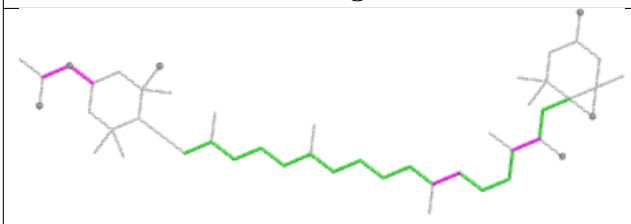

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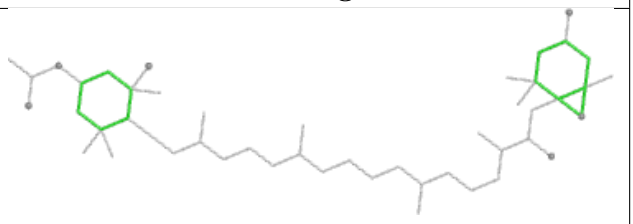
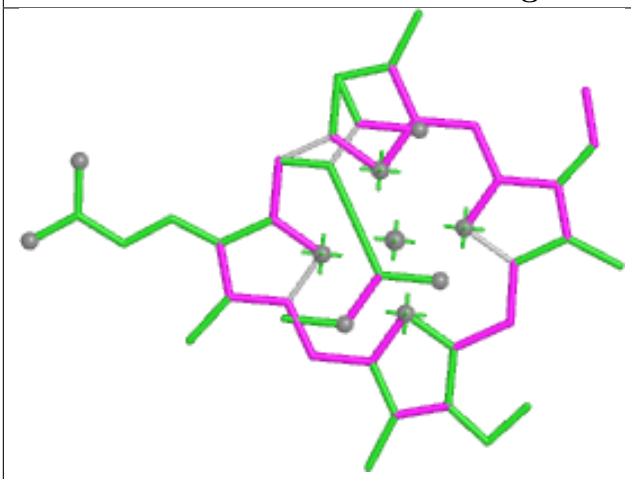


Rings

Ligand KC2 13 311



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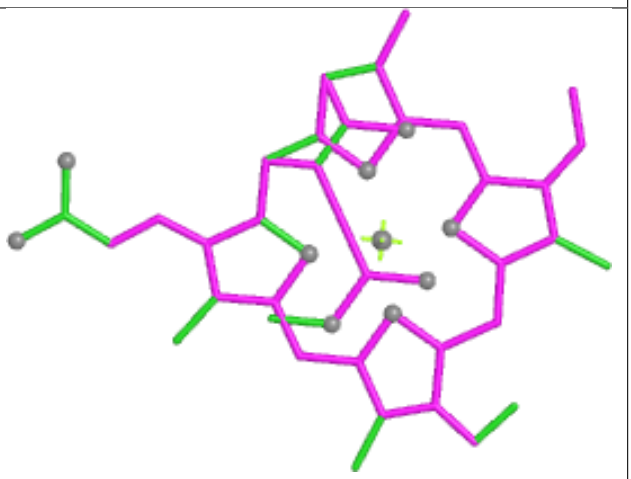

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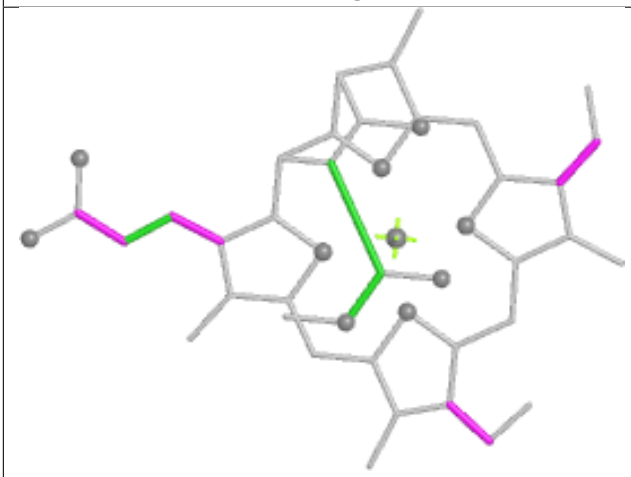

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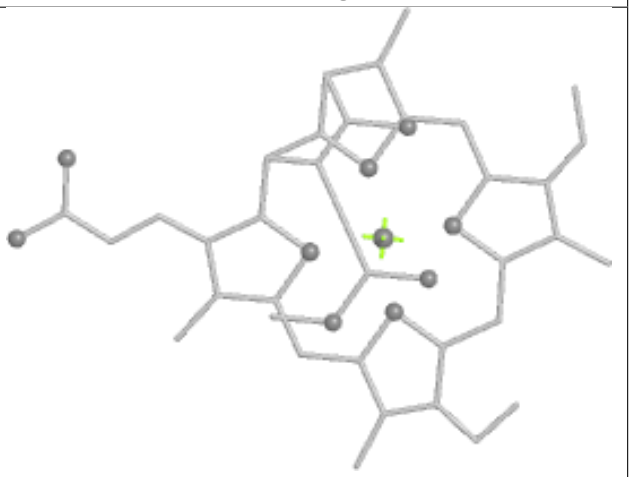
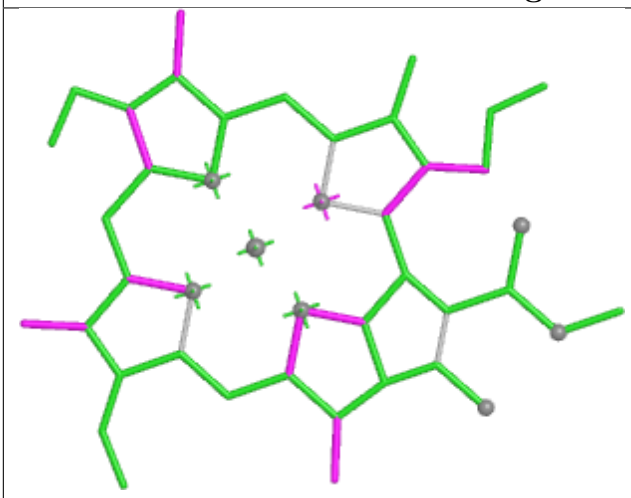


Rings

Ligand CLA P 606



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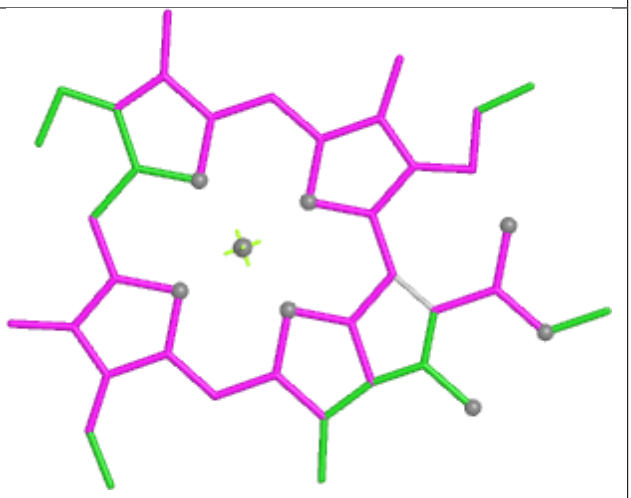
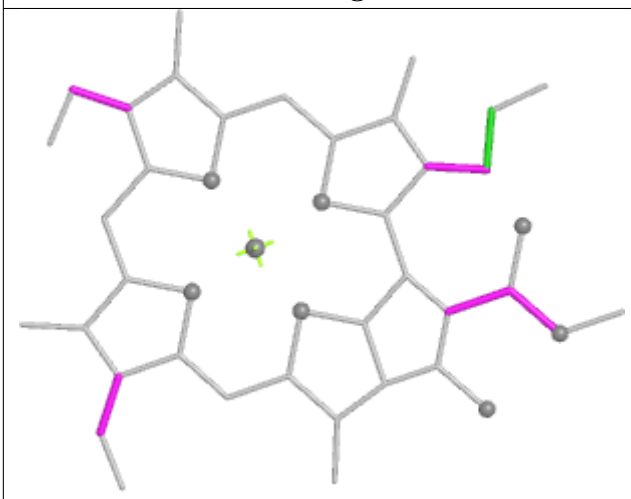


Bond angles



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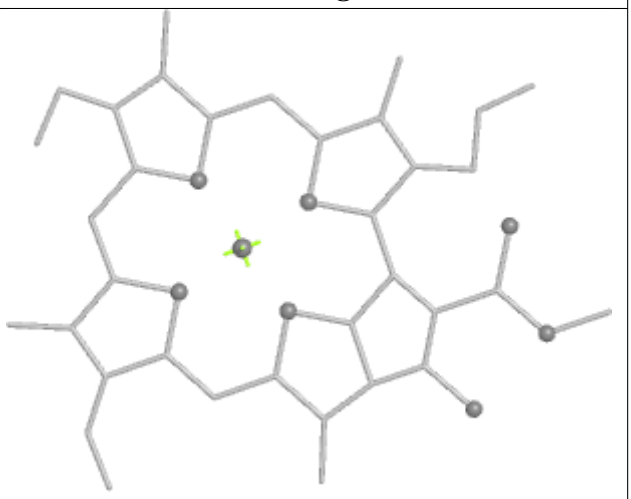
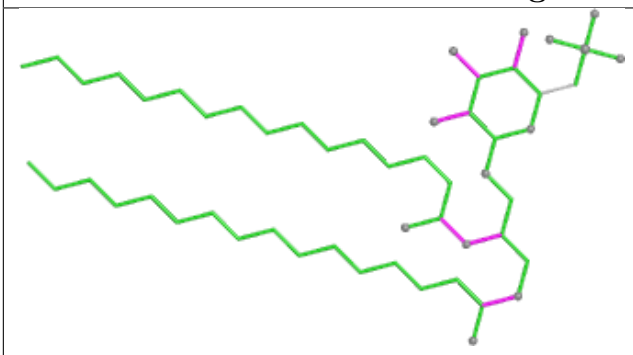


Rings

Ligand SQD a 408



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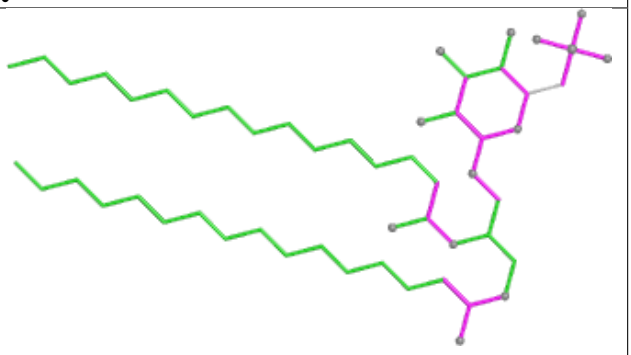
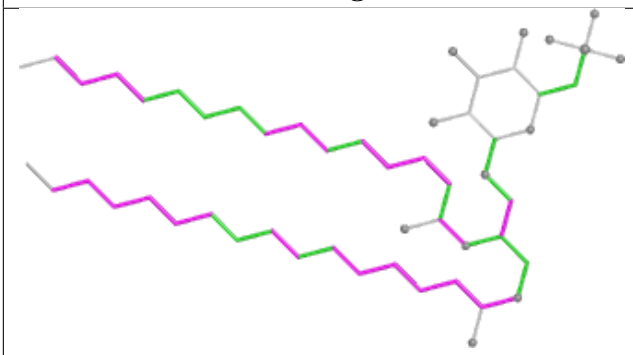


Bond angles



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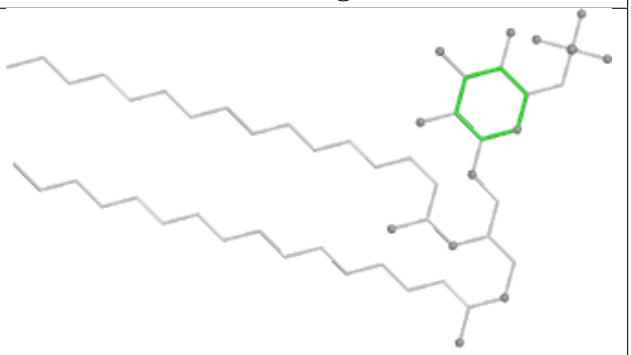
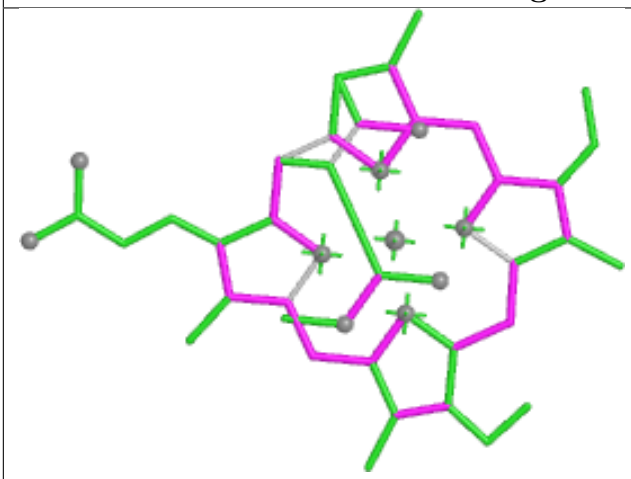


Rings

Ligand KC1 5 313



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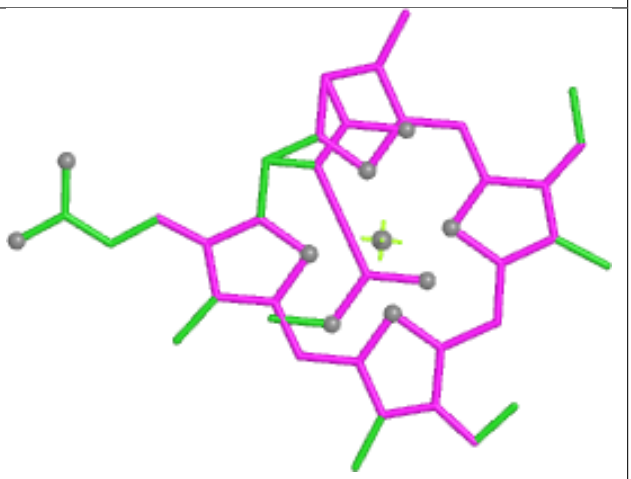
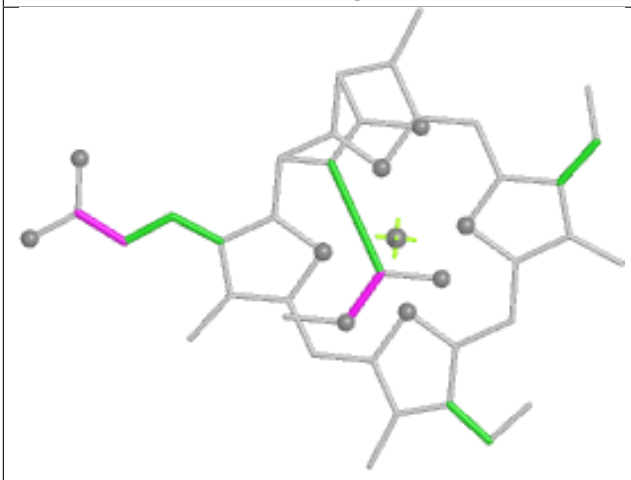


Bond angles



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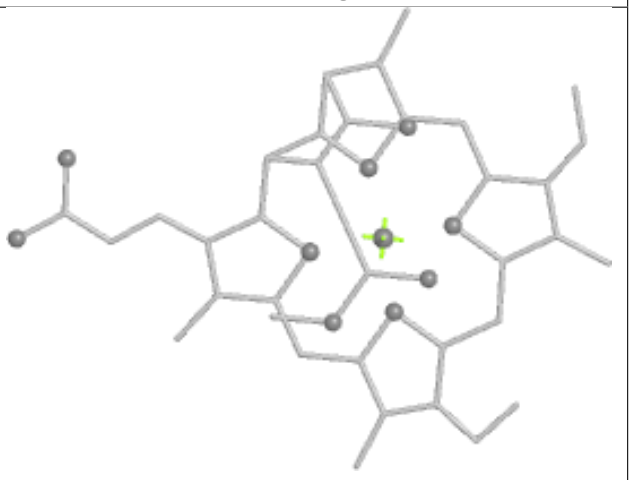
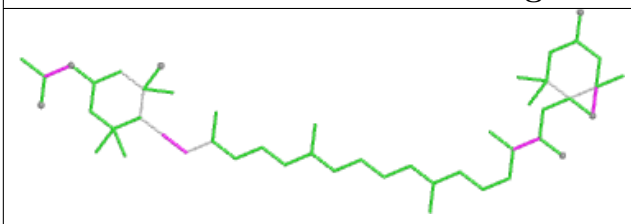


Rings

Ligand A86 10 306



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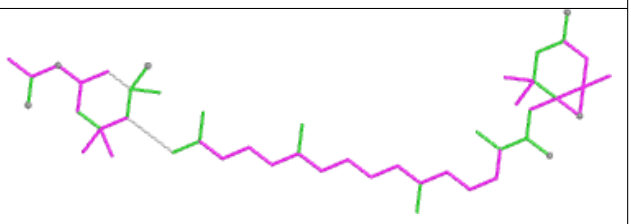
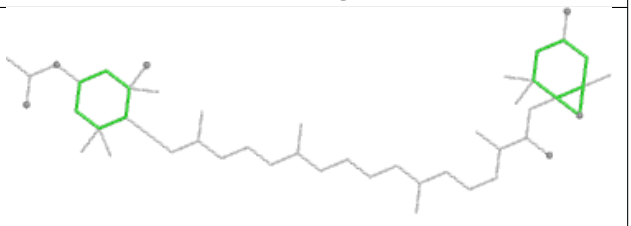


Bond angles

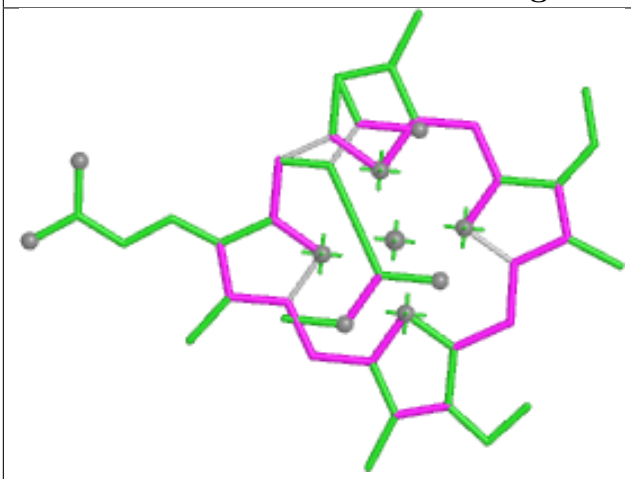


Torsions



Rings

Ligand KC1 3 314



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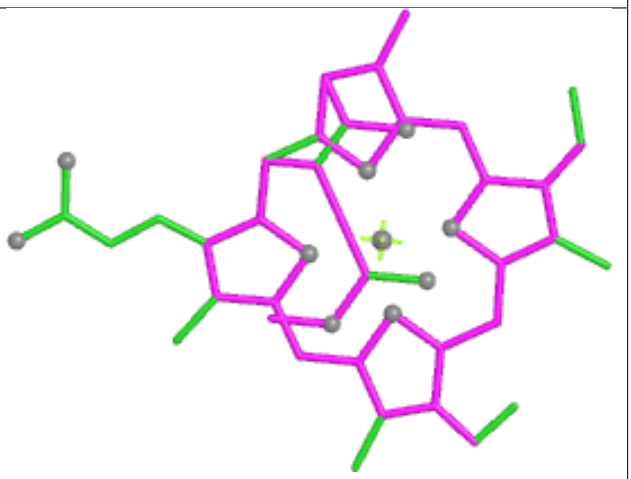
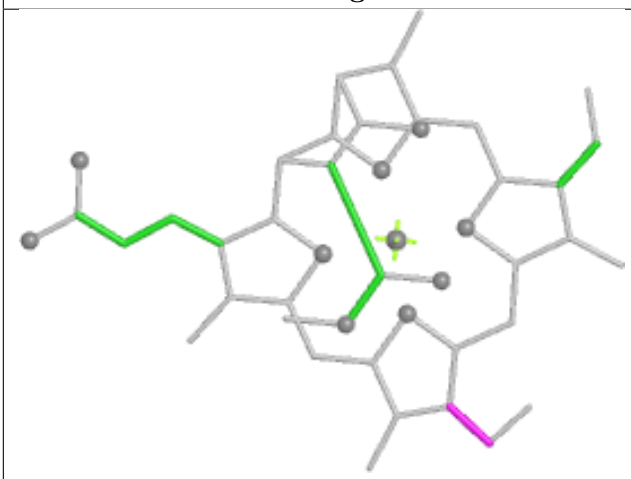


Bond angles



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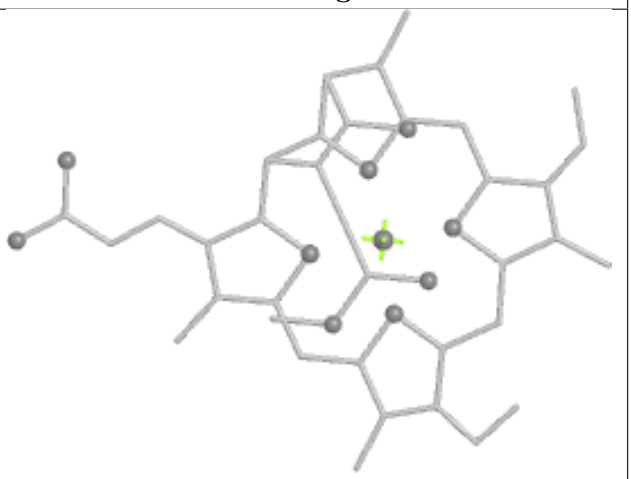
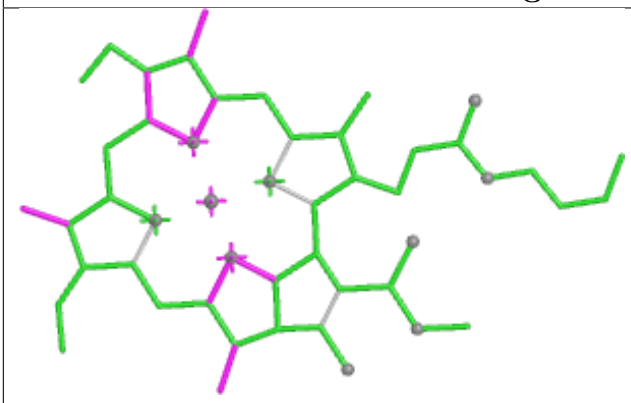


Rings

Ligand CLA A 404



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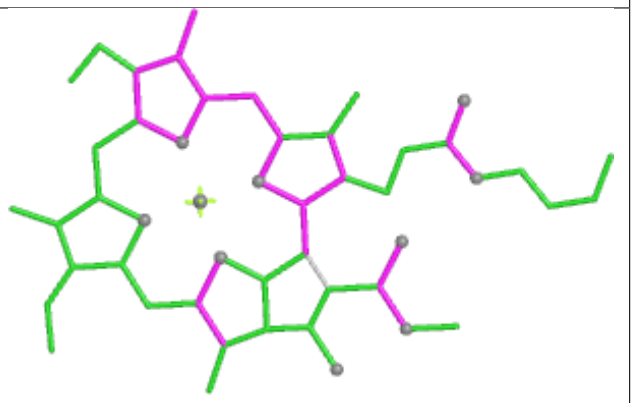

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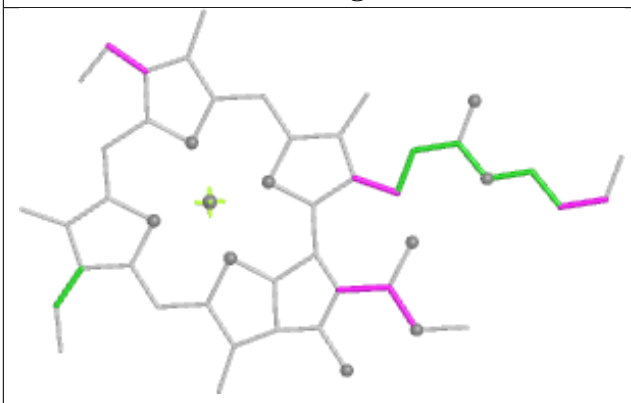

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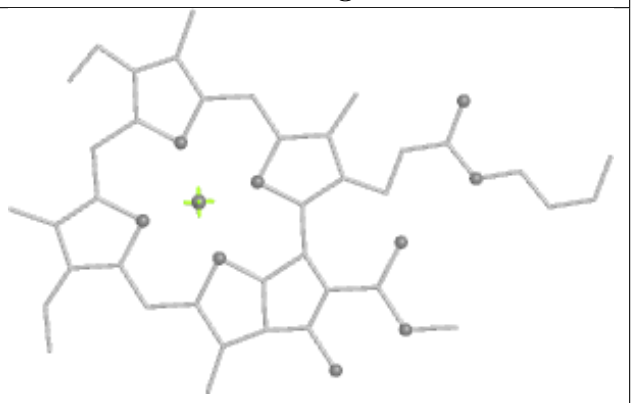
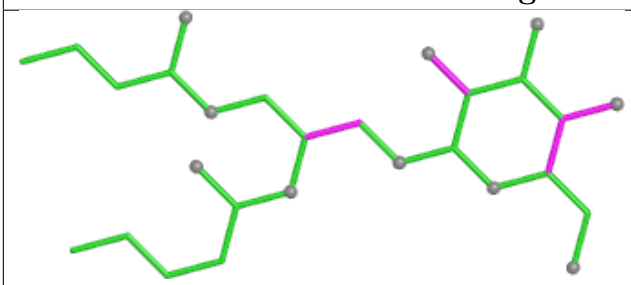


Rings

Ligand LMG N 101



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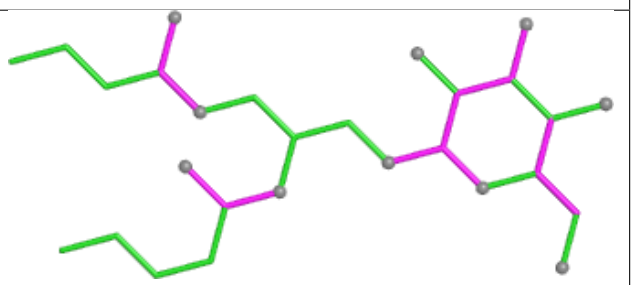

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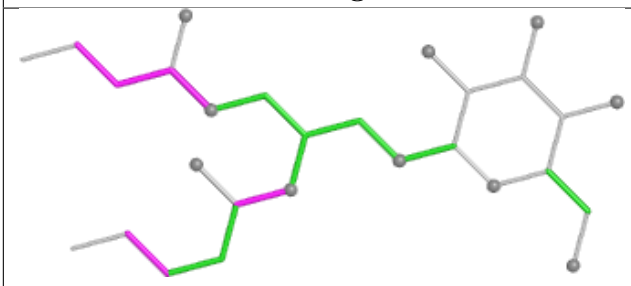

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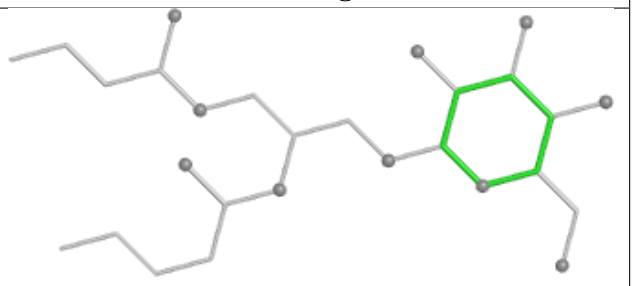
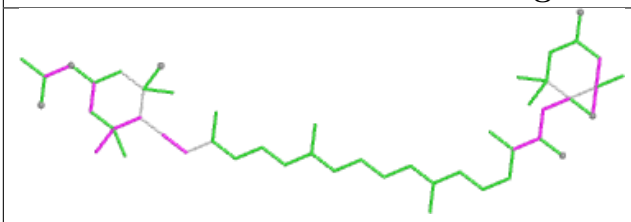


Rings

Ligand A86 6 305



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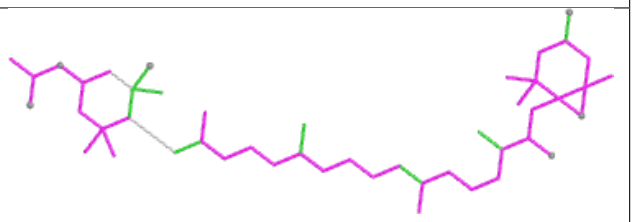

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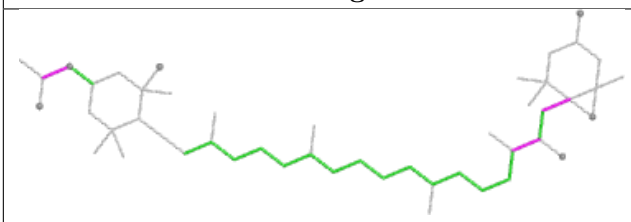

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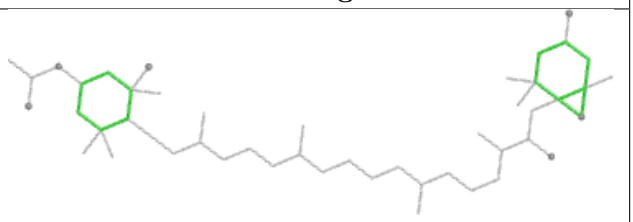
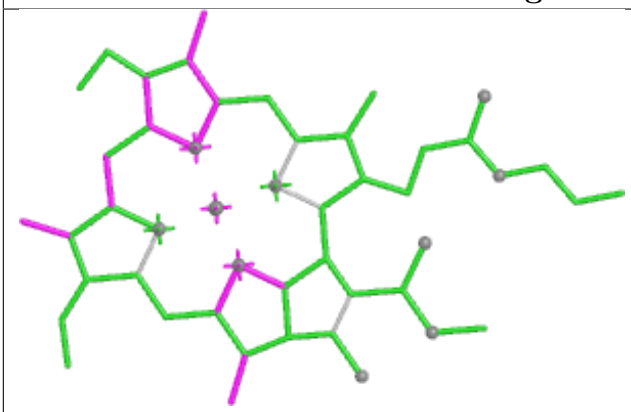


Rings

Ligand CLA P 604



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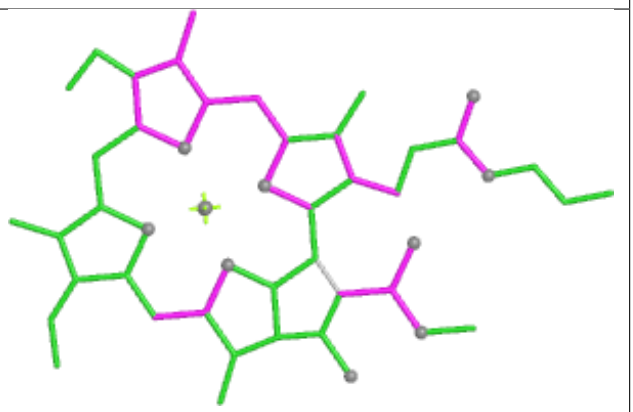

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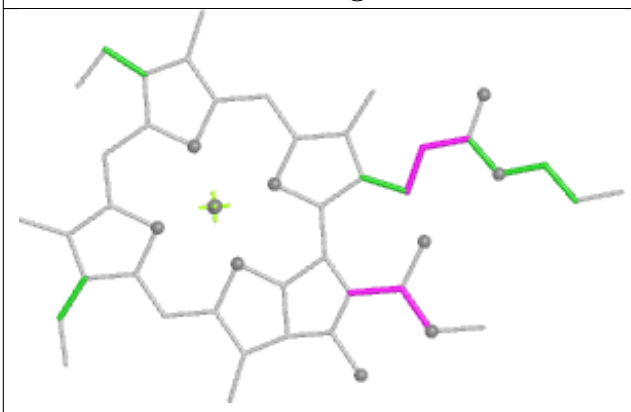

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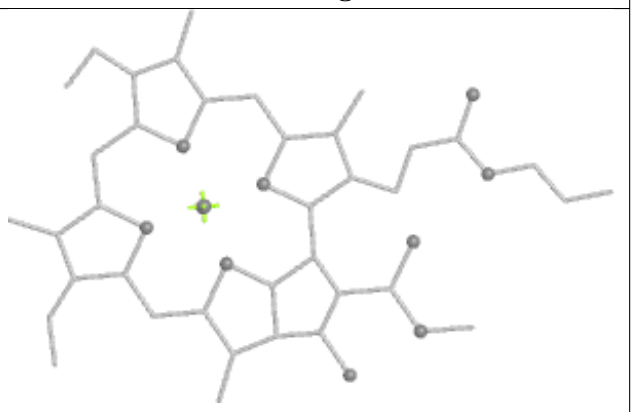
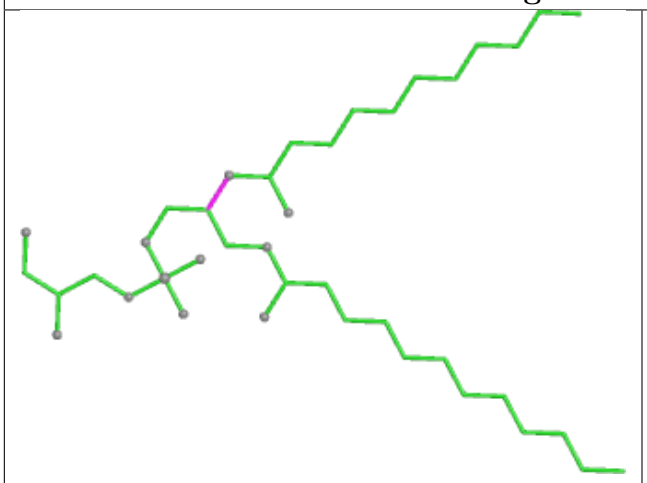


Rings

Ligand LHG w 202



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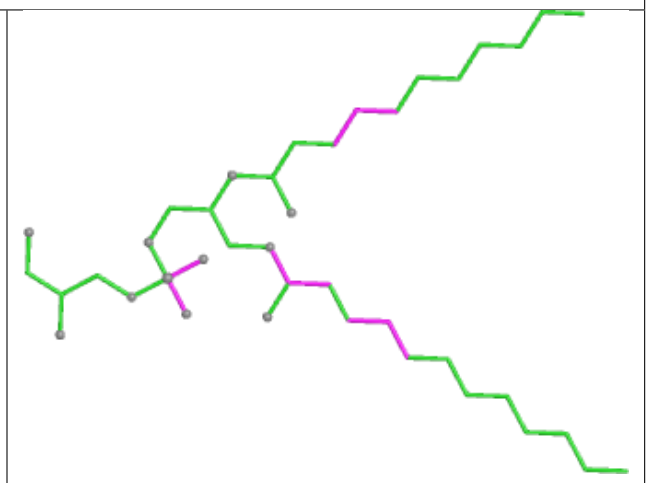

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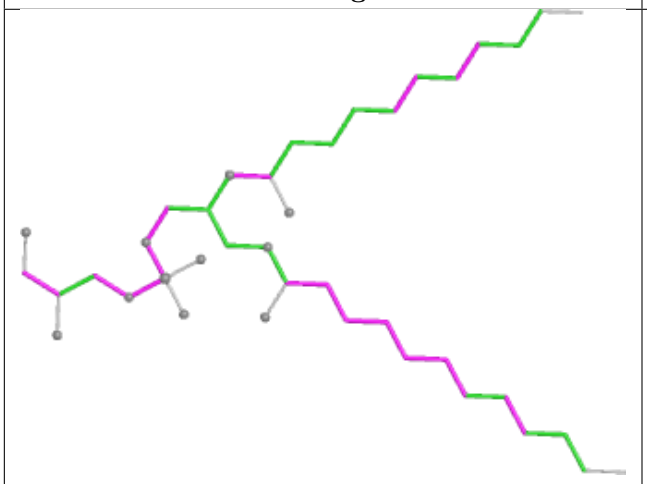

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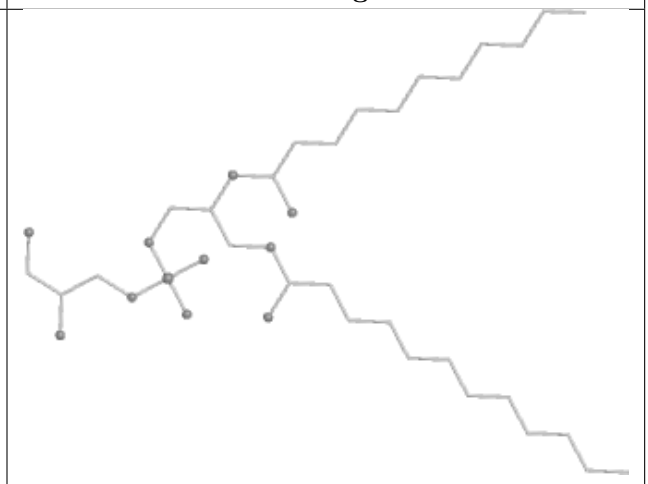
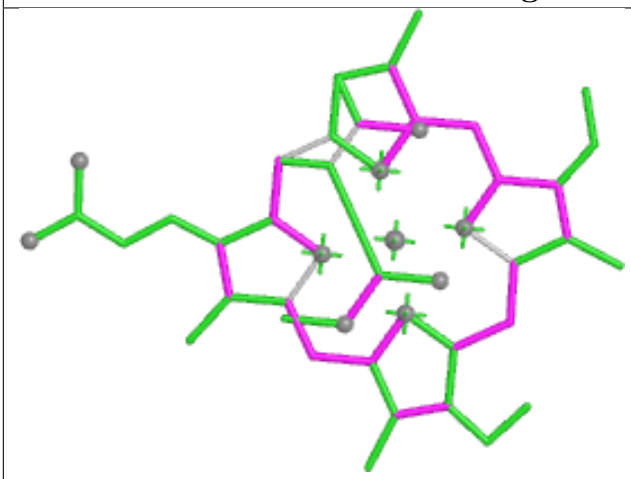


Rings

Ligand KC1 15 317



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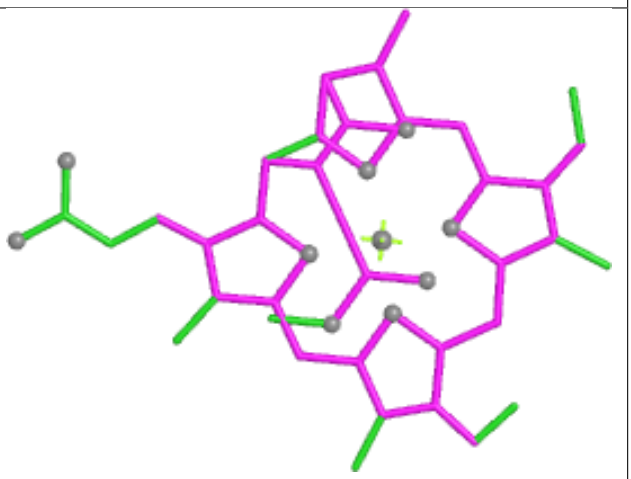

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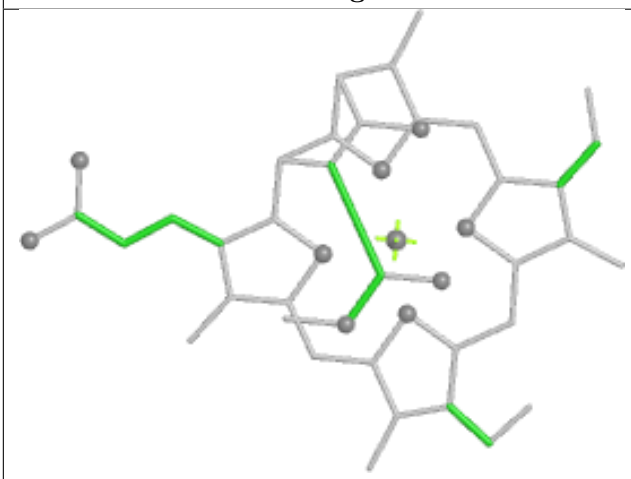

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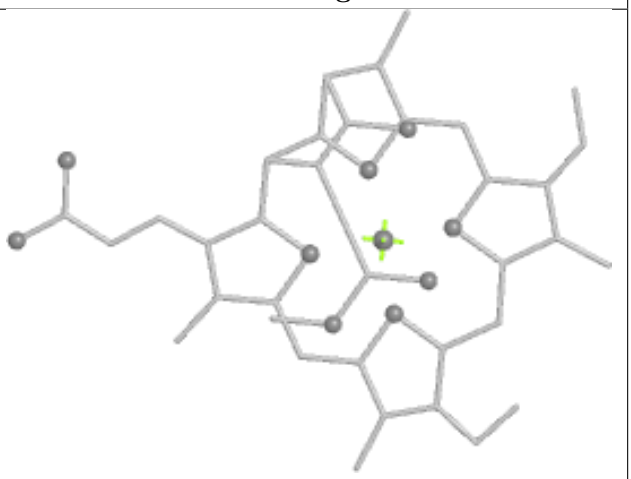
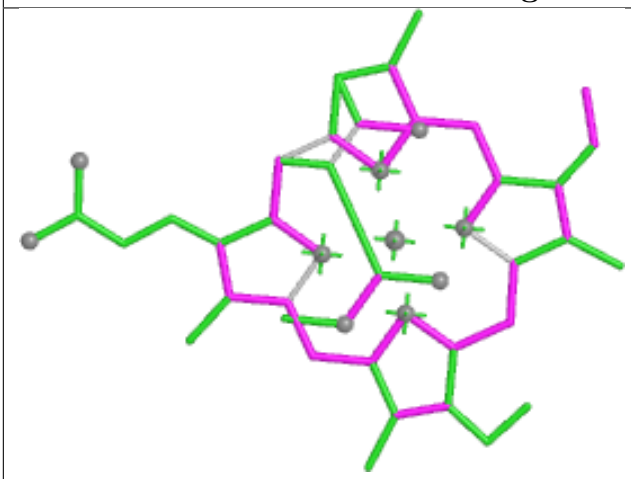


Rings

Ligand KC2 14 308



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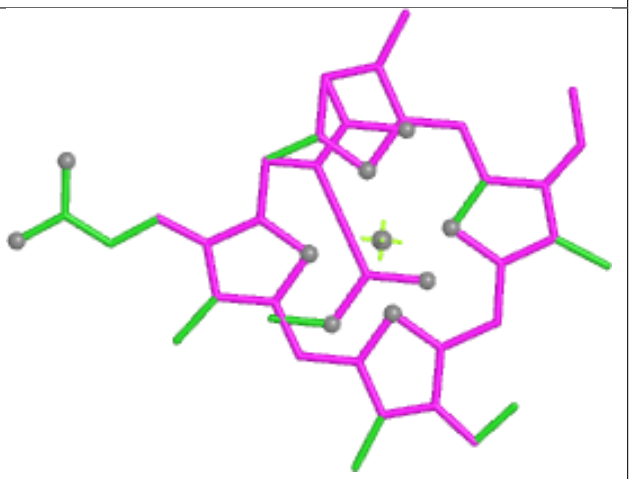

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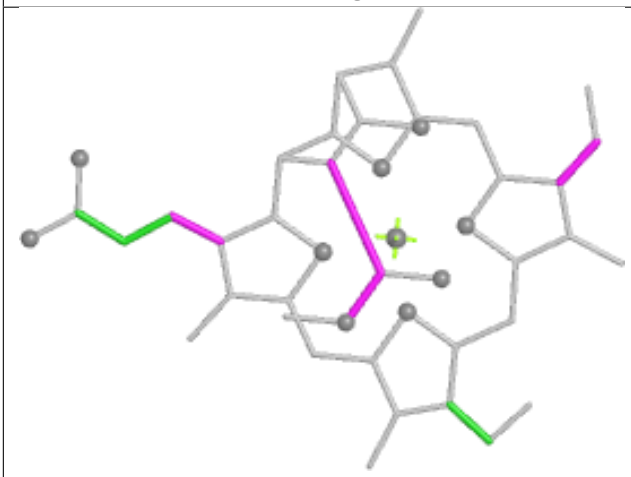

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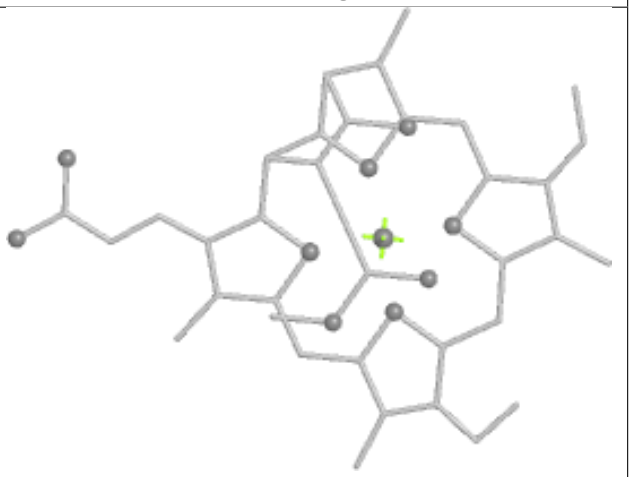
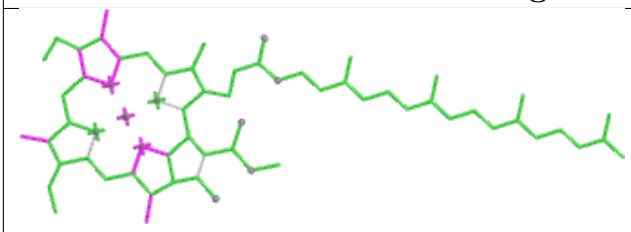


Rings

Ligand CLA c 502



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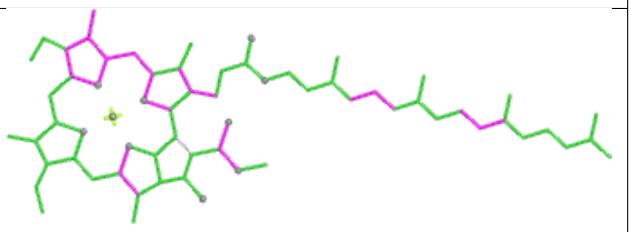
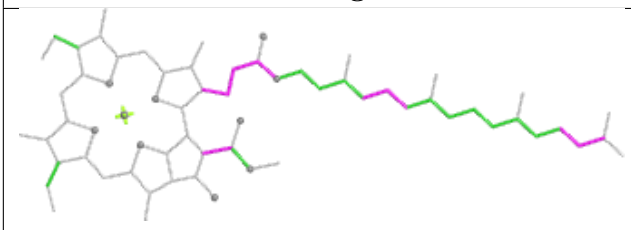


Bond angles



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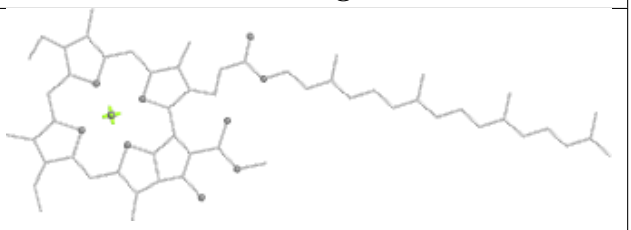
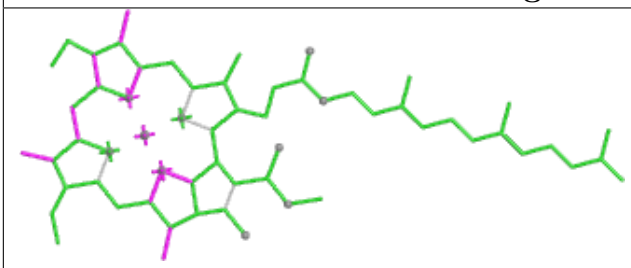
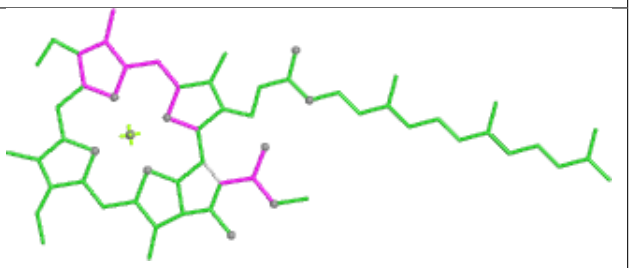


Rings

Ligand CLA A 406	
	
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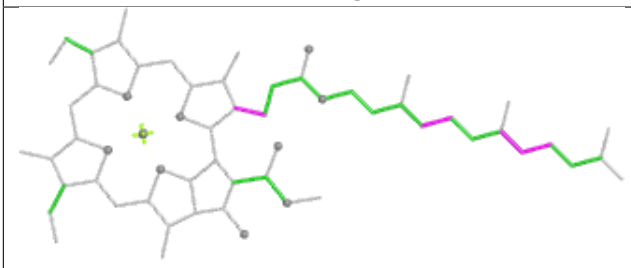	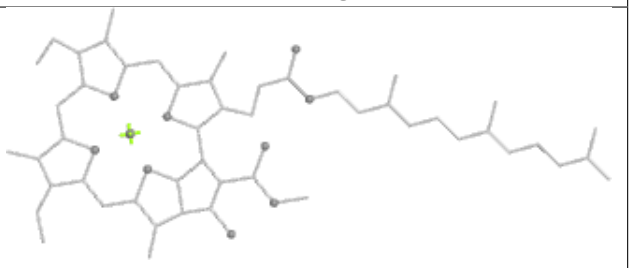
Torsions	Rings

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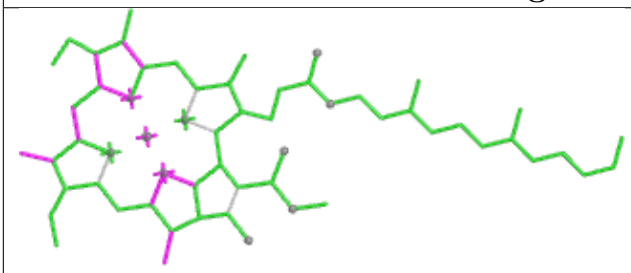	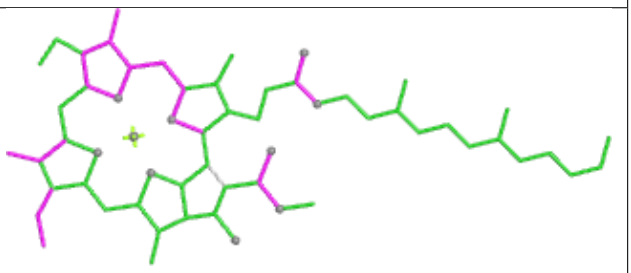
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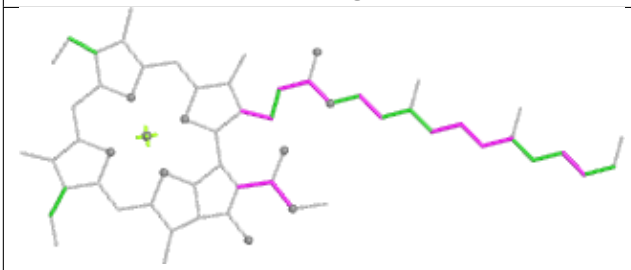
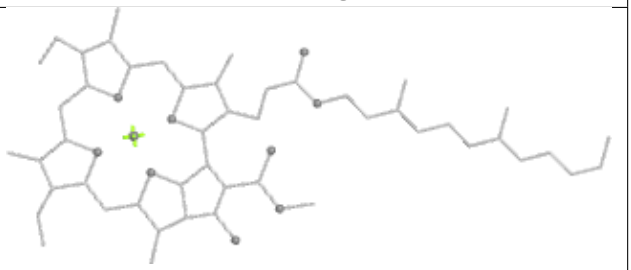
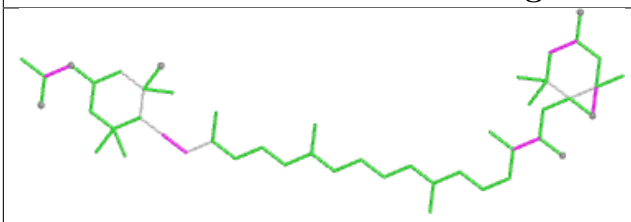
	
Torsions	Rings

Ligand A86 15 303



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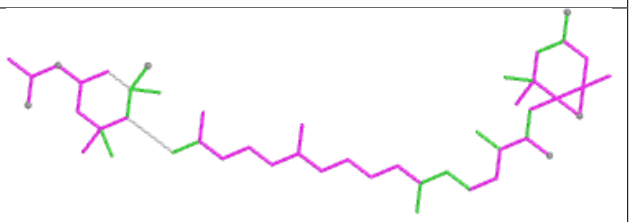
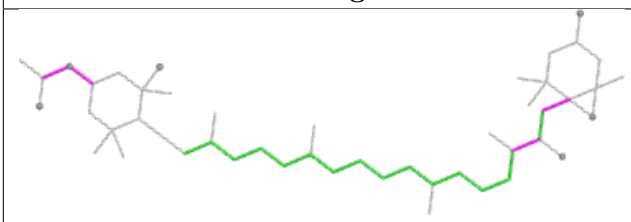


Bond angles



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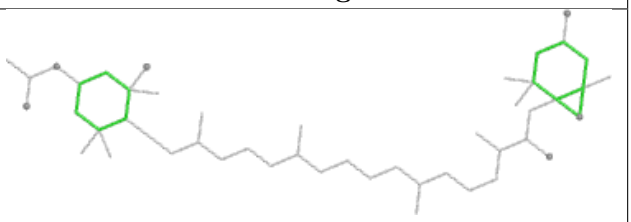
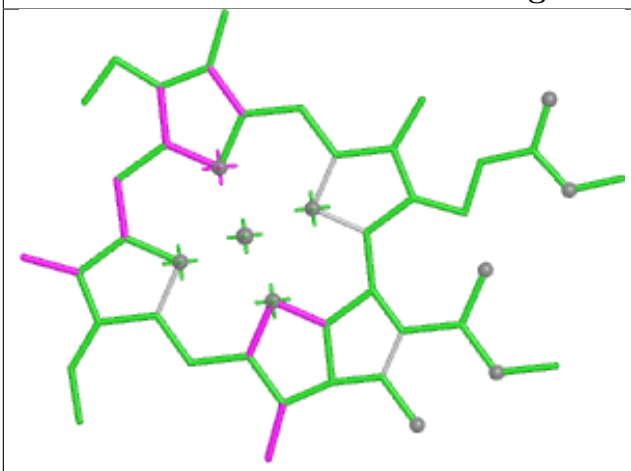


Rings

Ligand CLA 0 316



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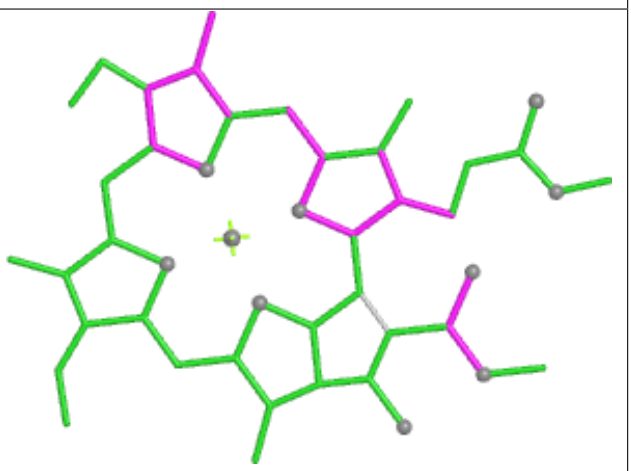
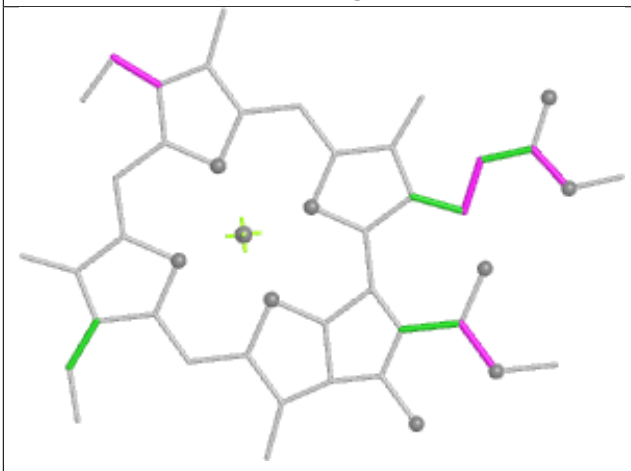


Bond angles



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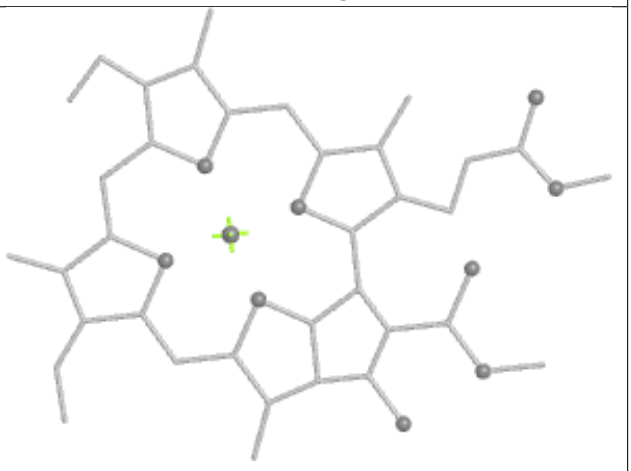
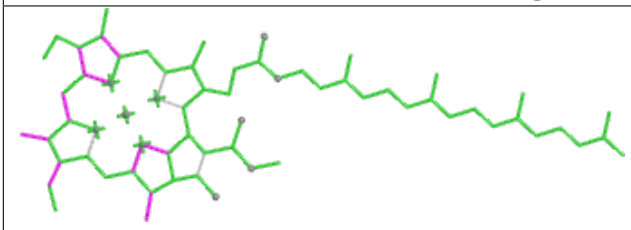


Rings

Ligand CLA 9 313



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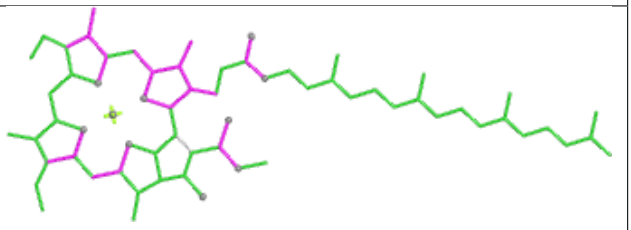
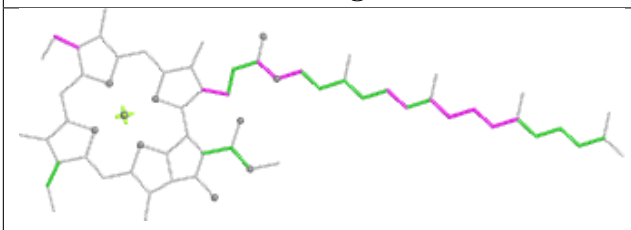


Bond angles



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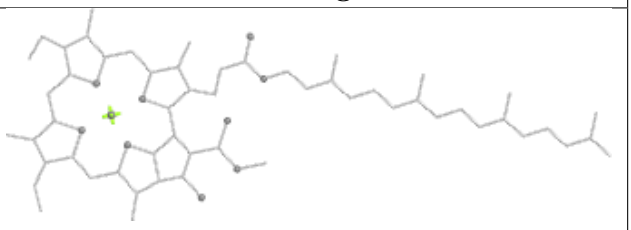
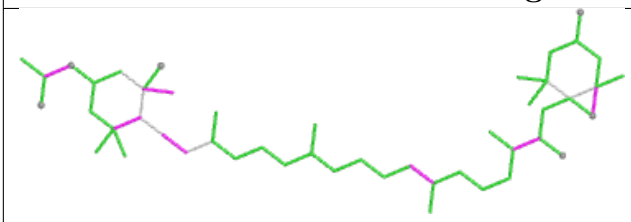


Rings

Ligand A86 10 303



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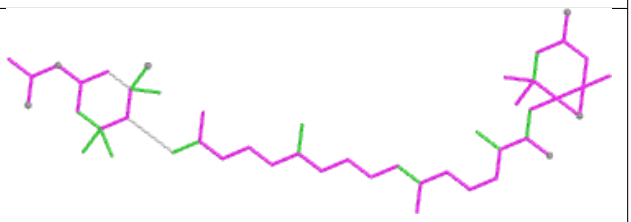
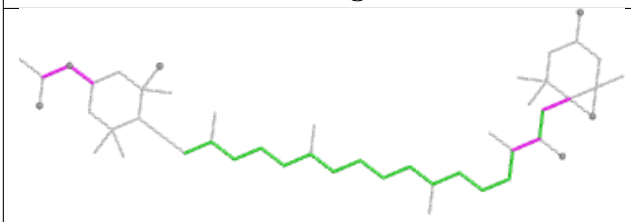


Bond angles



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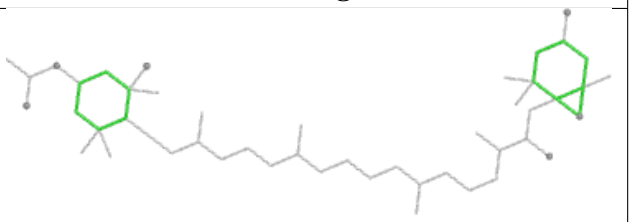

Rings

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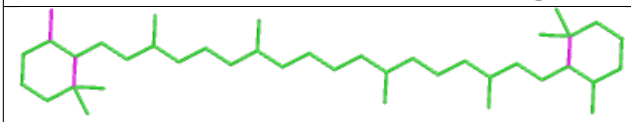

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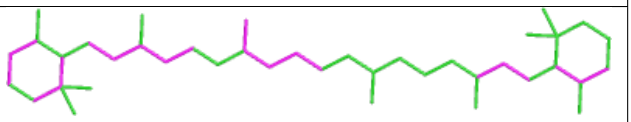

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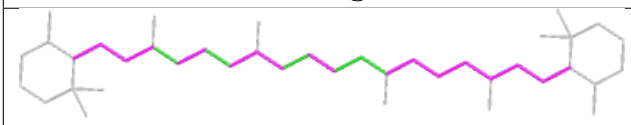

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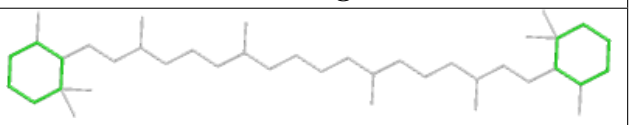

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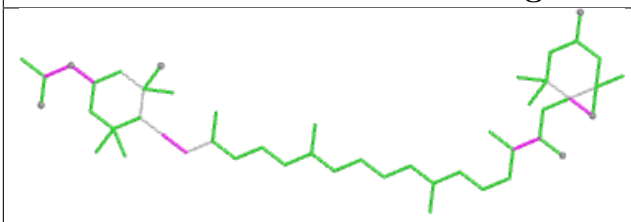

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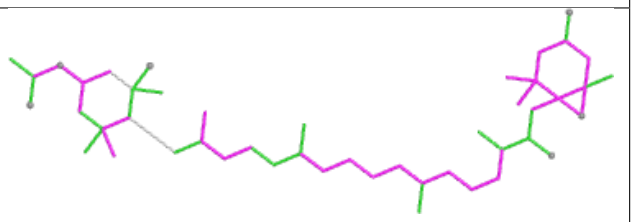

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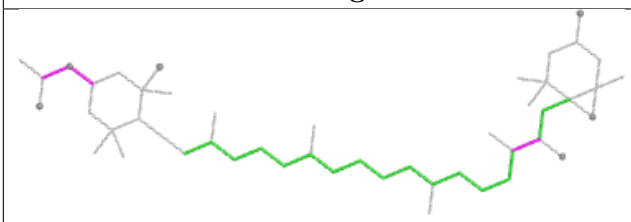

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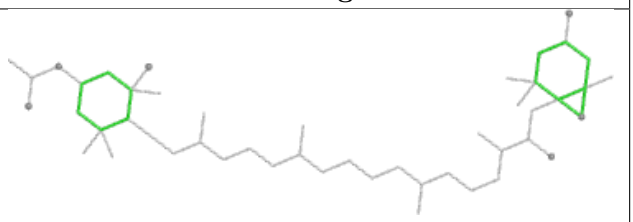

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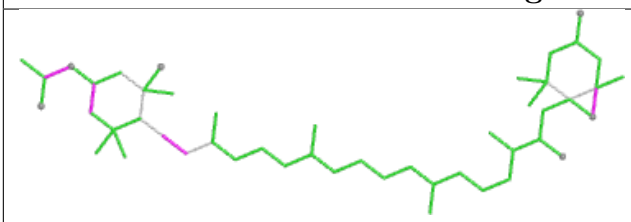

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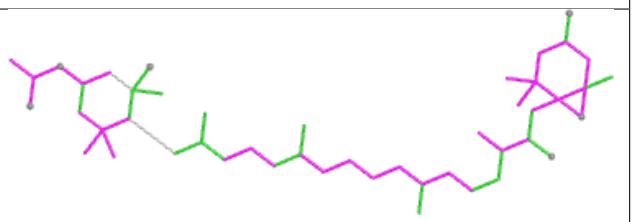

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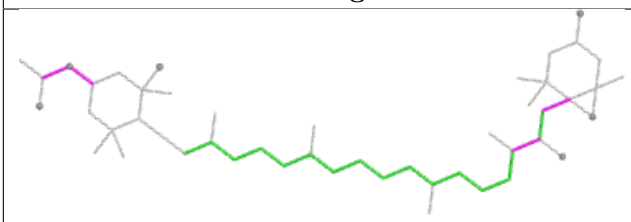

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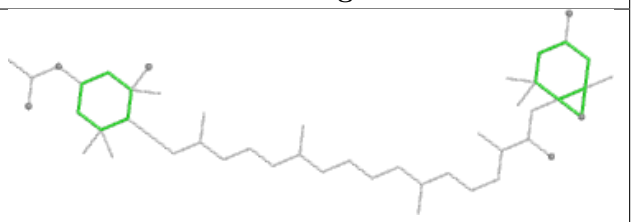

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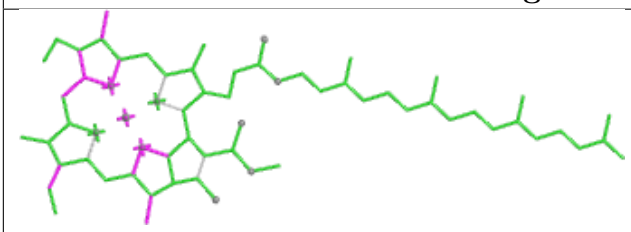

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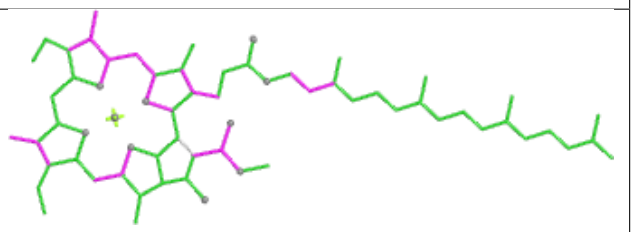

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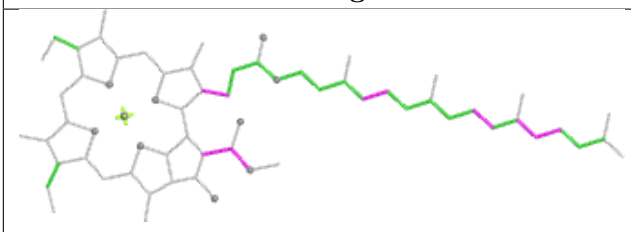

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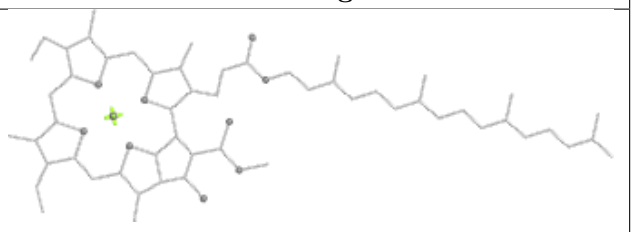

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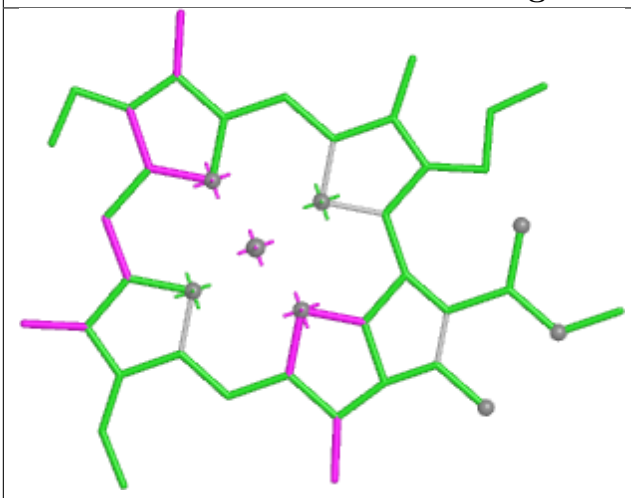

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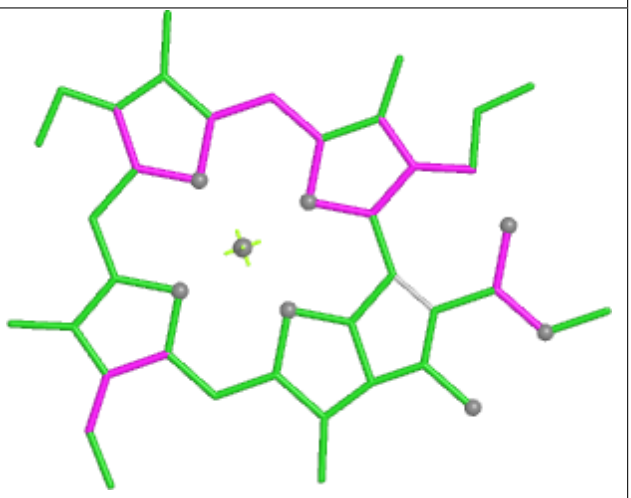

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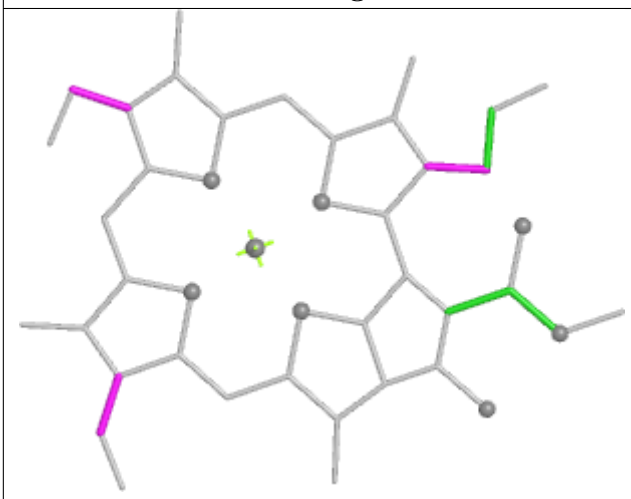

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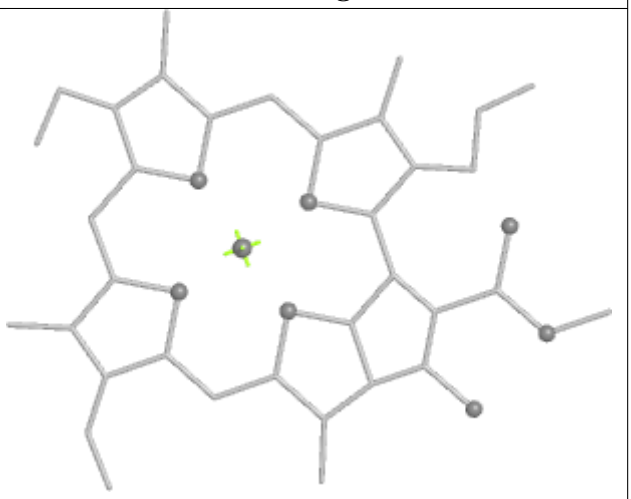

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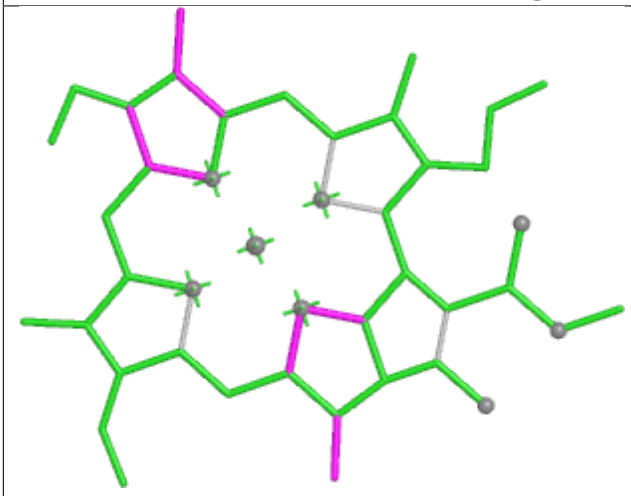

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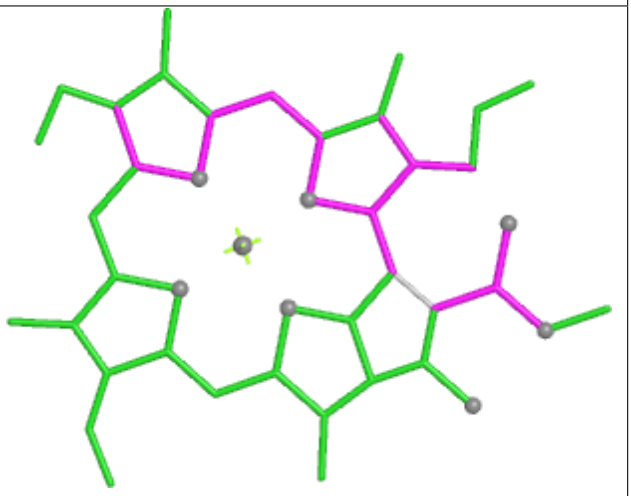

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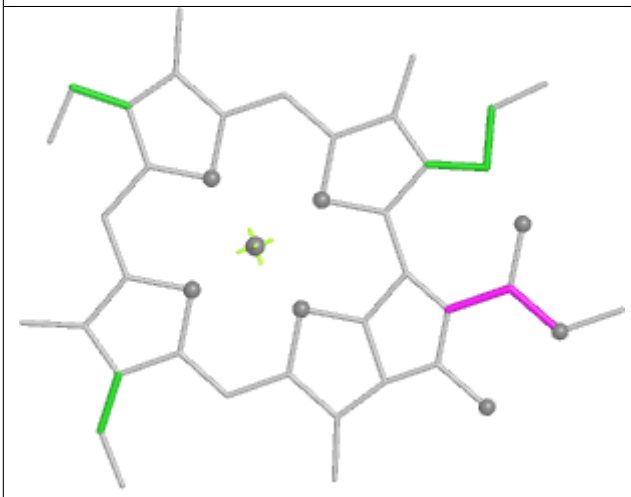

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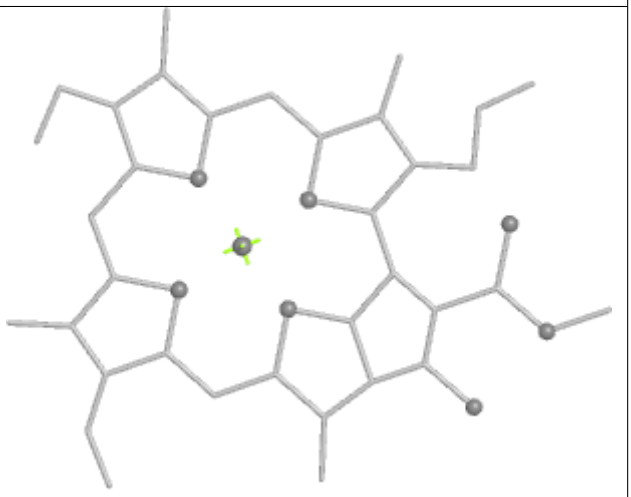

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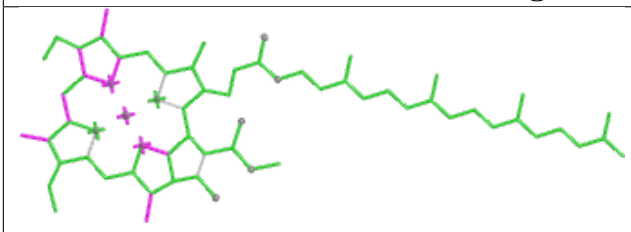

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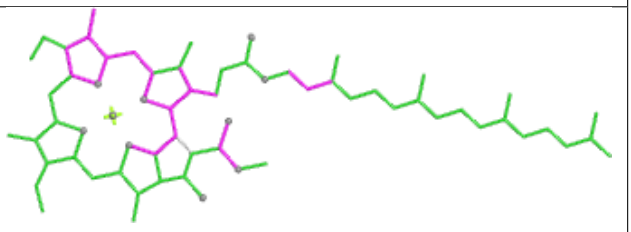

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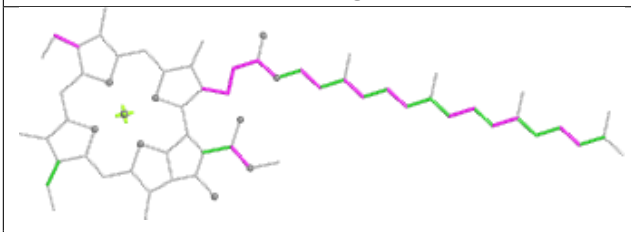

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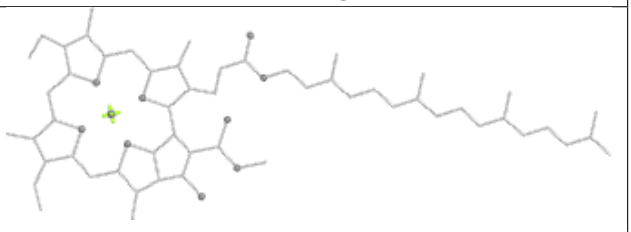

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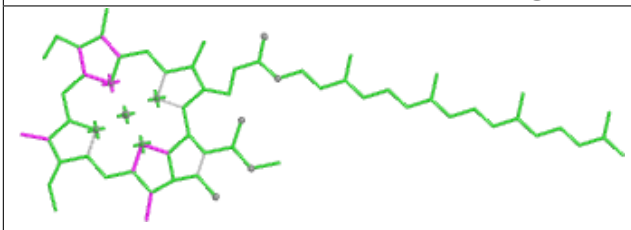

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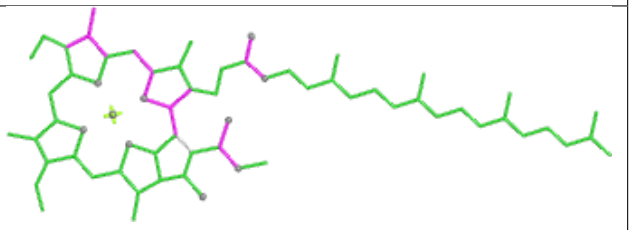

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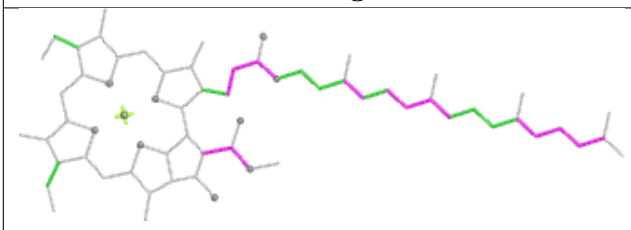

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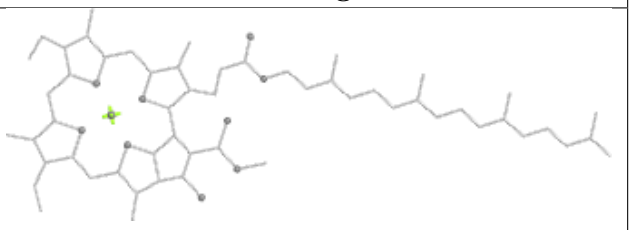

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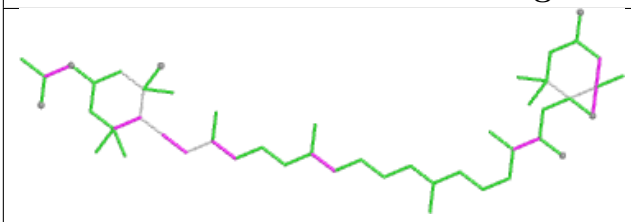

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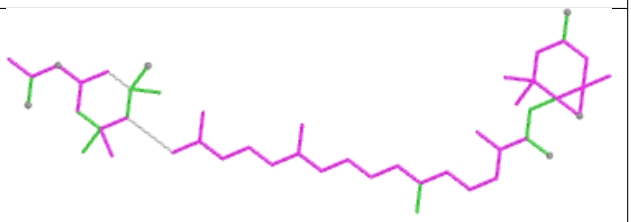

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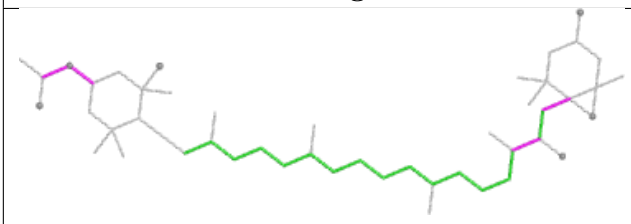

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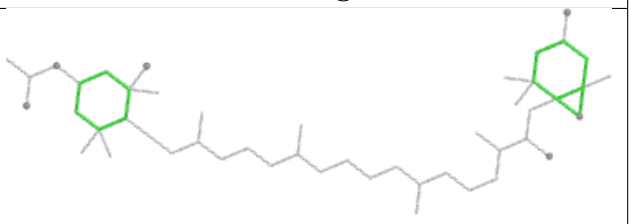

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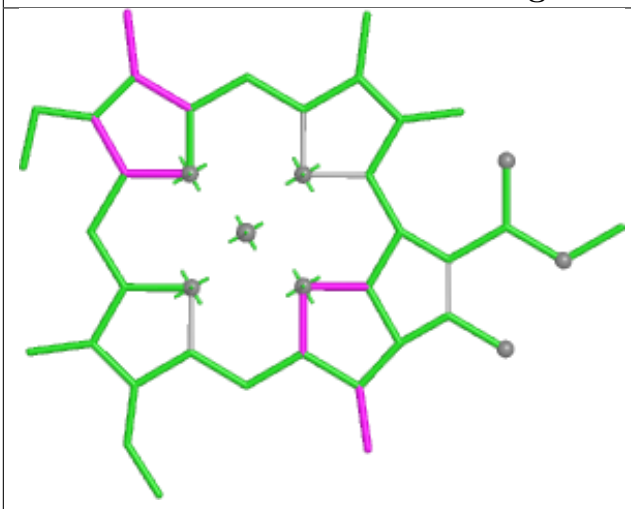

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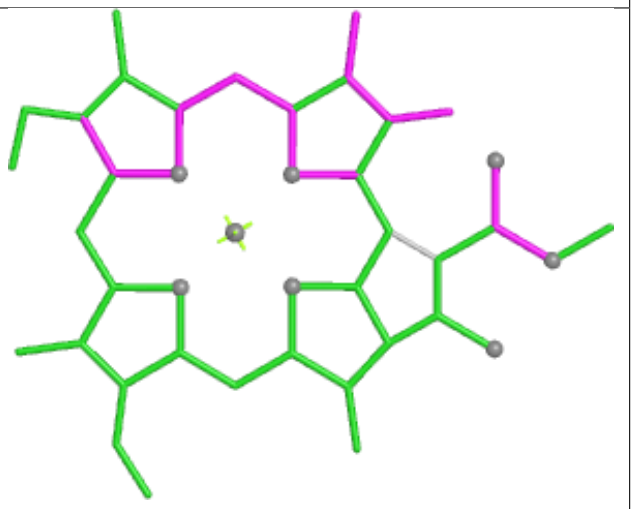

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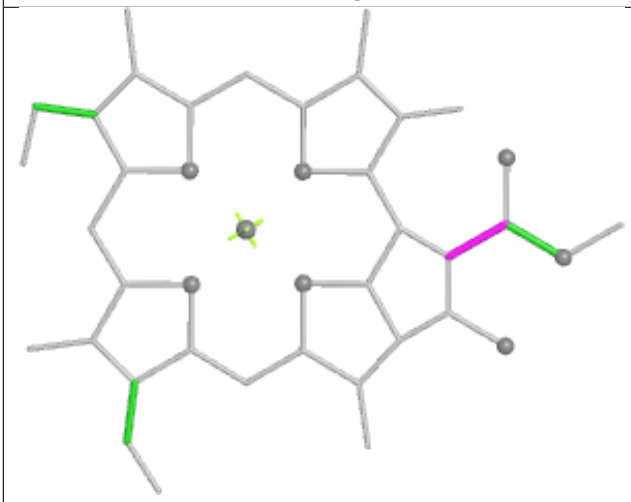

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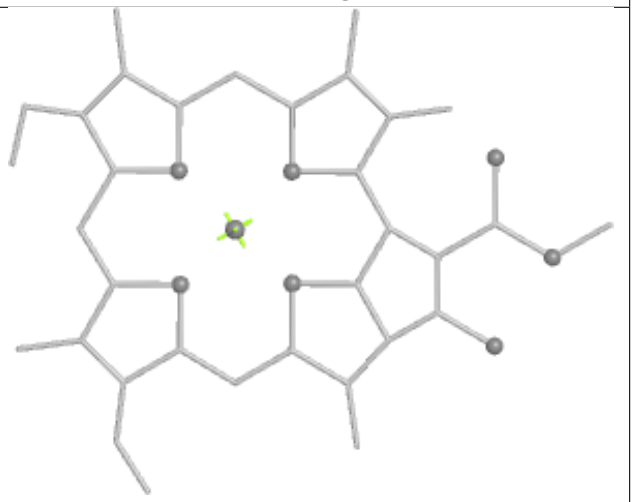

Rings

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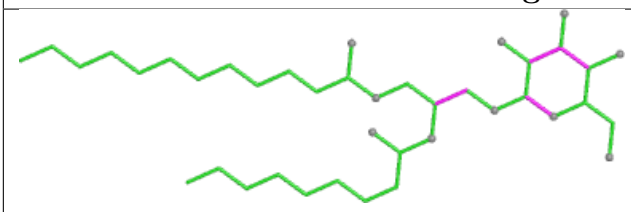

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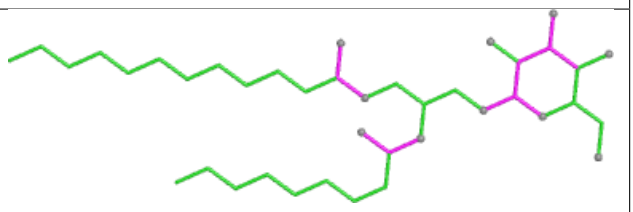

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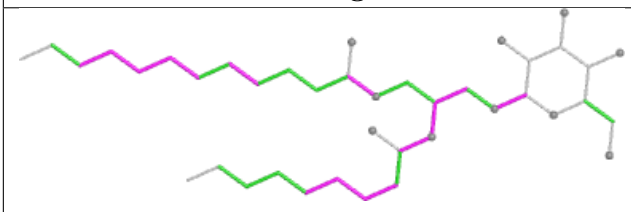

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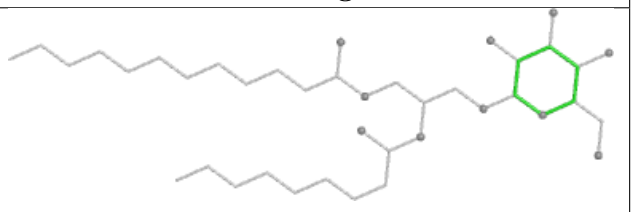

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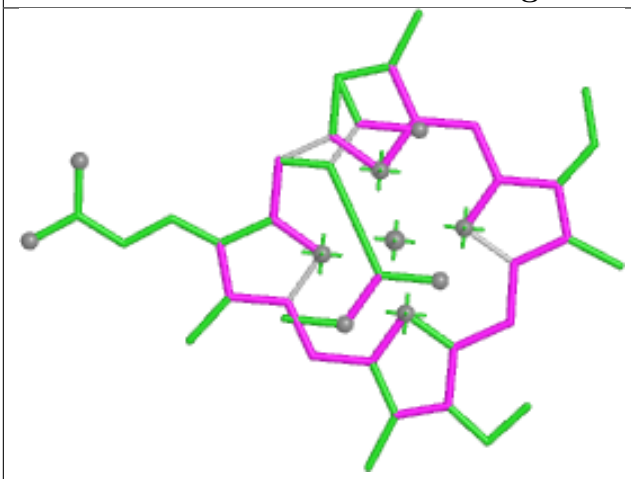

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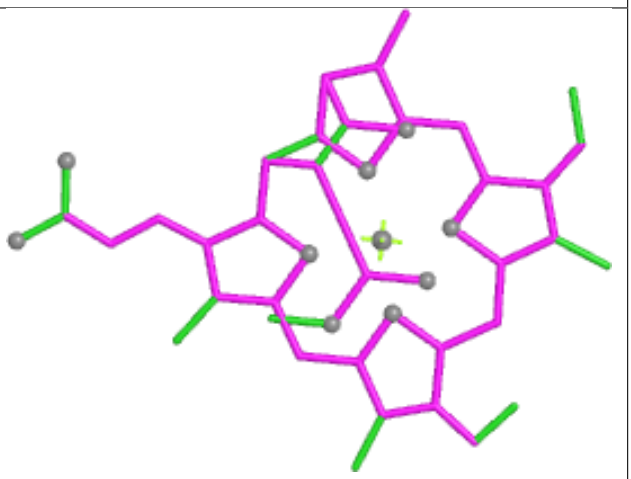

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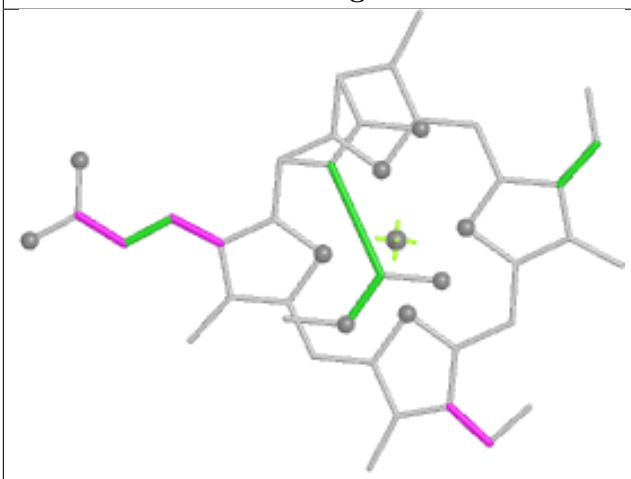

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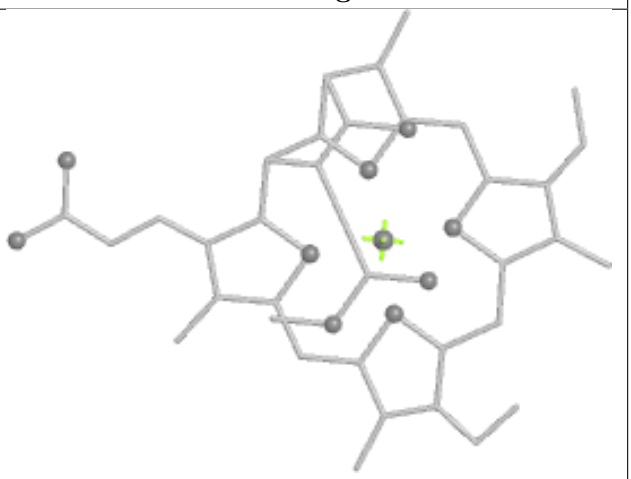

Rings

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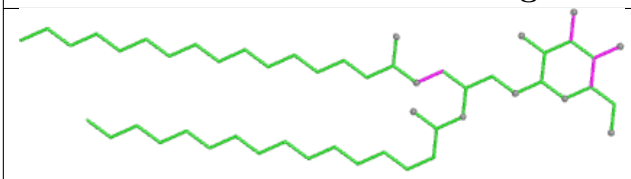

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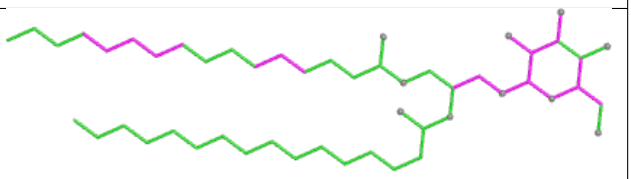

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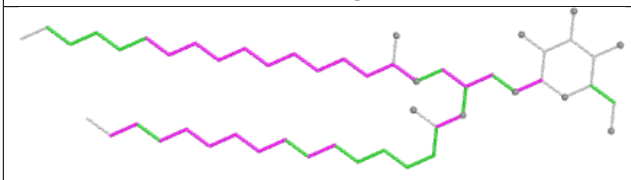

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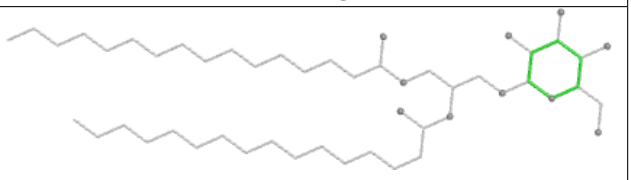

Rings

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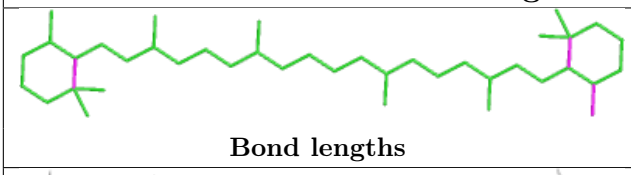

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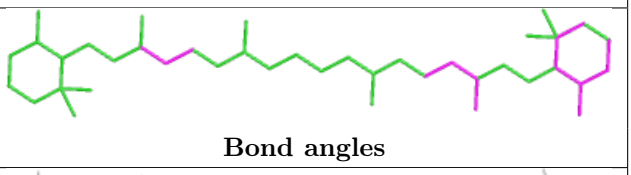
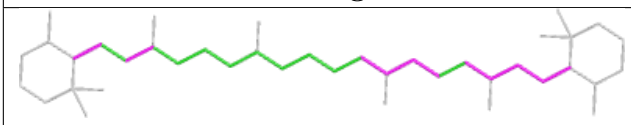


Bond angles



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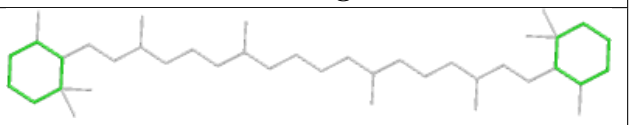
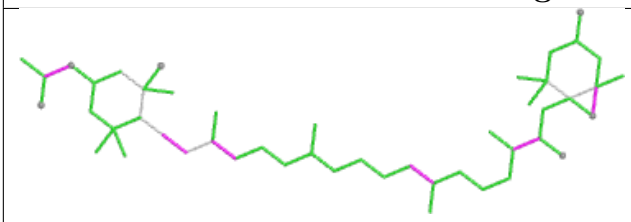


Rings

Ligand A86 6 304



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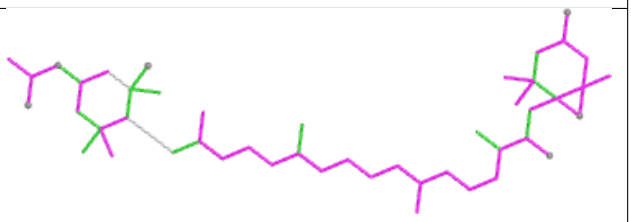
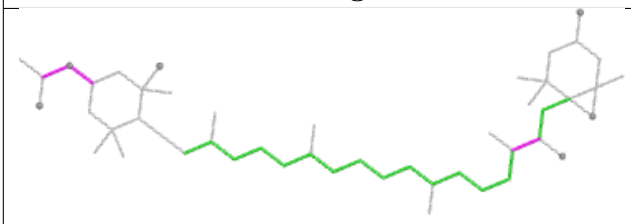
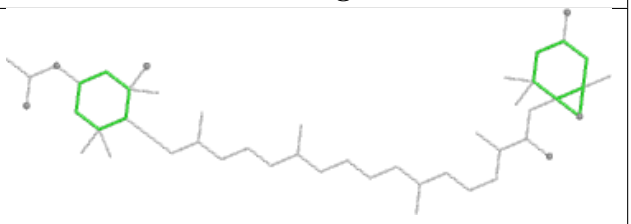


Bond angles

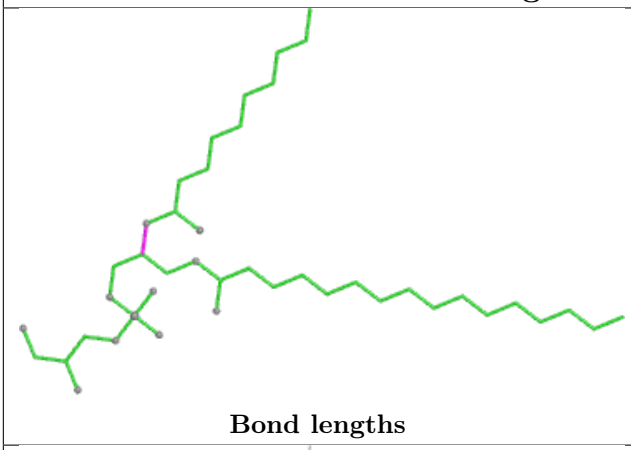


Torsions



Rings

Ligand LHG B 622



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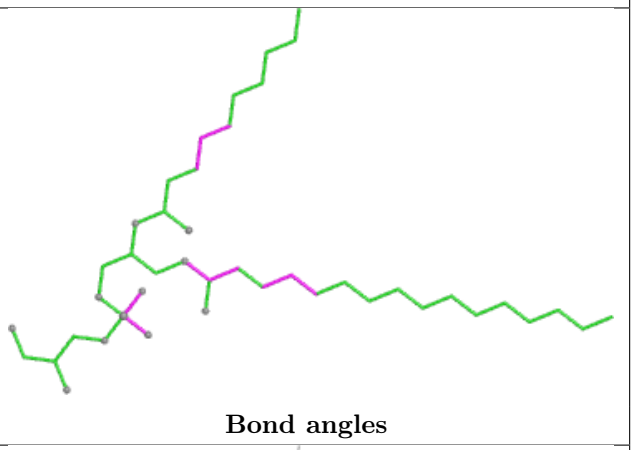

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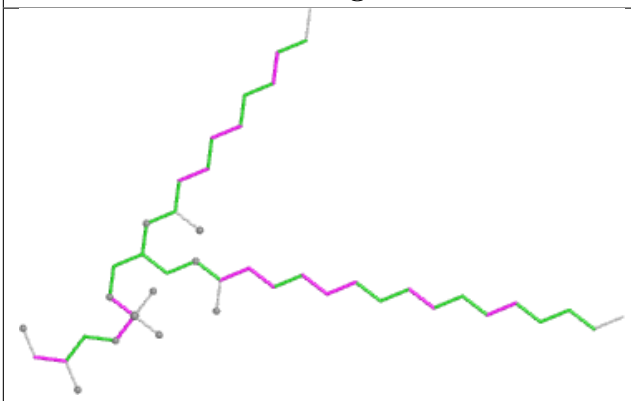

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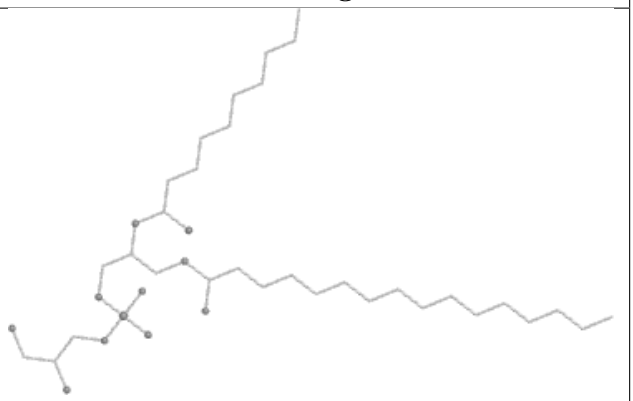
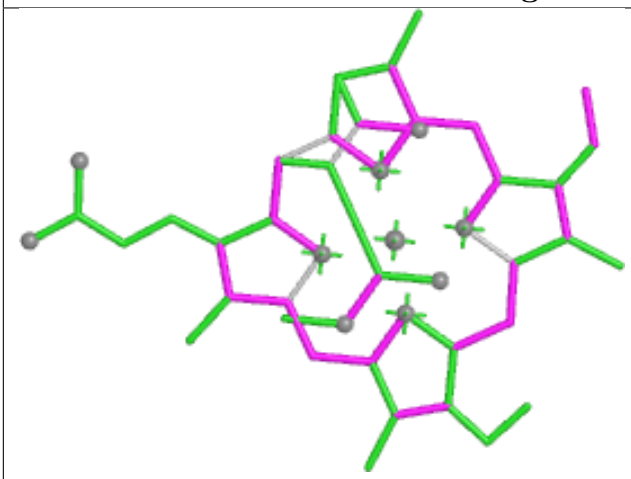


Rings

Ligand KC2 13 309



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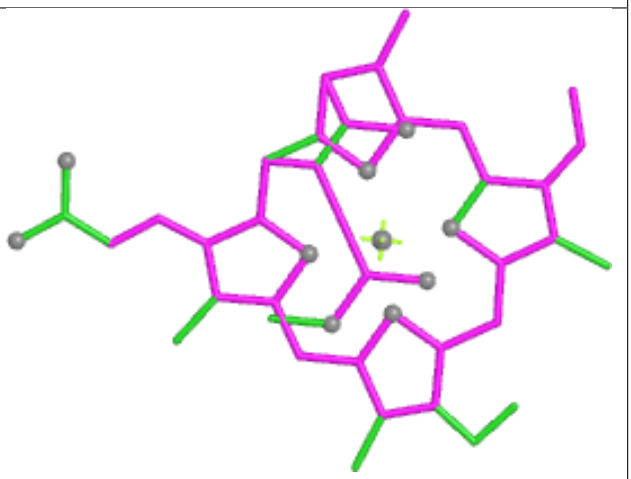

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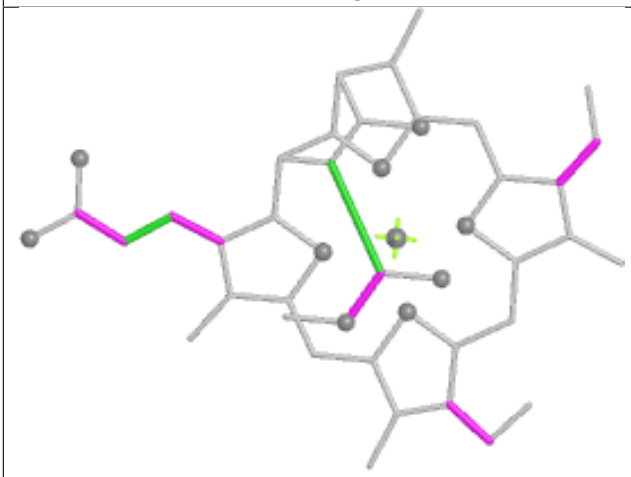

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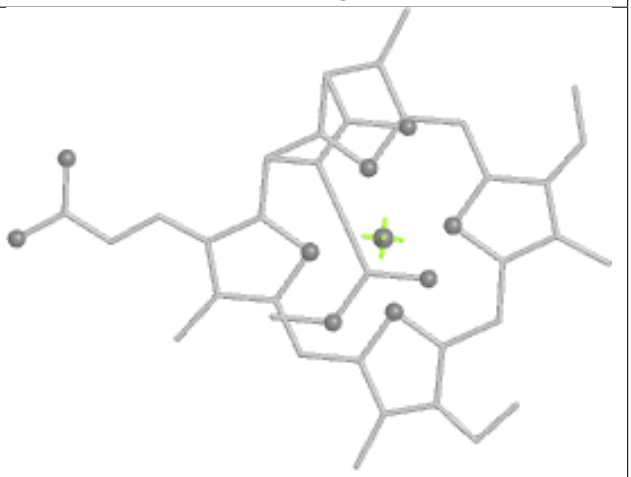
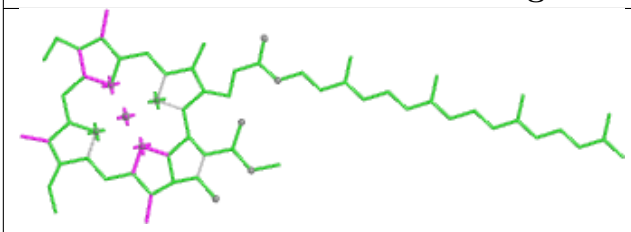


Rings

Ligand CLA b 610



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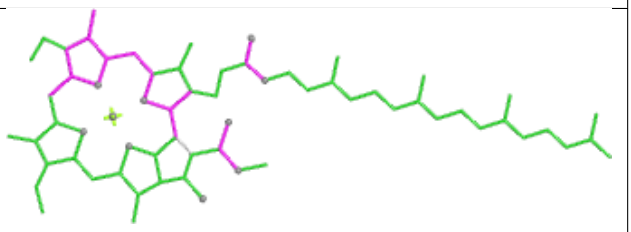

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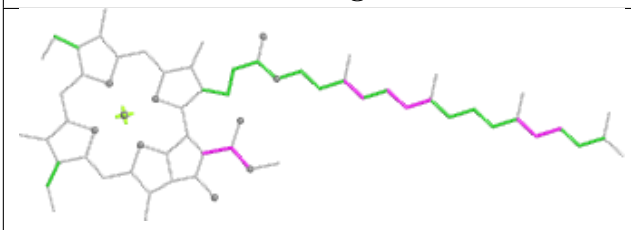

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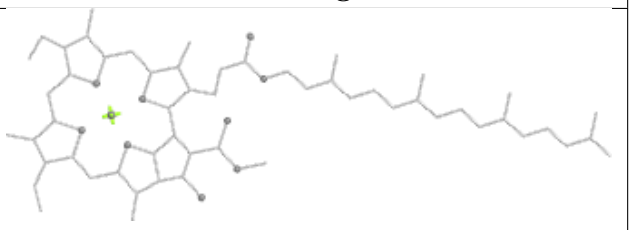
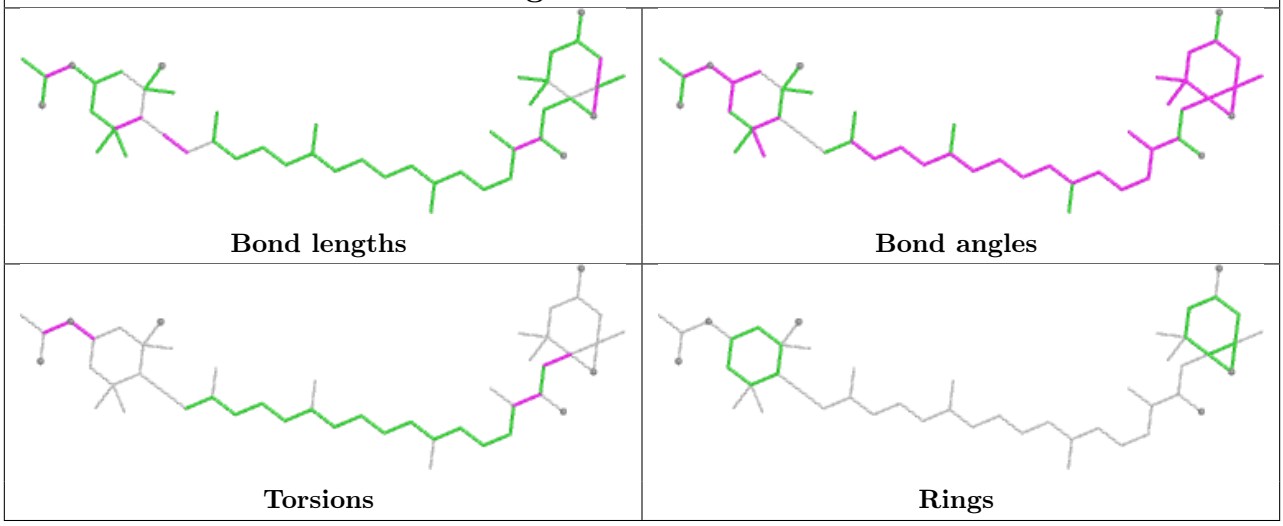


Rings

Ligand A86 17 303



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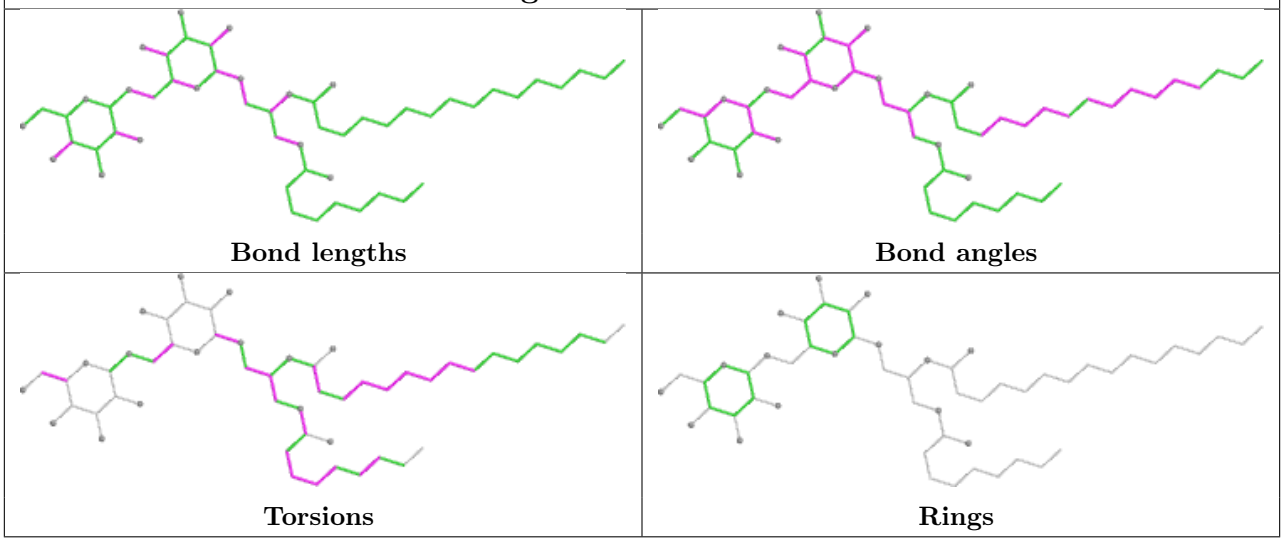

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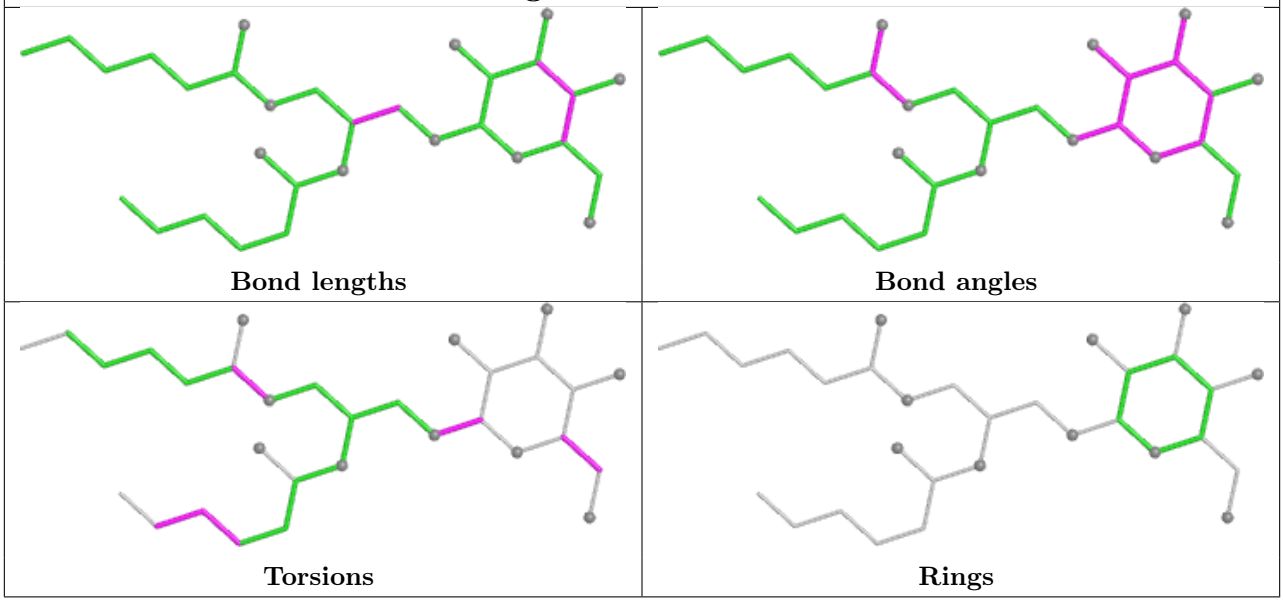

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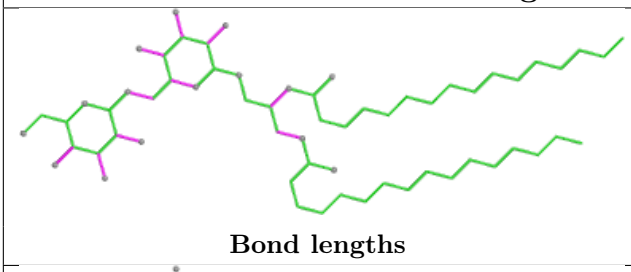

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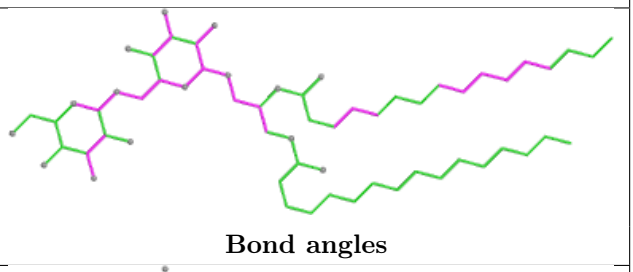

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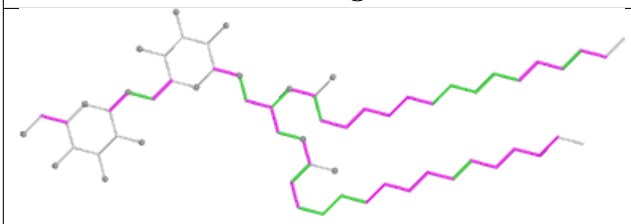

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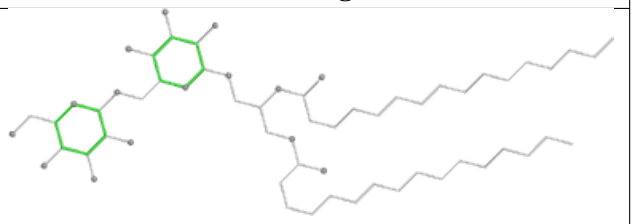
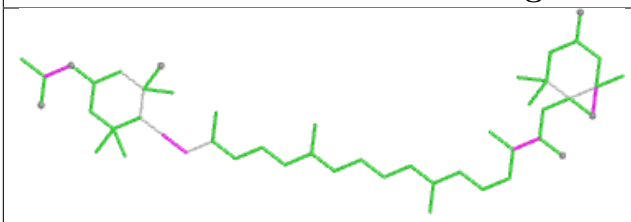


Rings

Ligand A86 17 304



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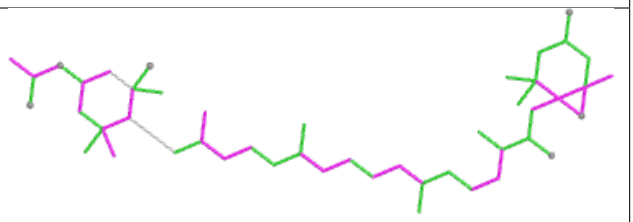
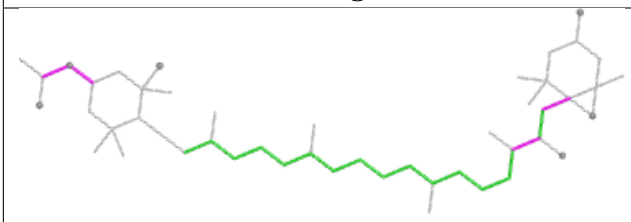


Bond angles



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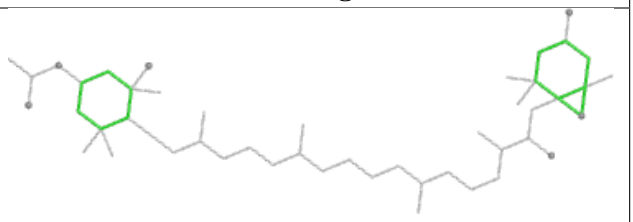
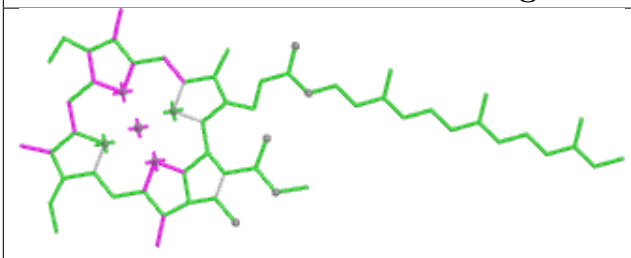


Rings

Ligand CLA 14 306



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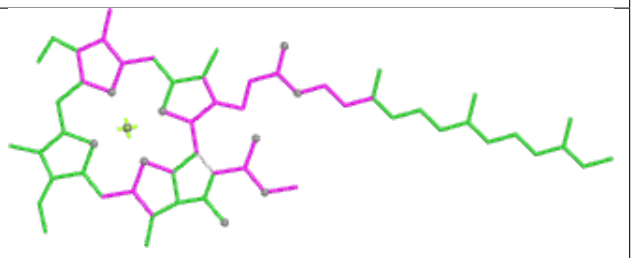
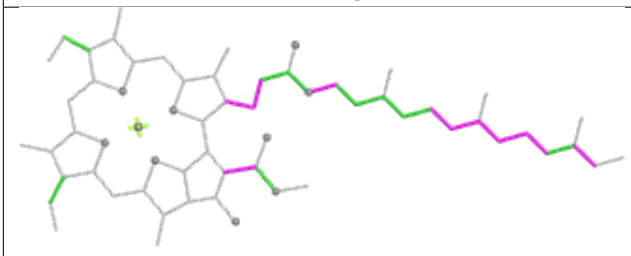


Bond angles



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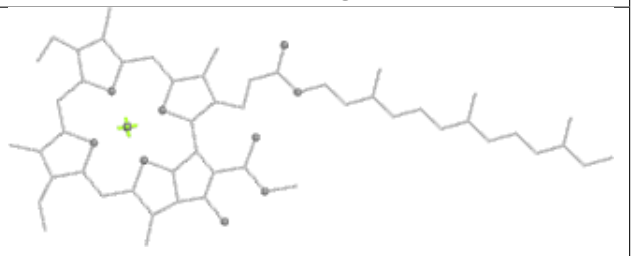
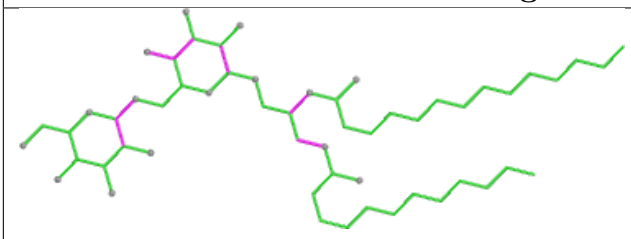


Rings

Ligand DGD w 204



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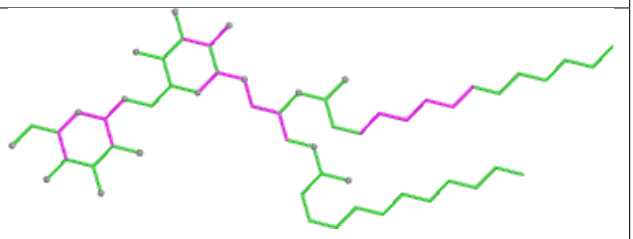
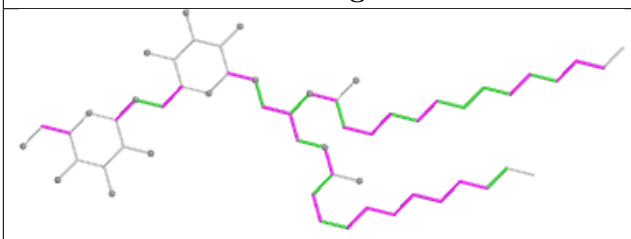


Bond angles



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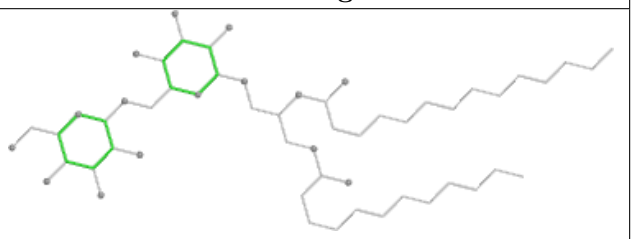
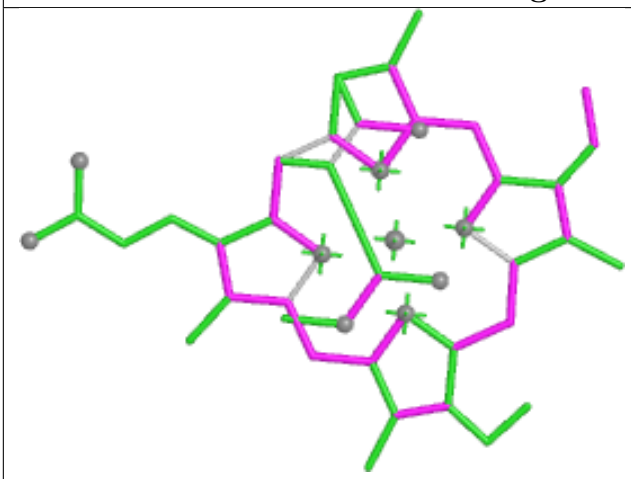


Rings

Ligand KC2 9 309



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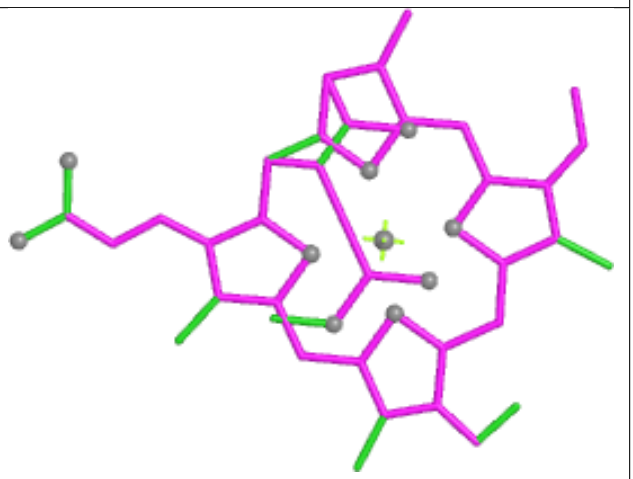

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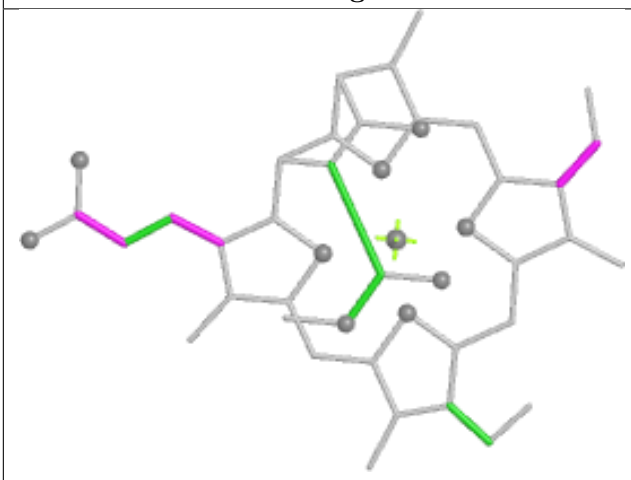

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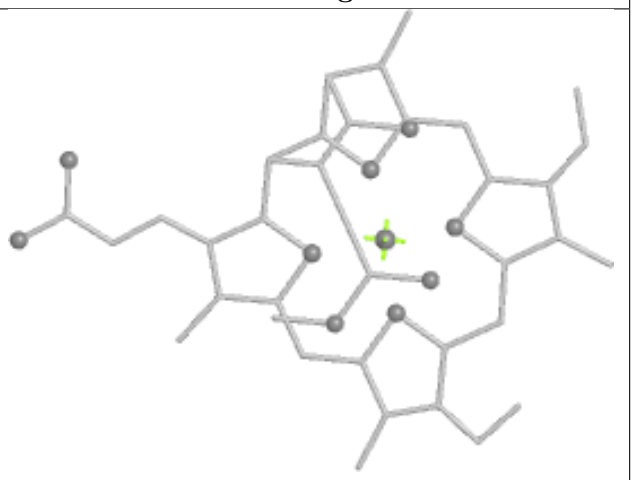
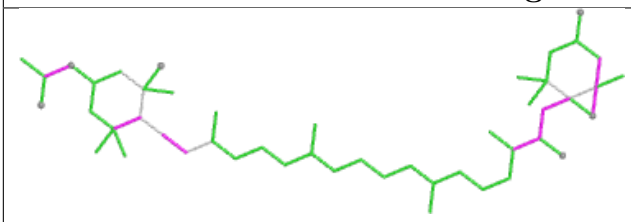


Rings

Ligand A86 11 306



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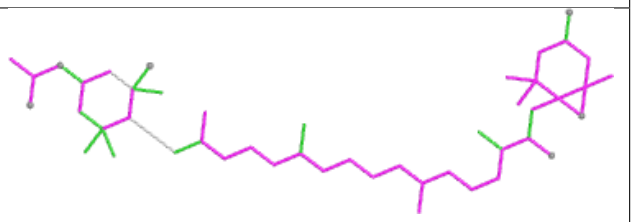

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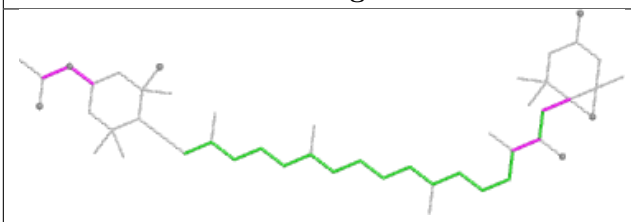

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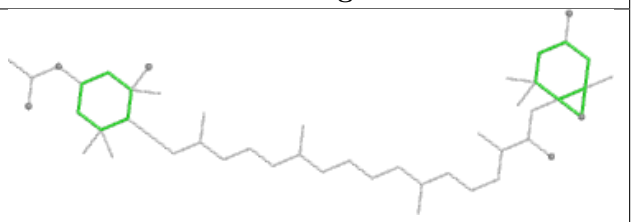
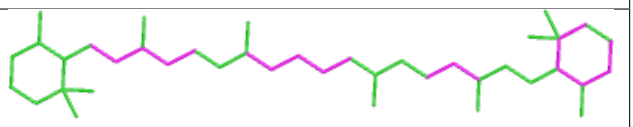


Rings

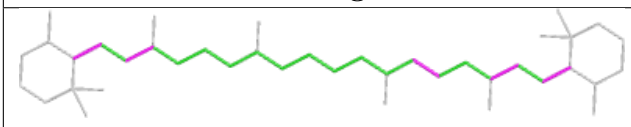
Ligand BCR c 516



Bond lengths



Bond angles



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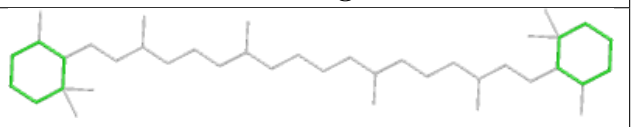
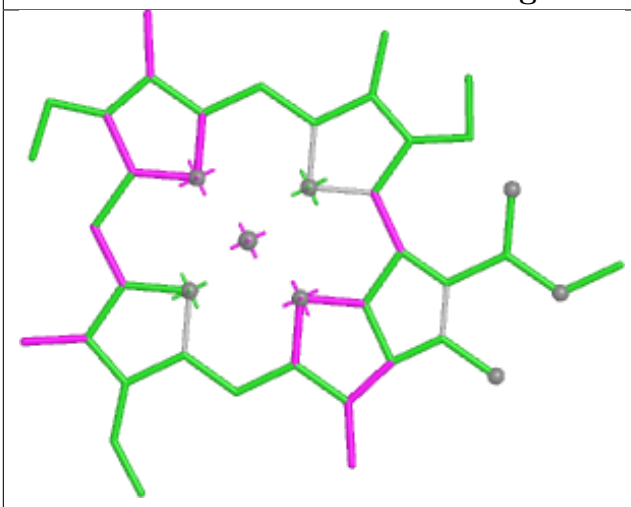


Rings

Ligand CLA 16 313



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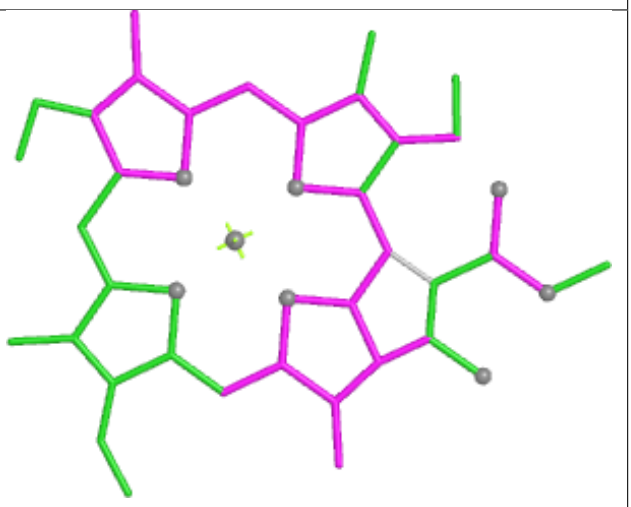
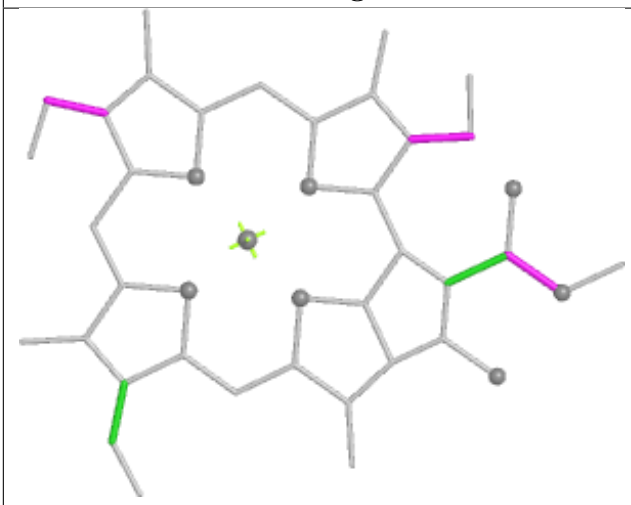


Bond angles

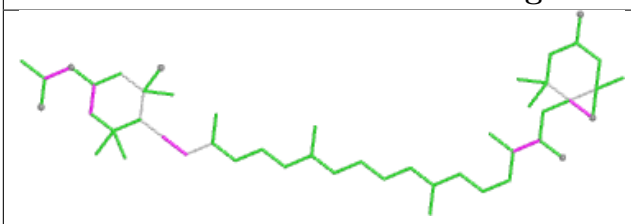


Torsions



Rings

Ligand A86 10 301



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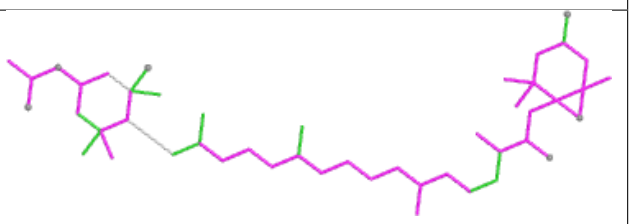
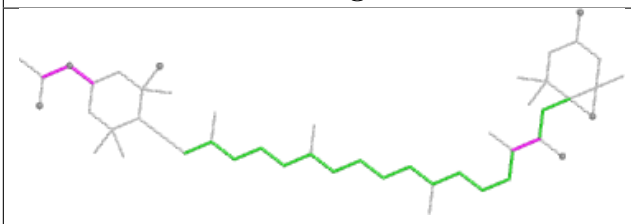


Bond angles



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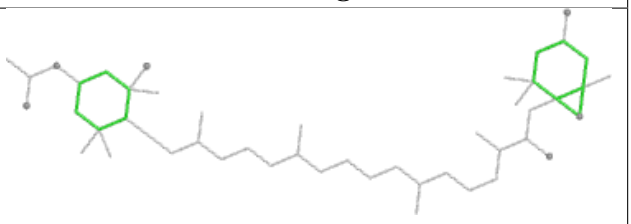
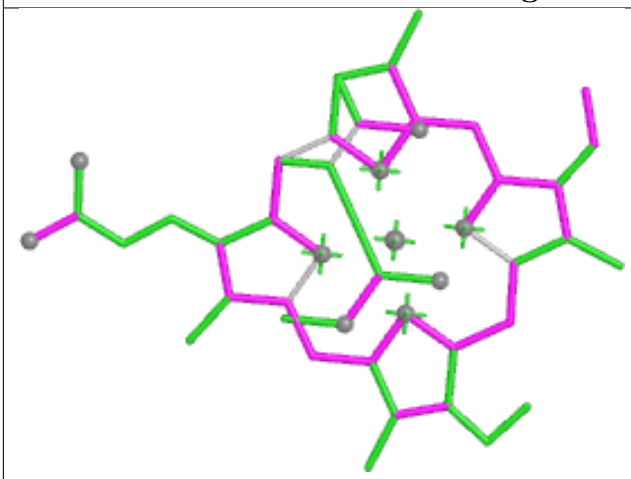


Rings

Ligand KC2 15 310



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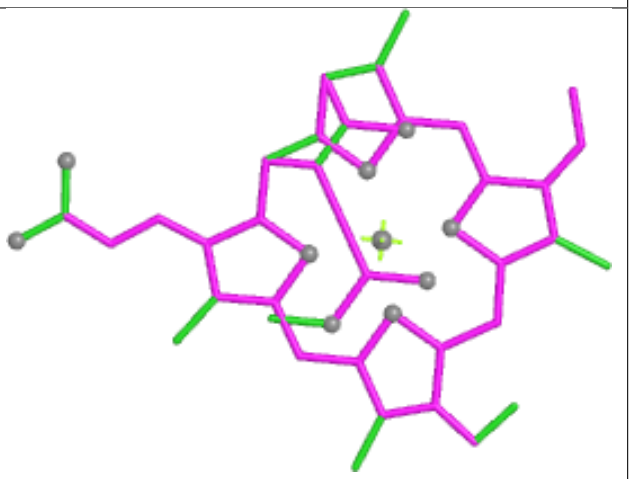

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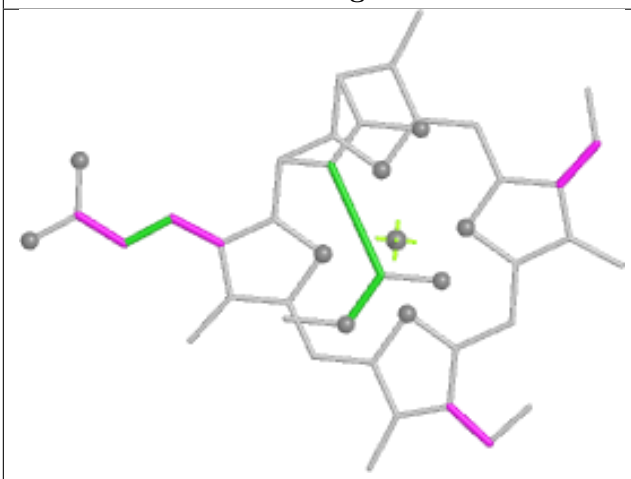

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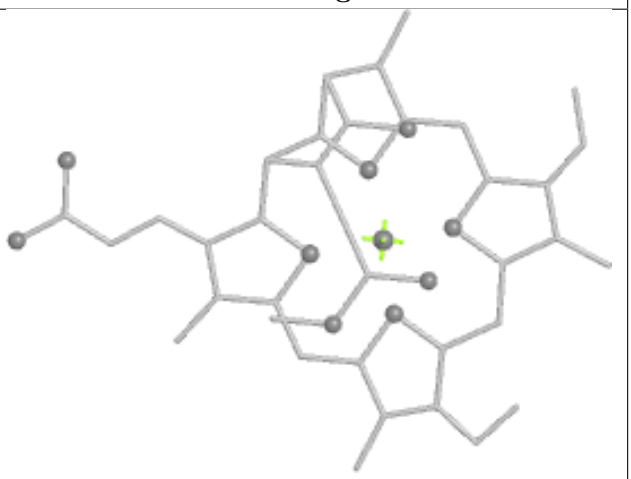
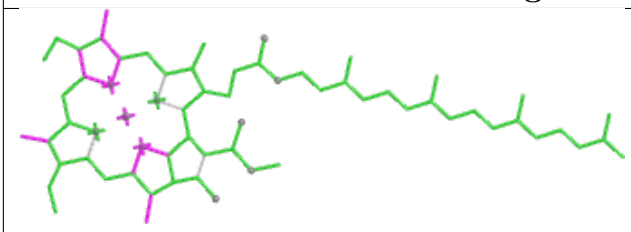
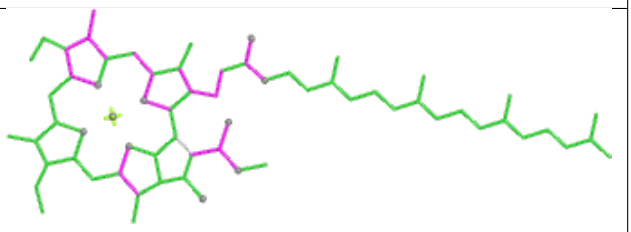


Rings

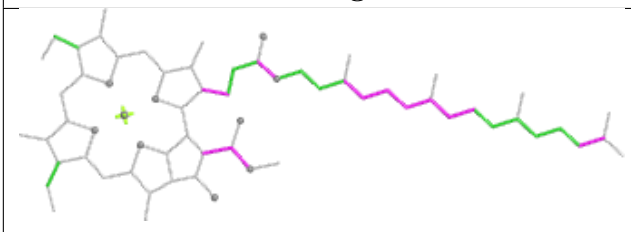
Ligand CLA B 614



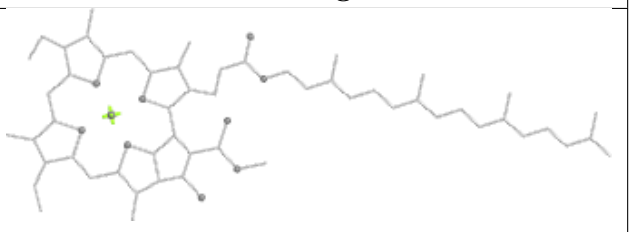
Bond lengths



Bond angles

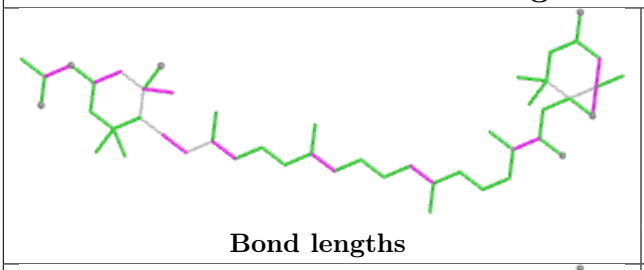


Torsions



Rings

Ligand A86 P 611



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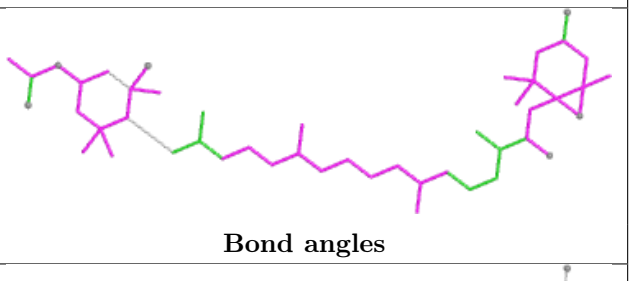

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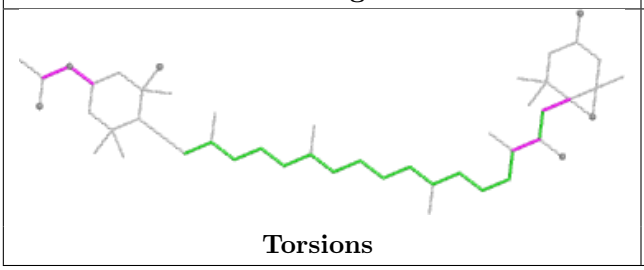

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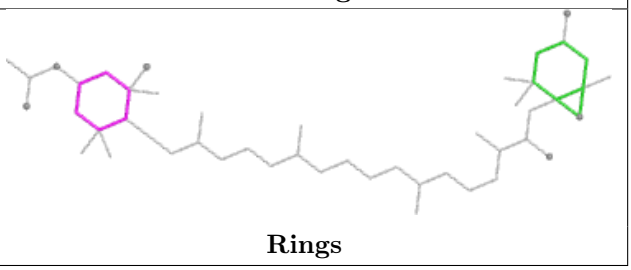
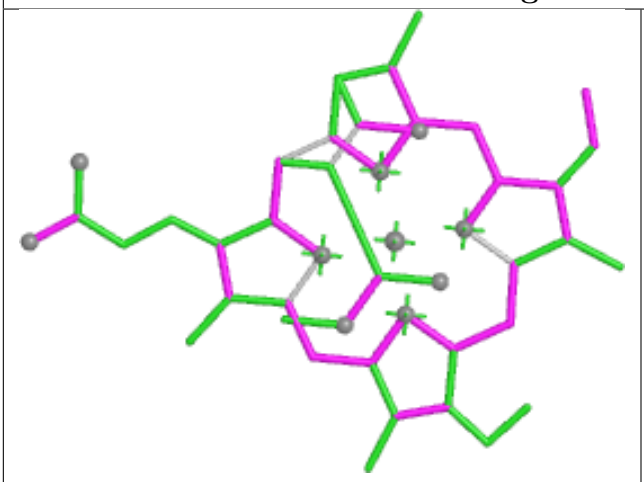


Rings

Ligand KC2 18 308



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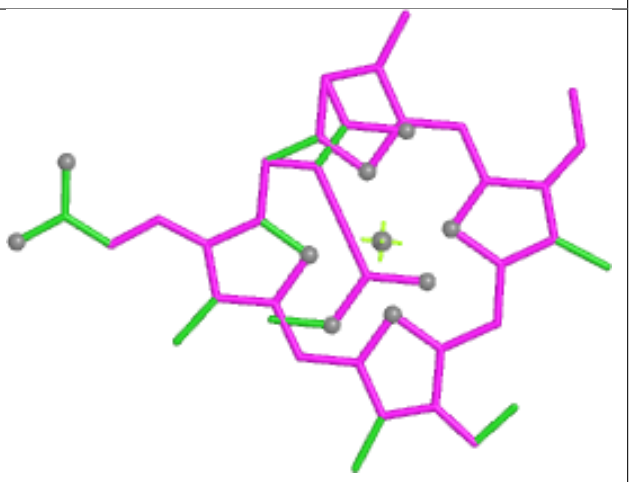

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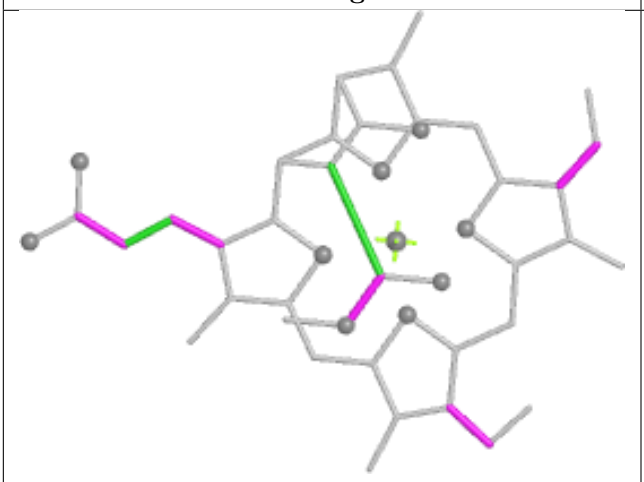

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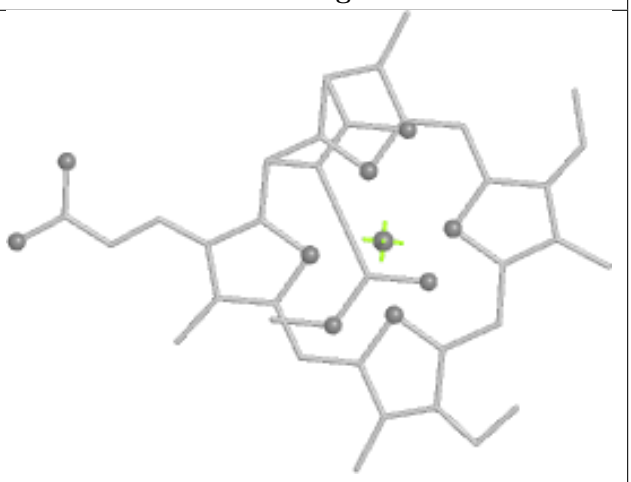
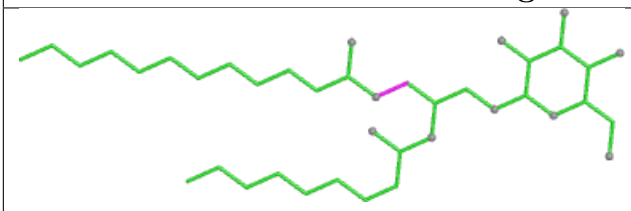


Rings

Ligand LMG m 101



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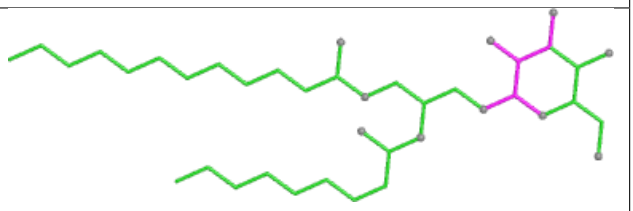

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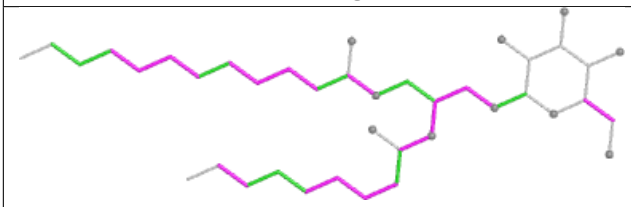

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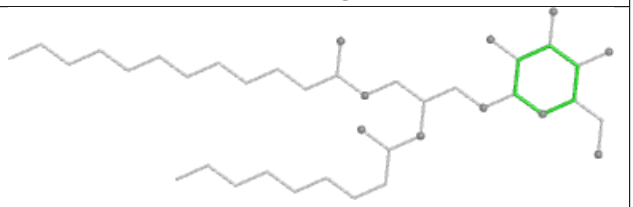
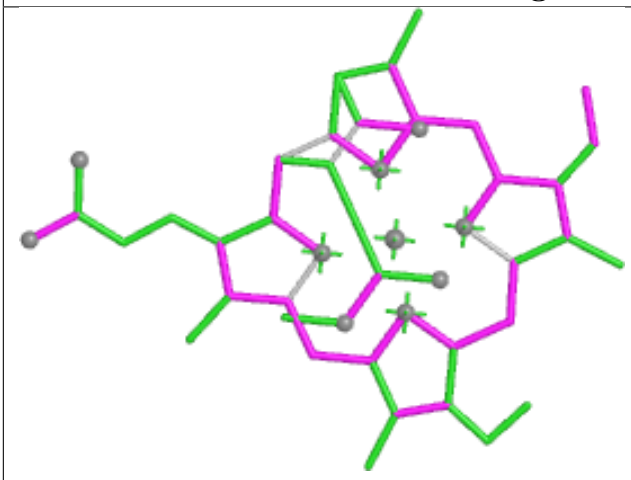


Rings

Ligand KC2 5 308



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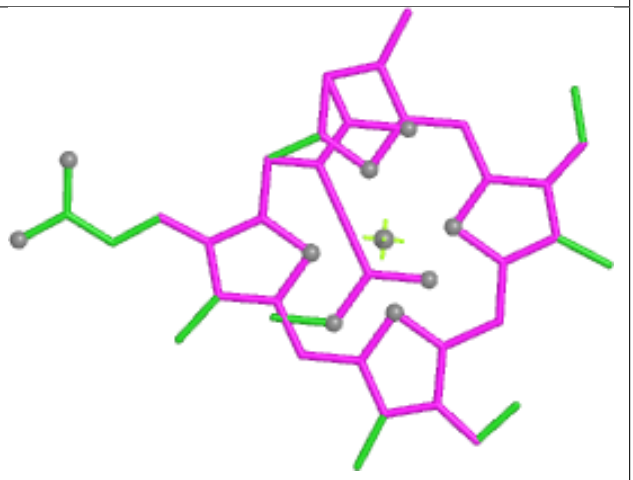

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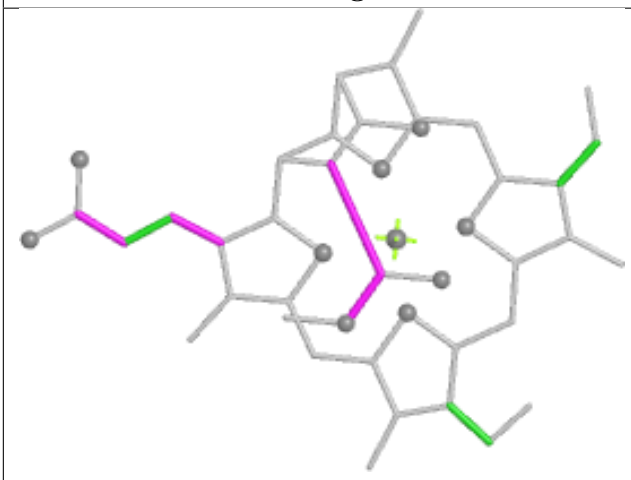

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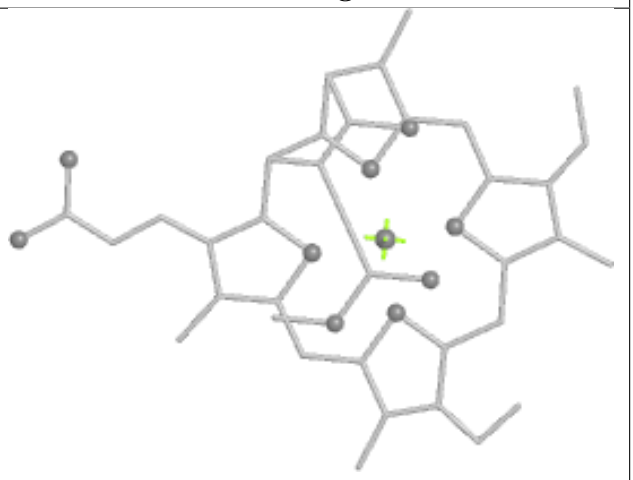
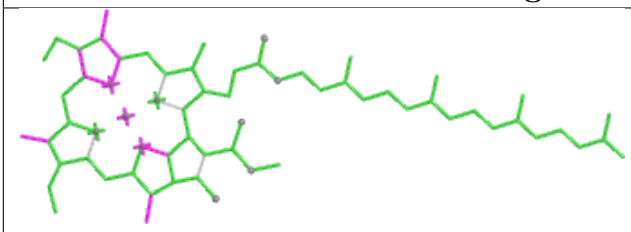


Rings

Ligand CLA C 512



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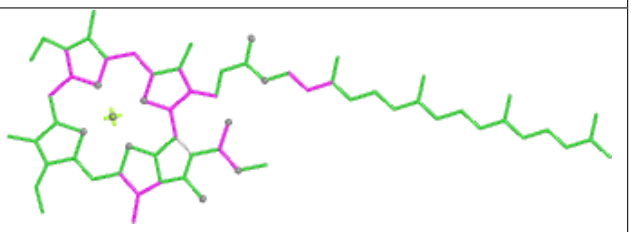
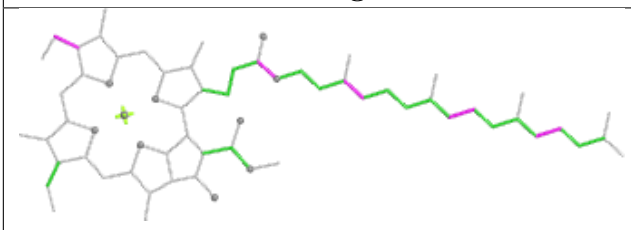


Bond angles



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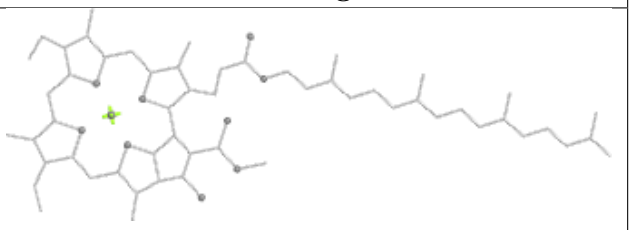
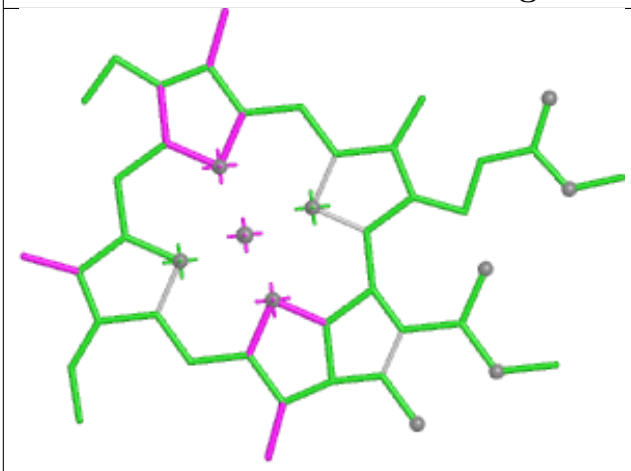


Rings

Ligand CLA 11 312



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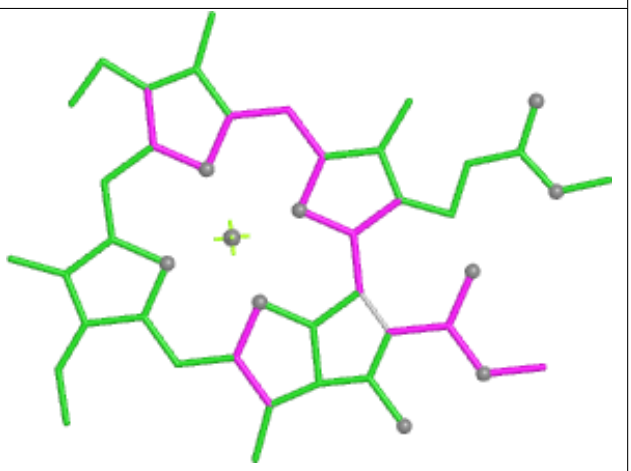

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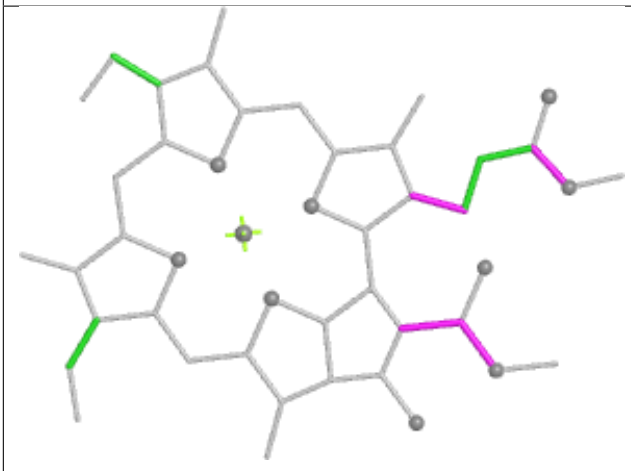

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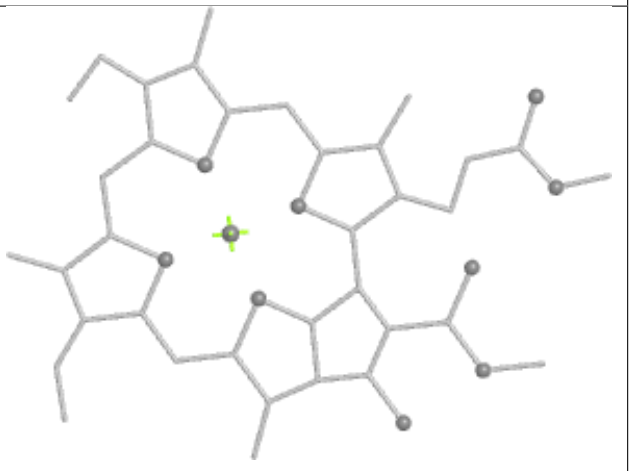
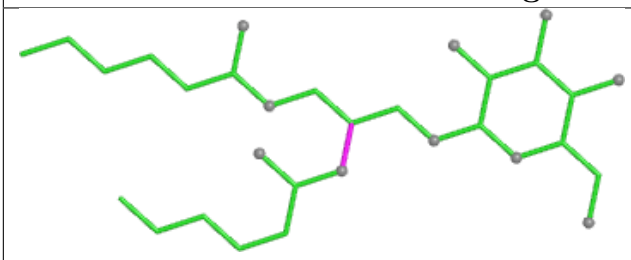


Rings

Ligand LMG p 614



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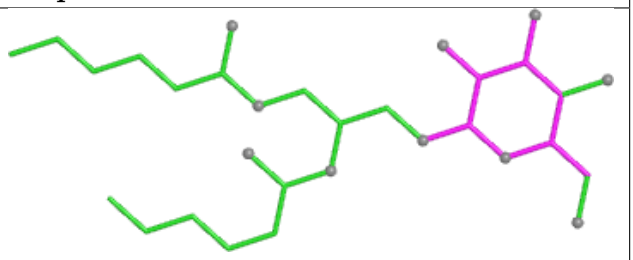

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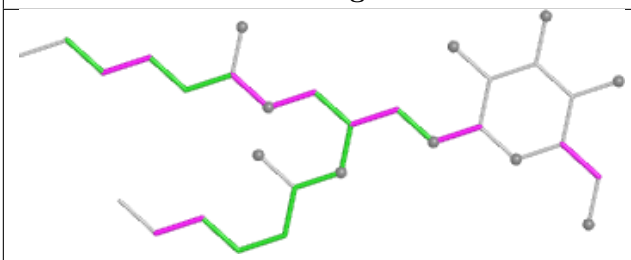

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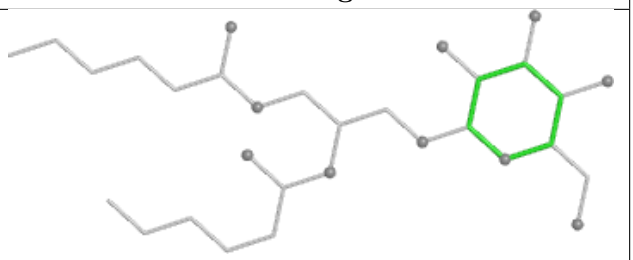
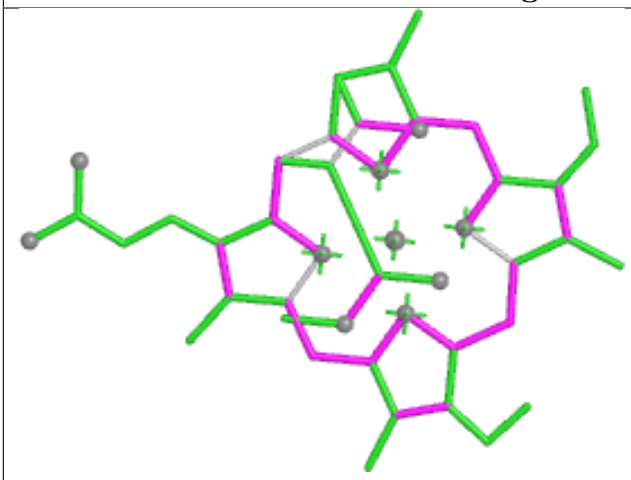


Rings

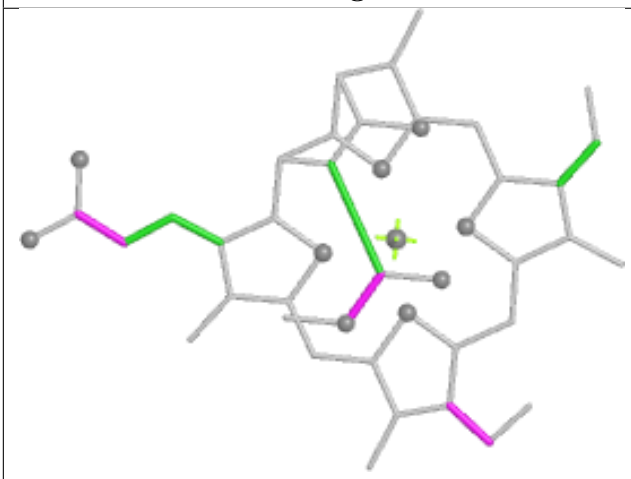
Ligand KC1 13 314



Bond lengths



Bond angles



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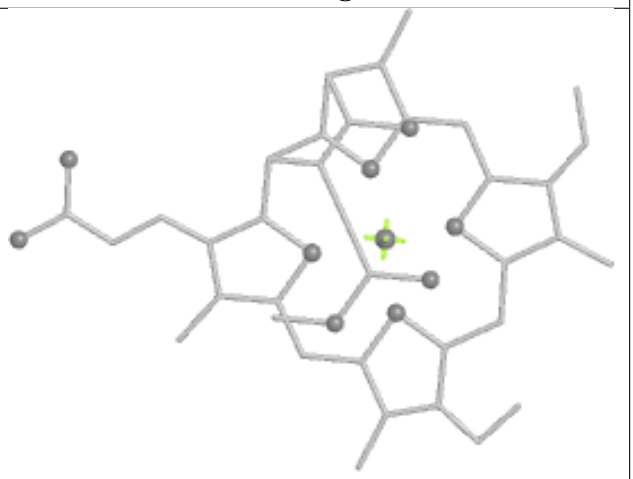
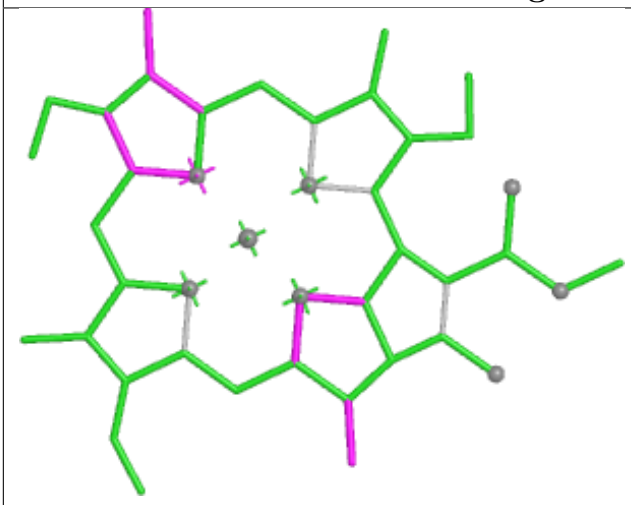


Rings

Ligand CLA 5 306



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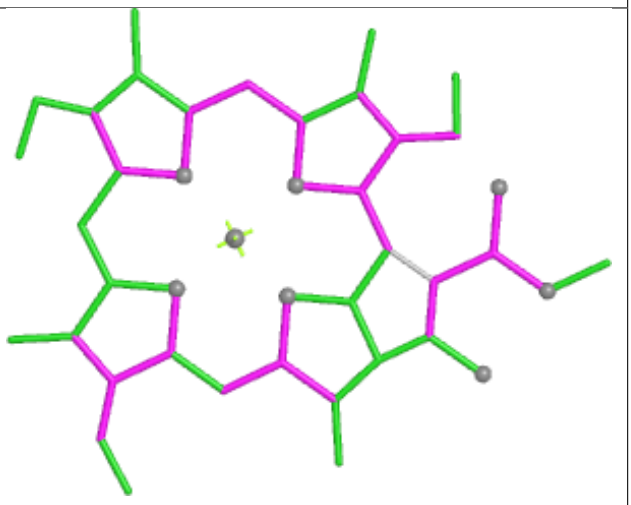
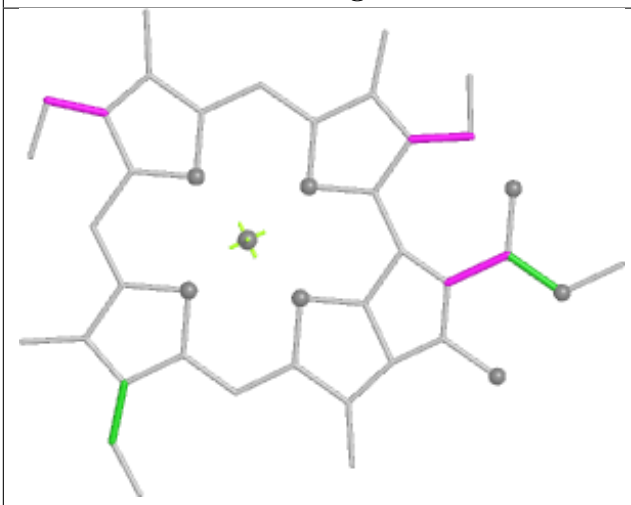


Bond angles

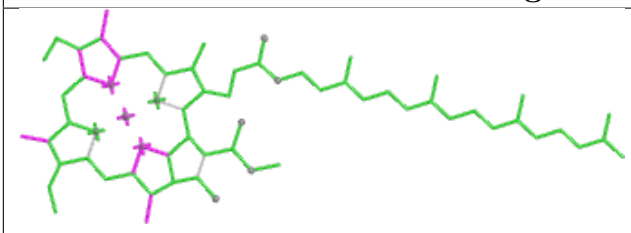


Torsions



Rings

Ligand CLA C 504



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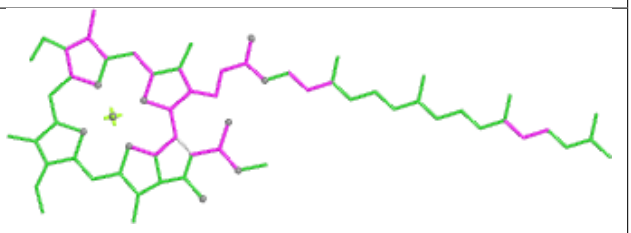
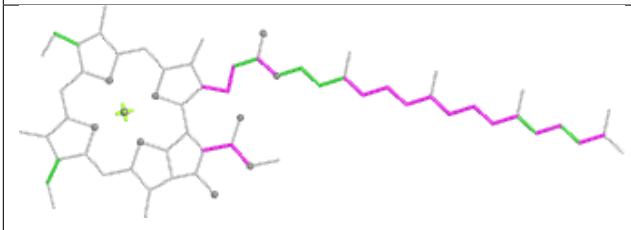


Bond angles



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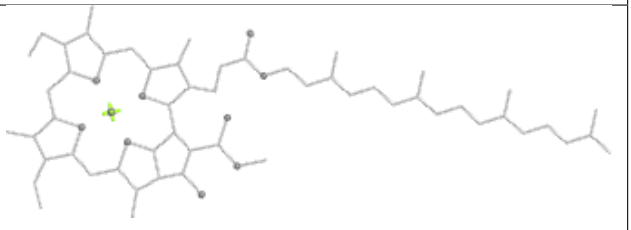
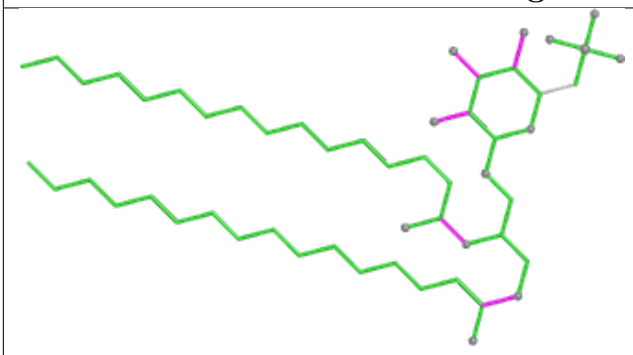


Rings

Ligand SQD b 601



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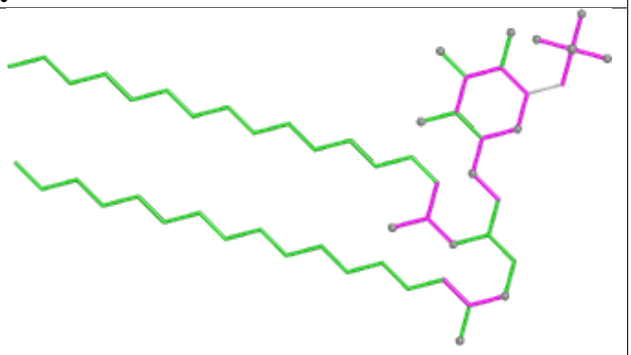
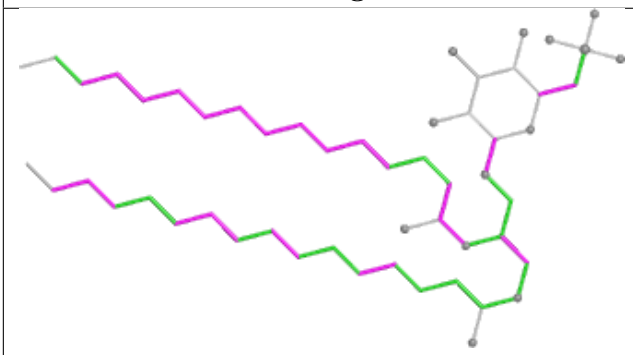


Bond angles



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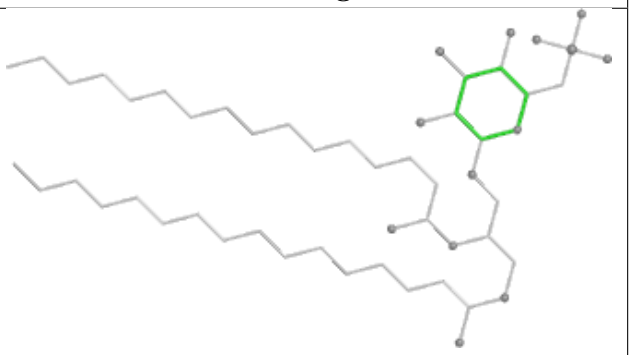
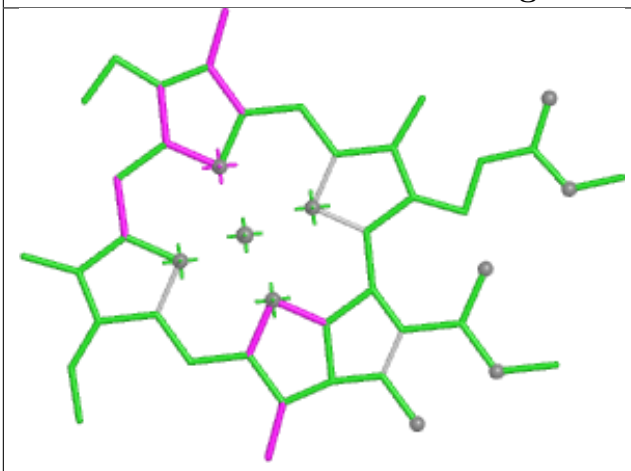


Rings

Ligand CLA 10 312



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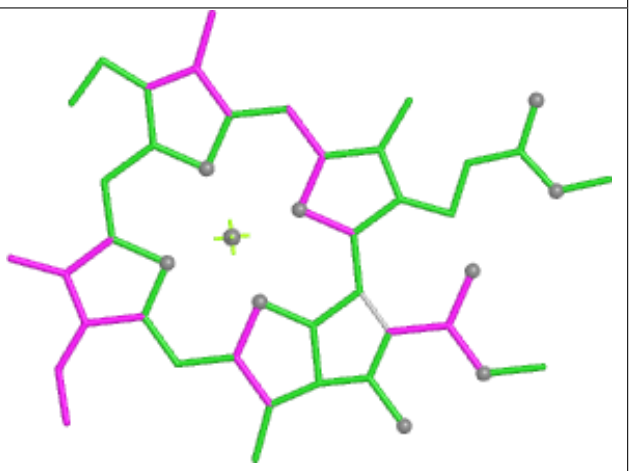

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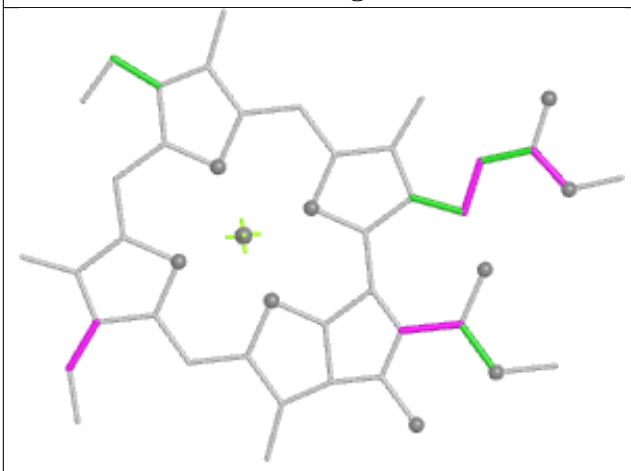

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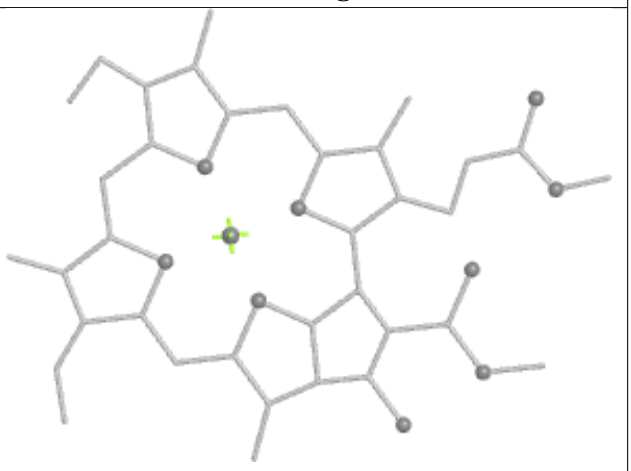
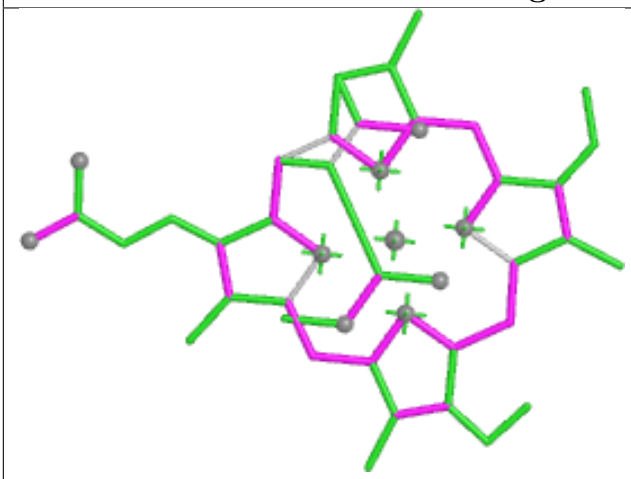


Rings

Ligand KC1 p 609



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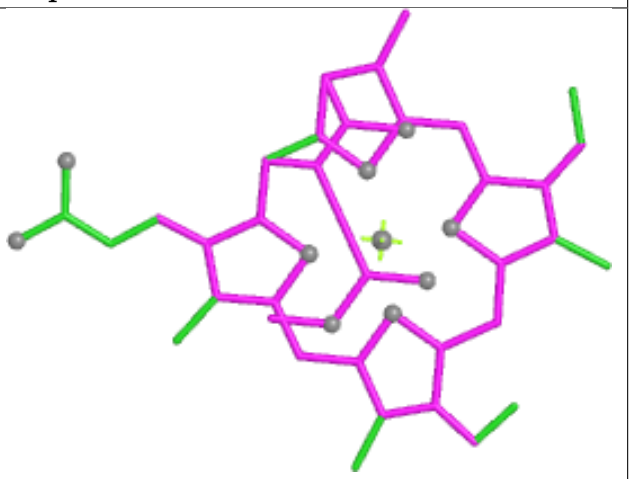
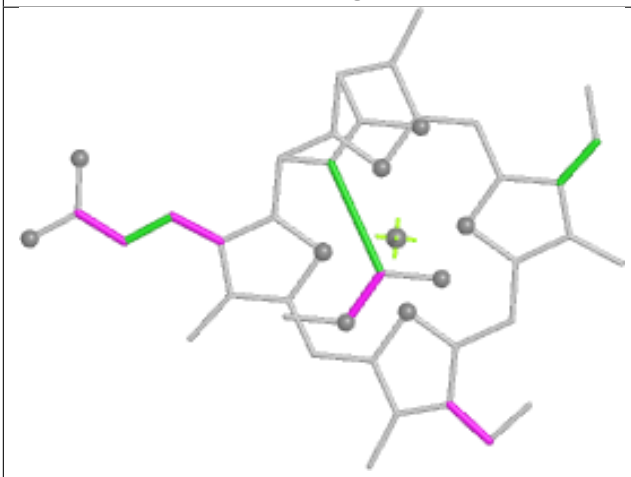


Bond angles



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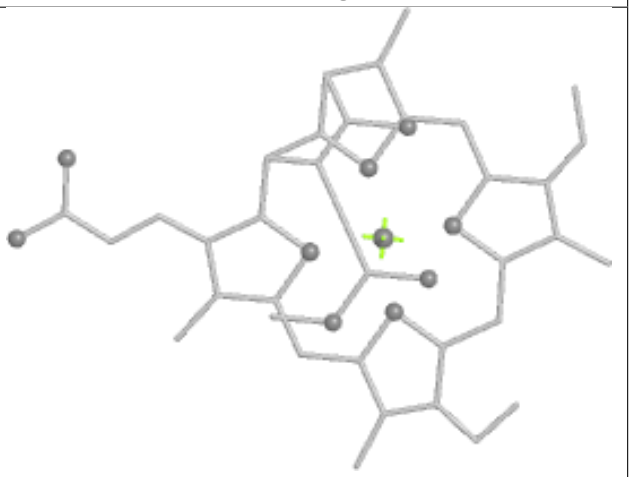
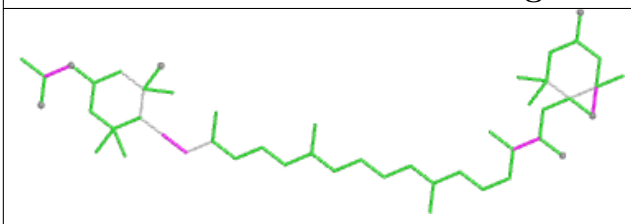


Rings

Ligand A86 11 303



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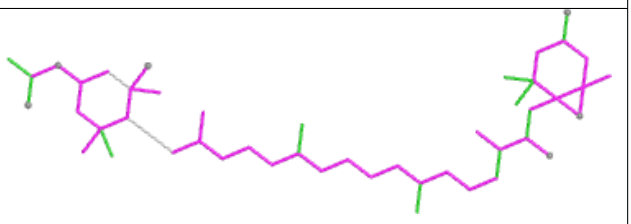
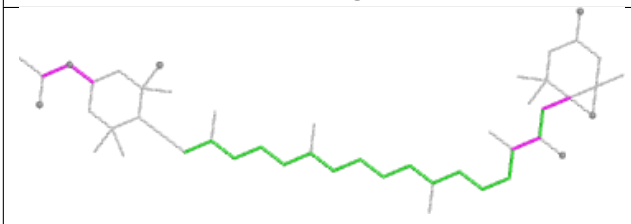


Bond angles



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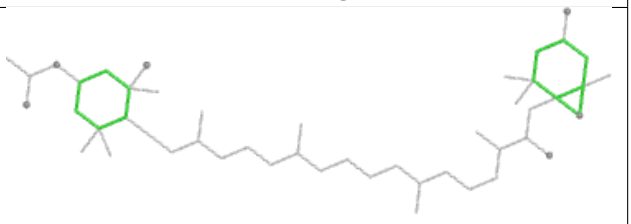
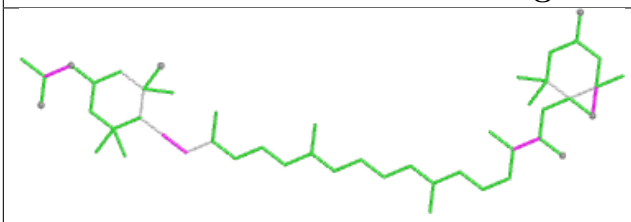


Rings

Ligand A86 4 304



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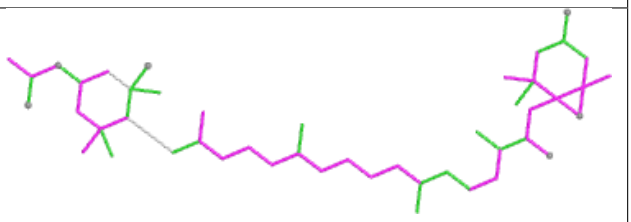
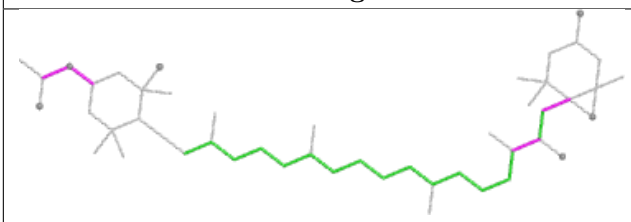


Bond angles



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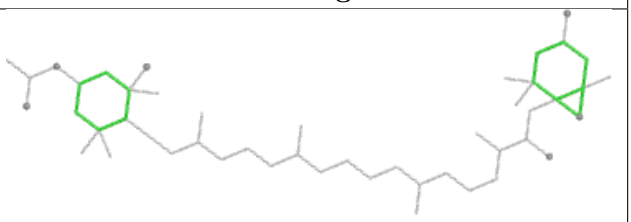
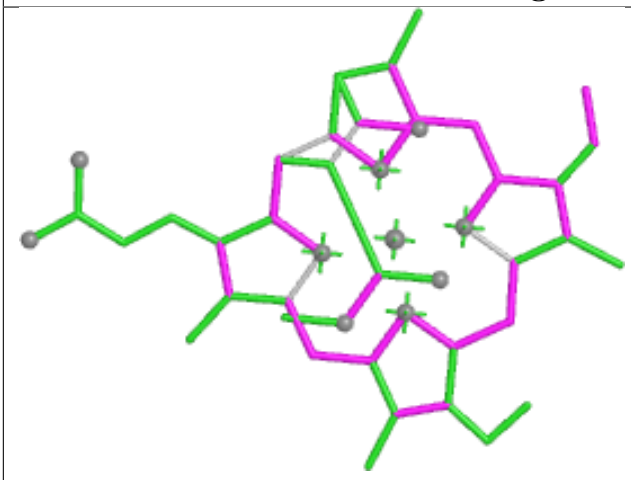


Rings

Ligand KC2 1 309



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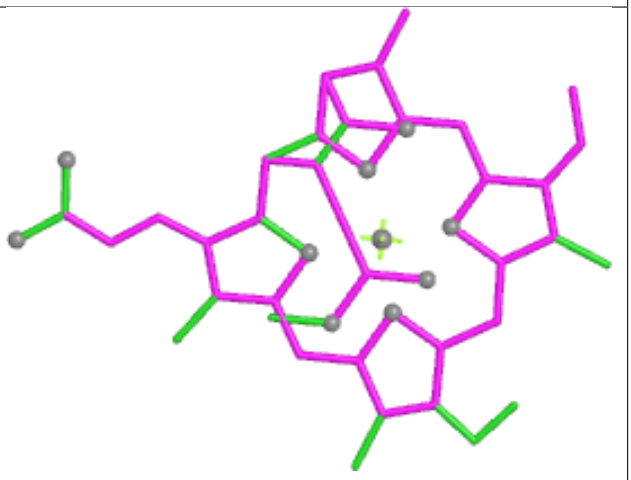

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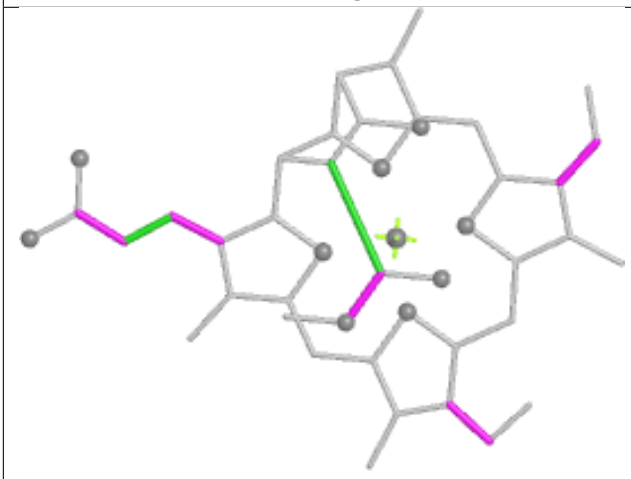

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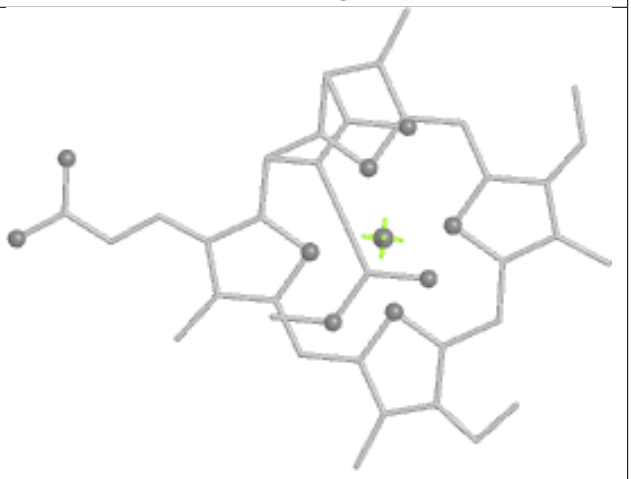

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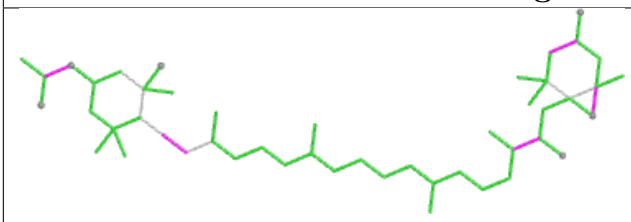

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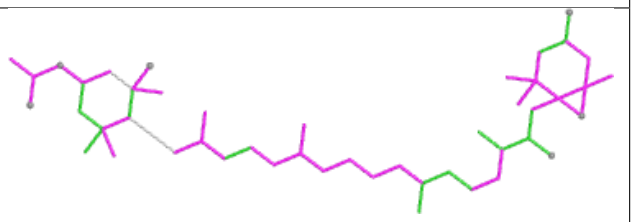

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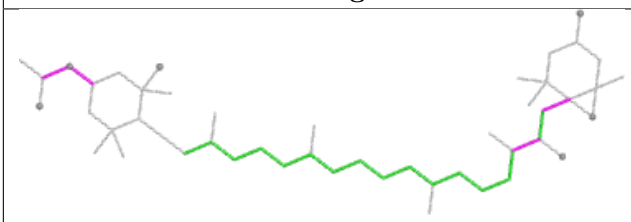

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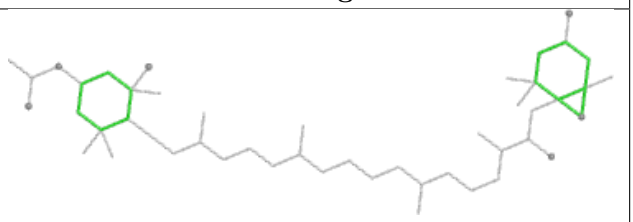

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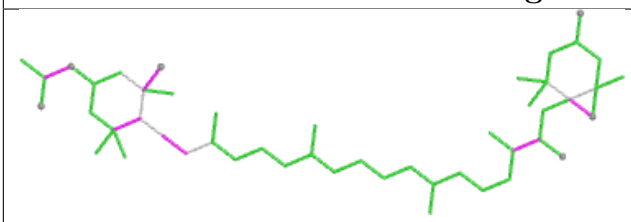

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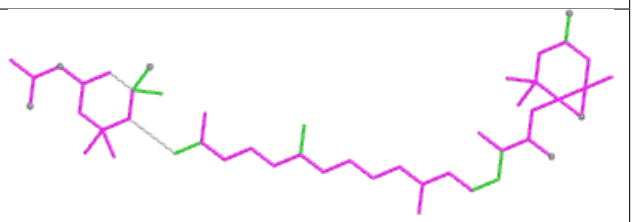

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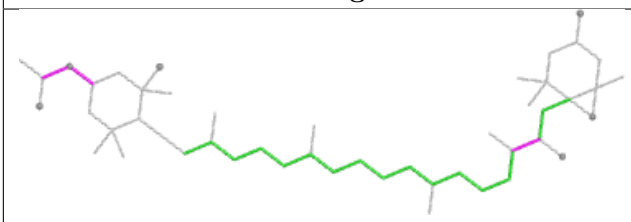

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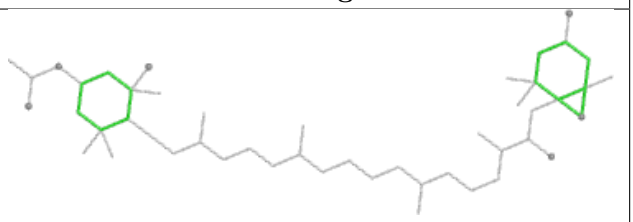

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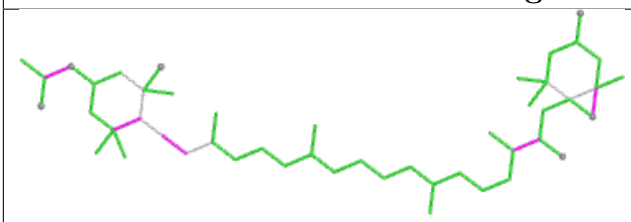

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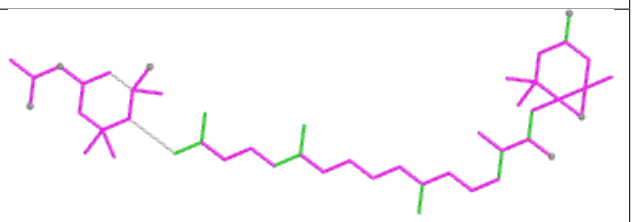

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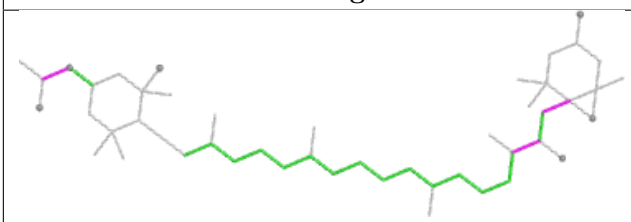

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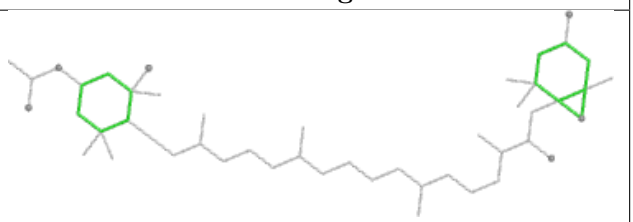

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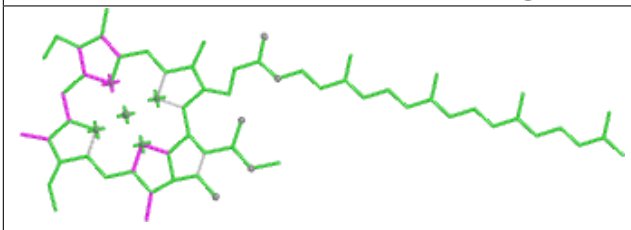

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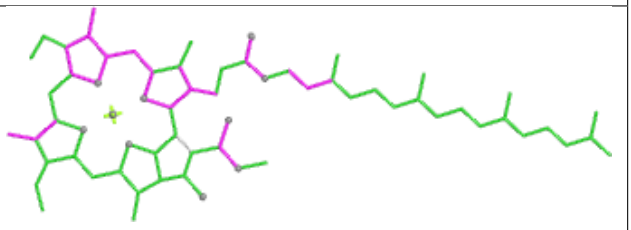

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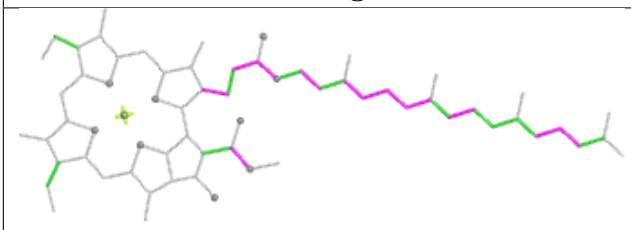

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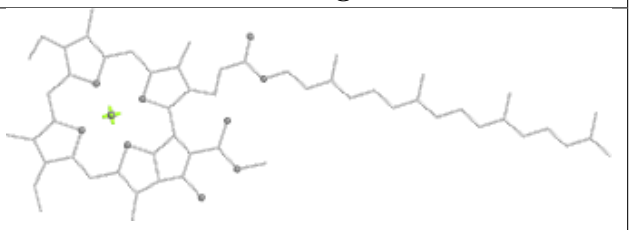

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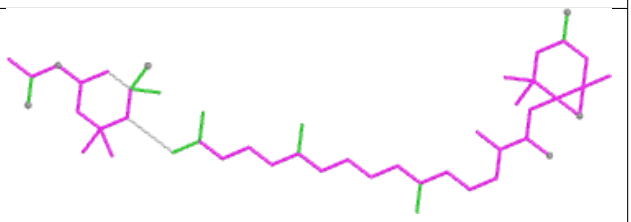

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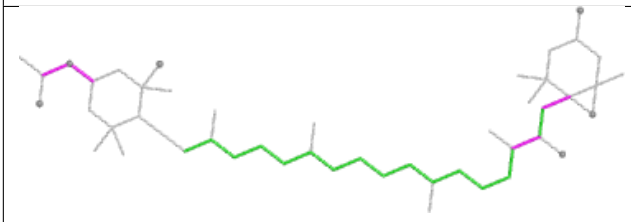

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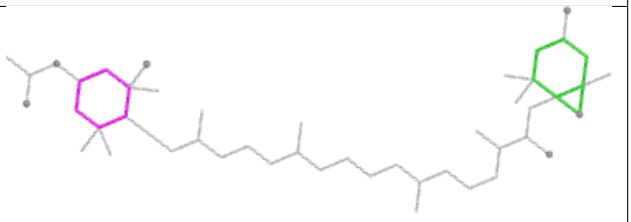

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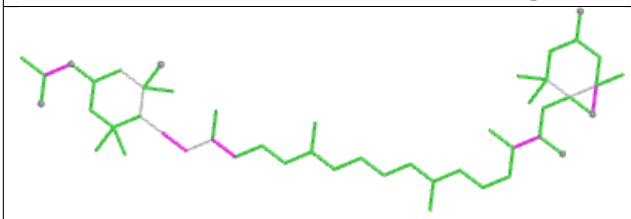

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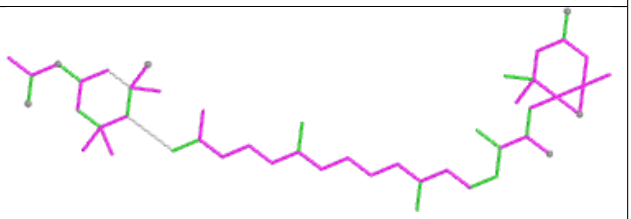

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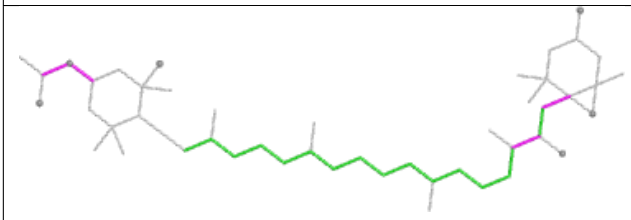

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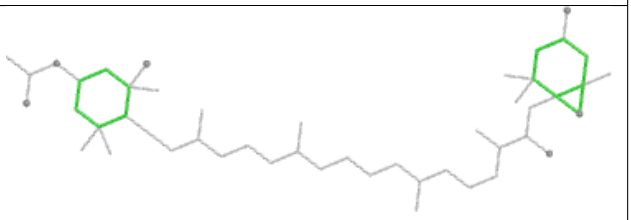

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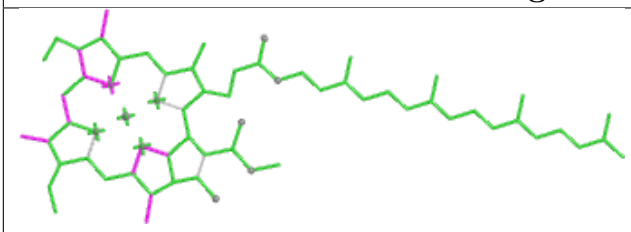

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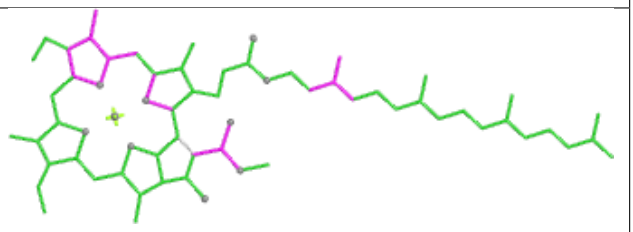

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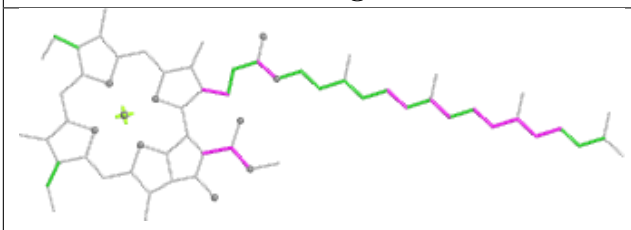

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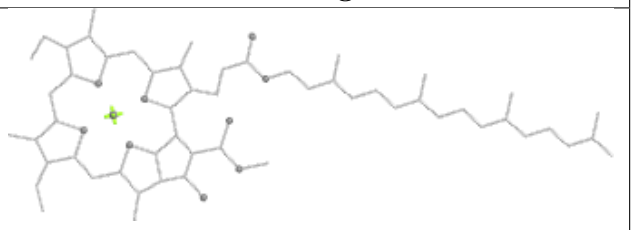

Rings

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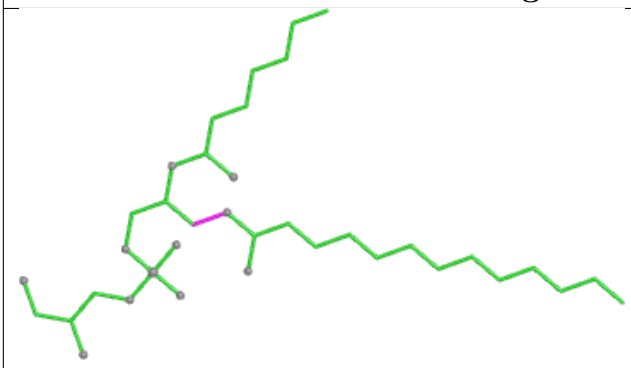

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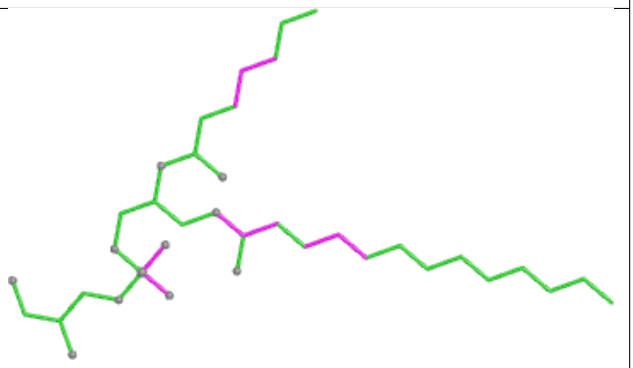

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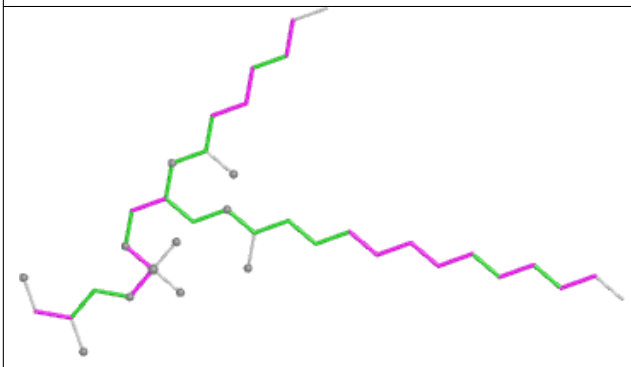

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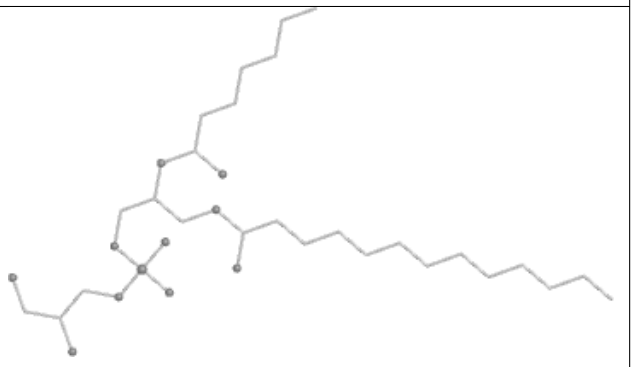

Rings

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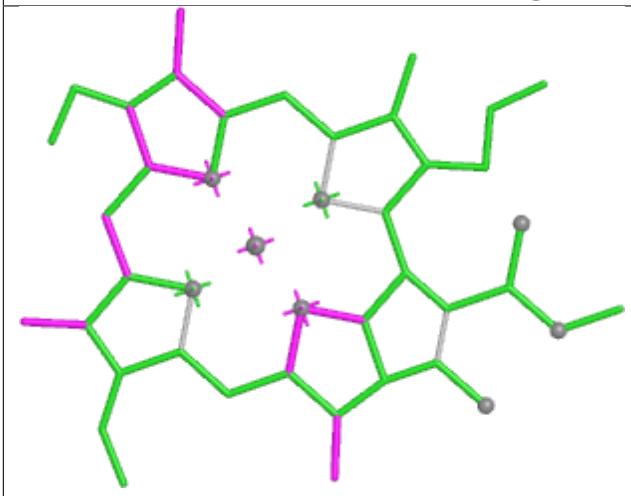

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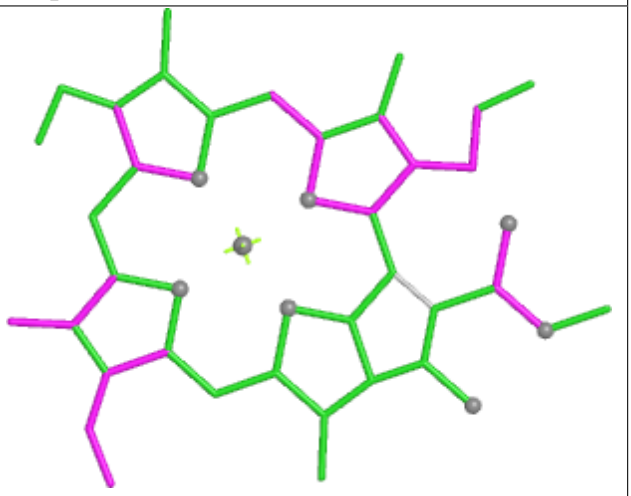

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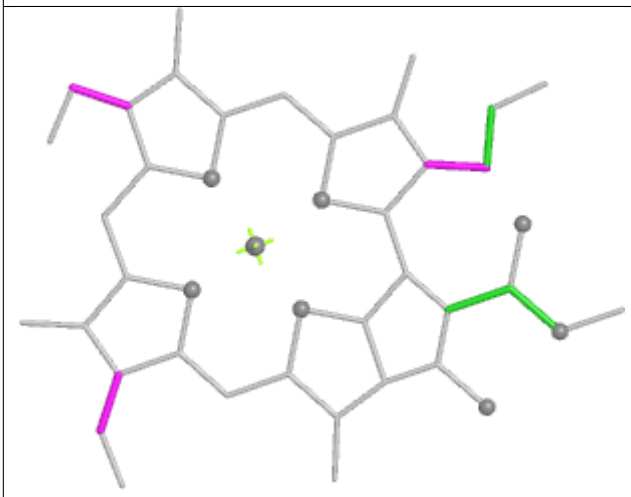

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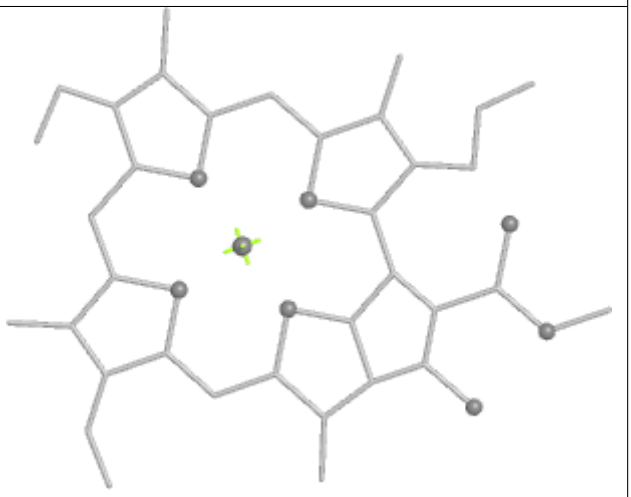
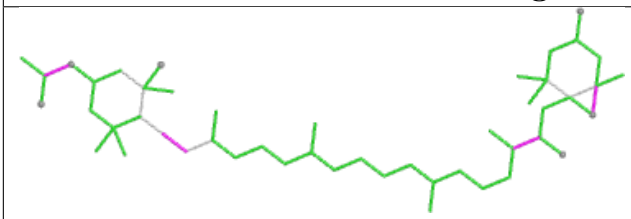


Rings

Ligand A86 P 613



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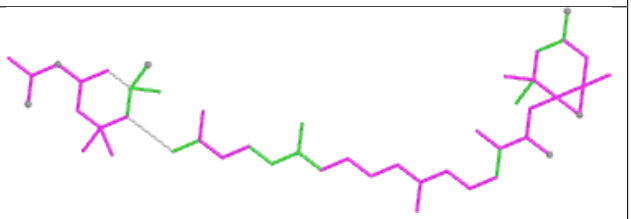

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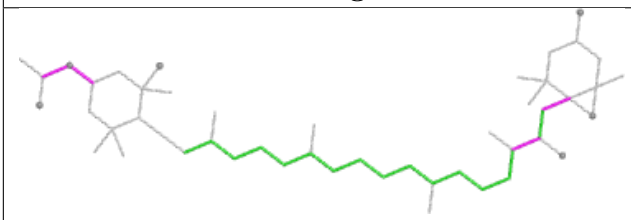

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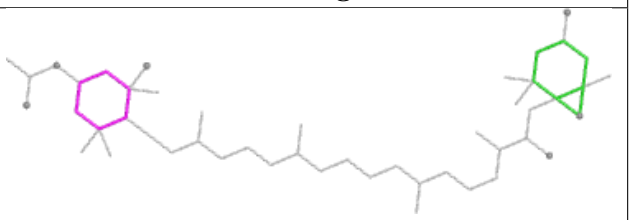
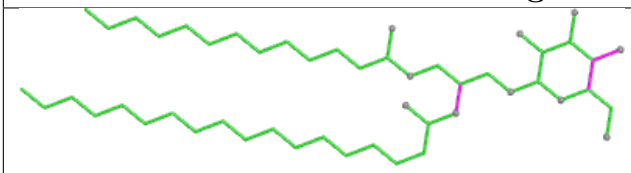


Rings

Ligand LMG j 101



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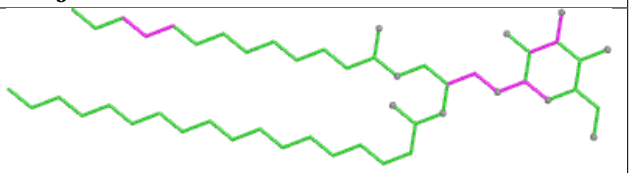
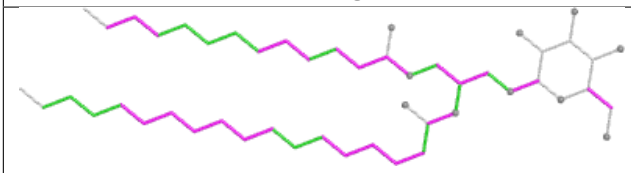


Bond angles



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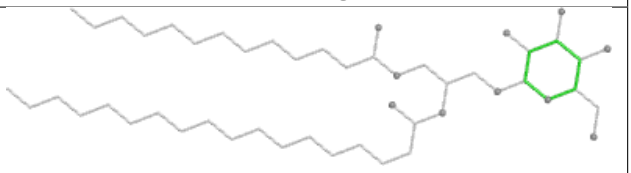
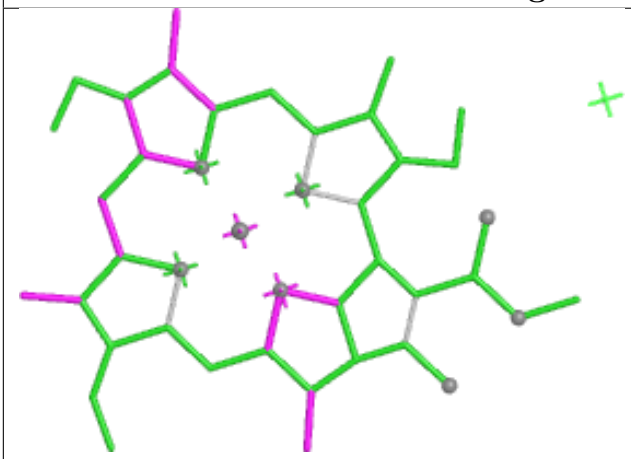


Rings

Ligand CLA 0 313



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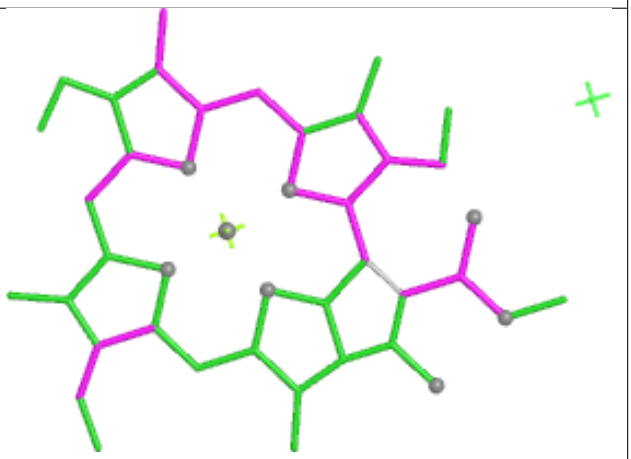
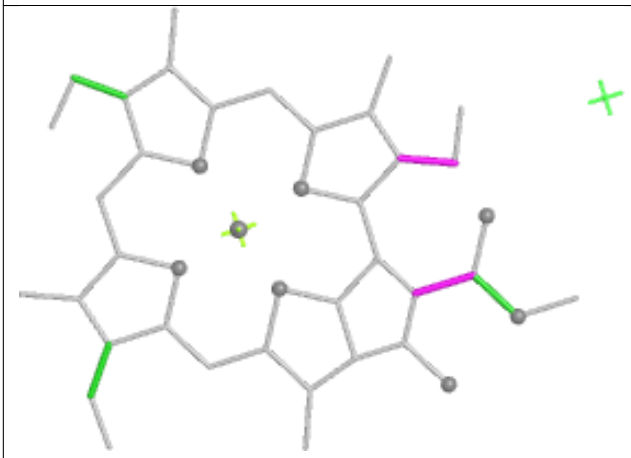


Bond angles



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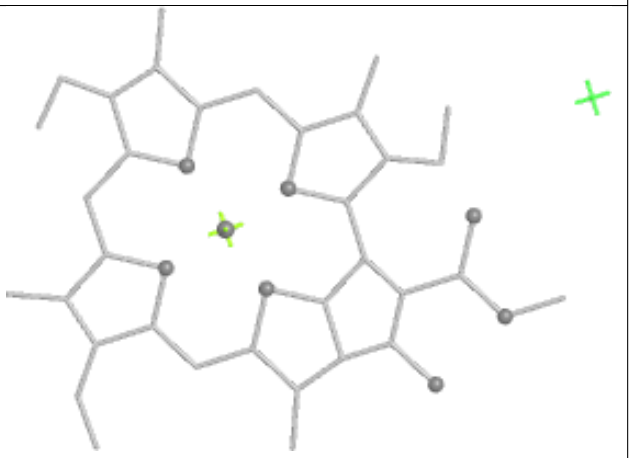
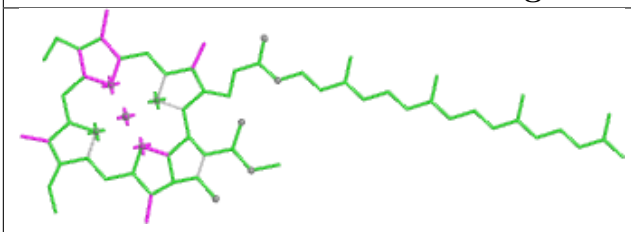


Rings

Ligand CLA B 612



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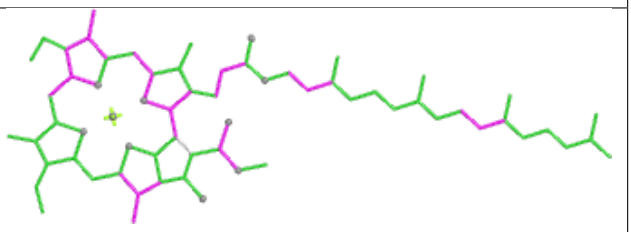
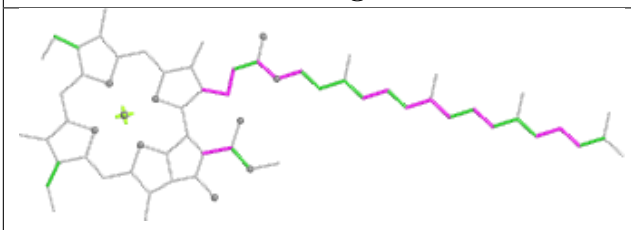


Bond angles



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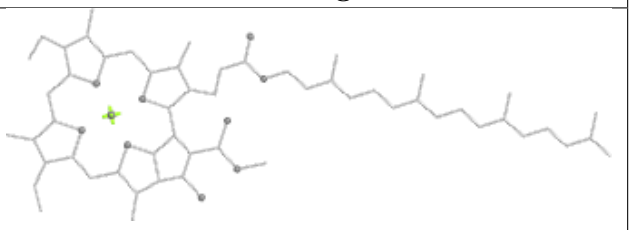
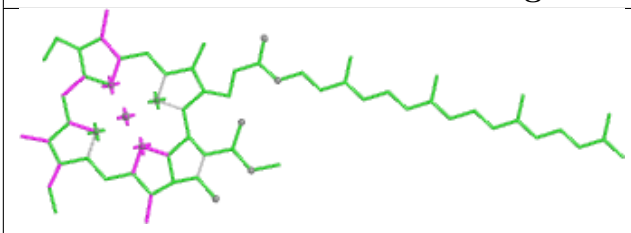
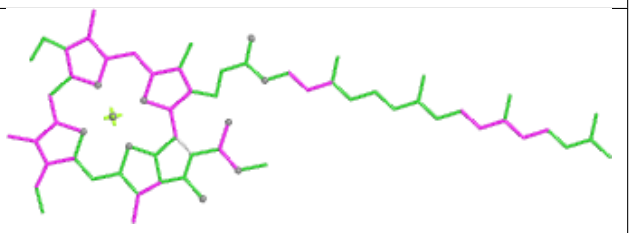


Rings

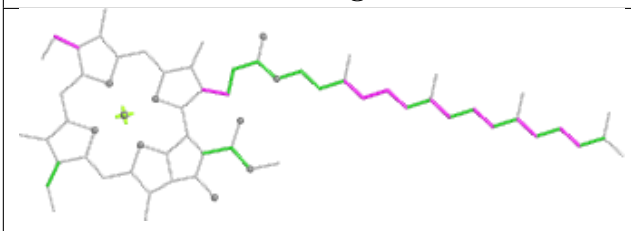
Ligand CLA C 503



Bond lengths



Bond angles



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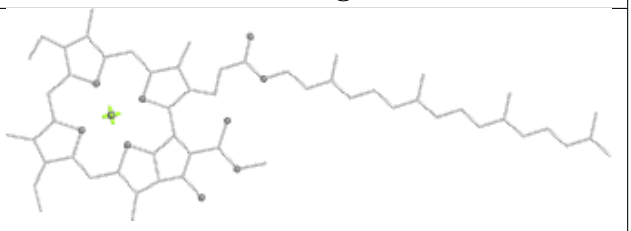
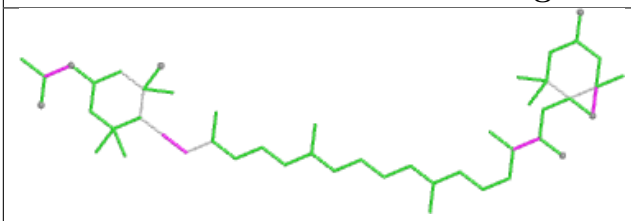


Rings

Ligand A86 7 303



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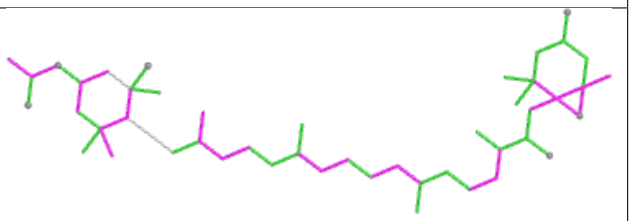

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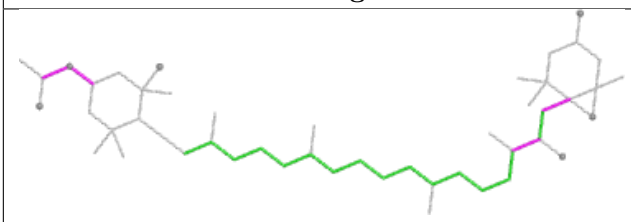

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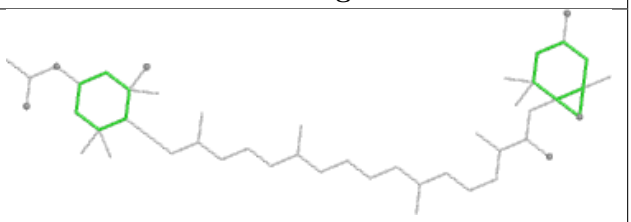
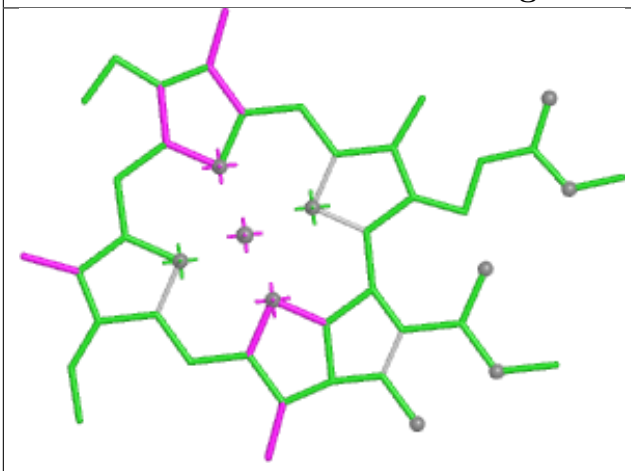


Rings

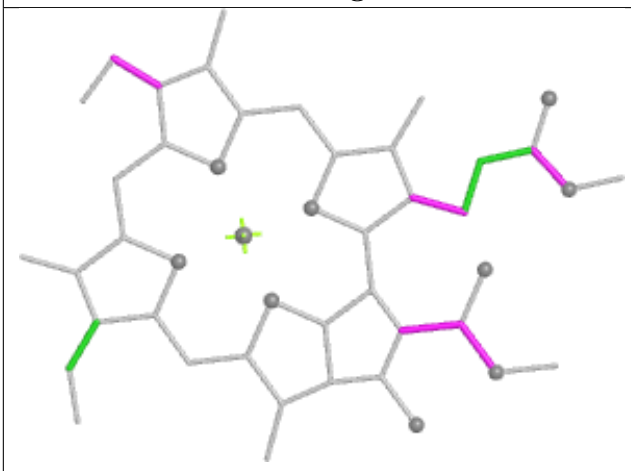
Ligand CLA 18 311



Bond lengths



Bond angles



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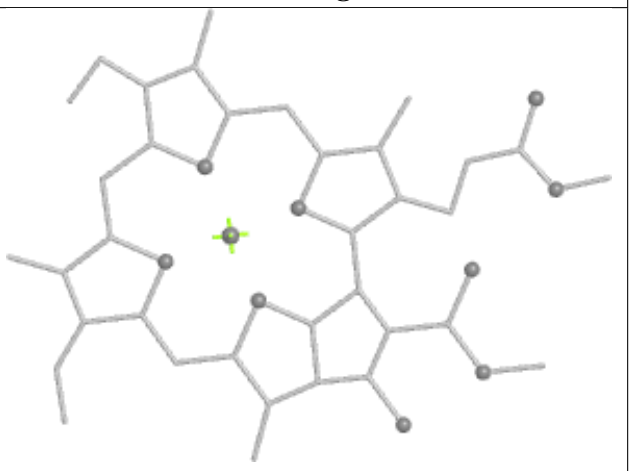
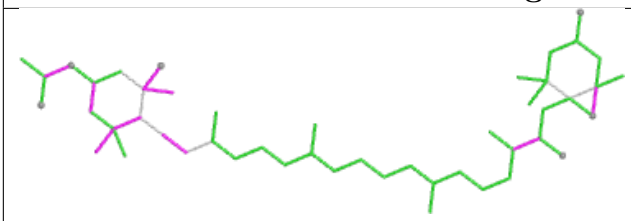


Rings

Ligand A86 17 302



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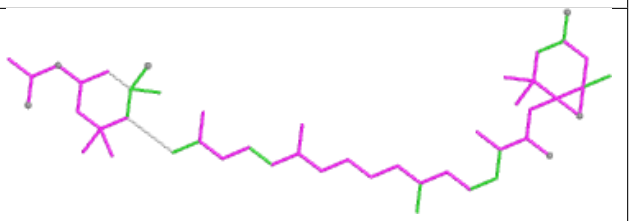

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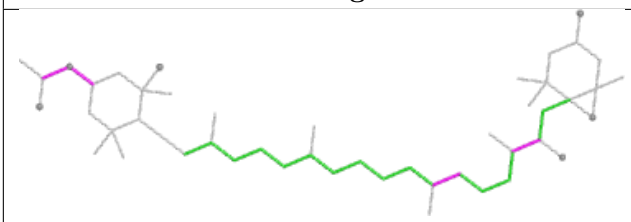

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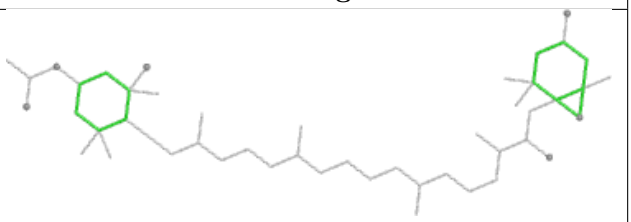
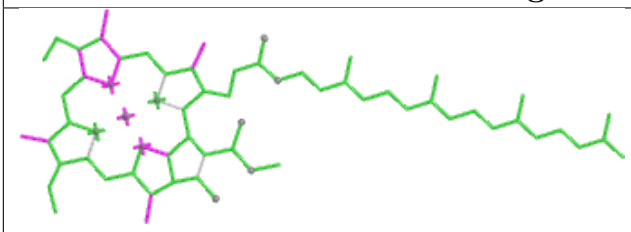


Rings

Ligand CLA b 613



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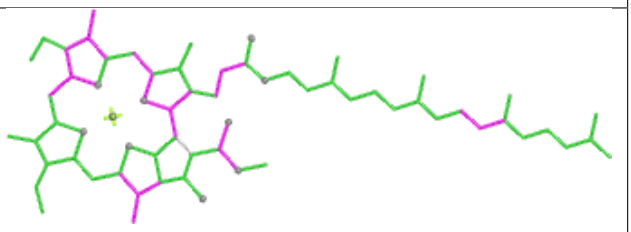
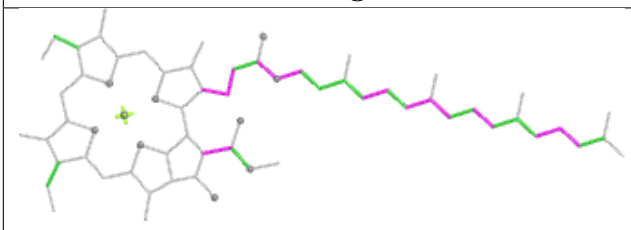


Bond angles



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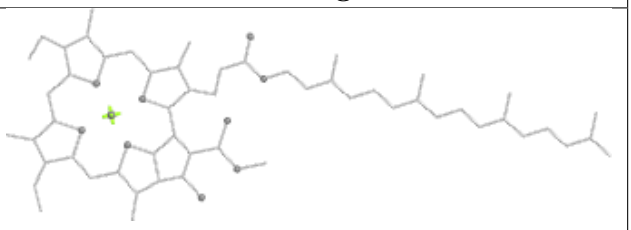
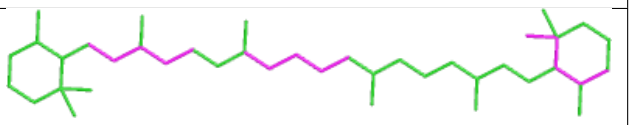


Rings

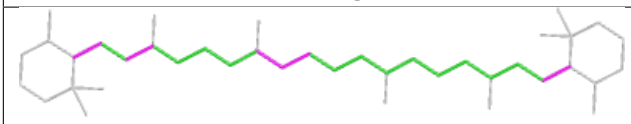
Ligand BCR a 407



Bond lengths



Bond angles



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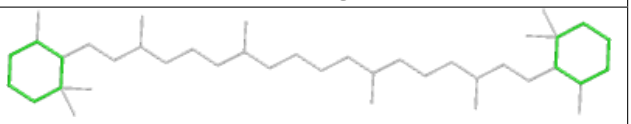
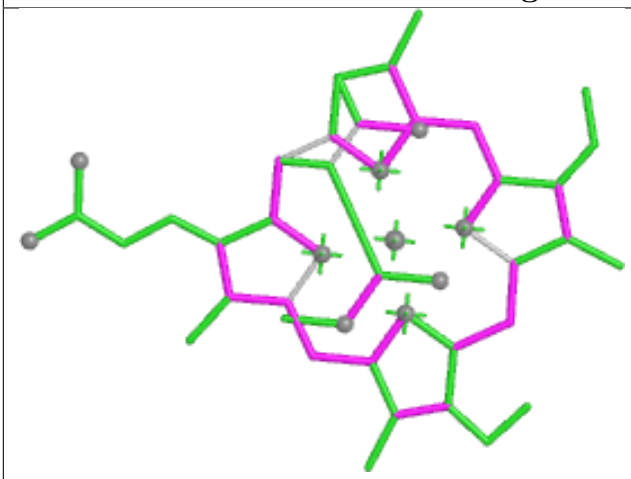


Rings

Ligand KC1 17 314



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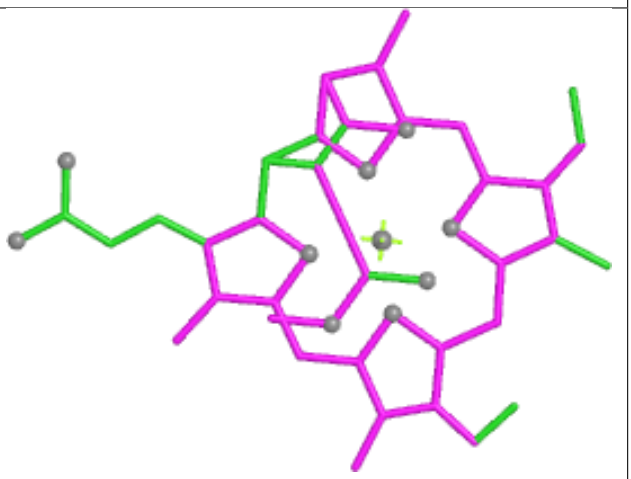
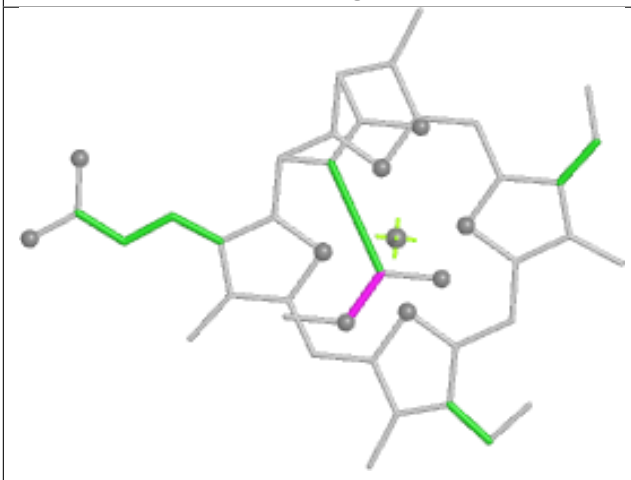


Bond angles



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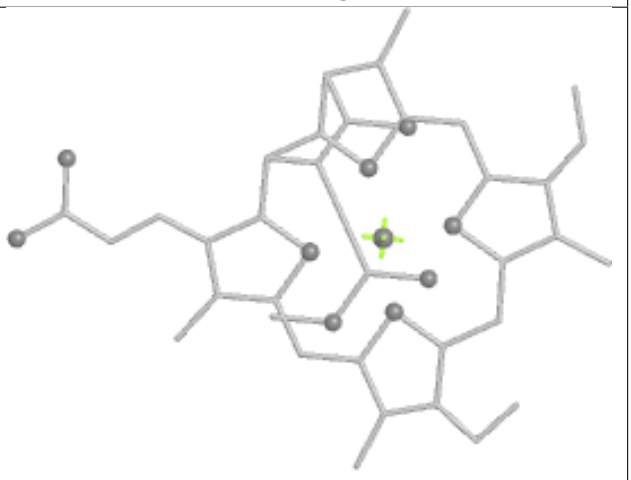
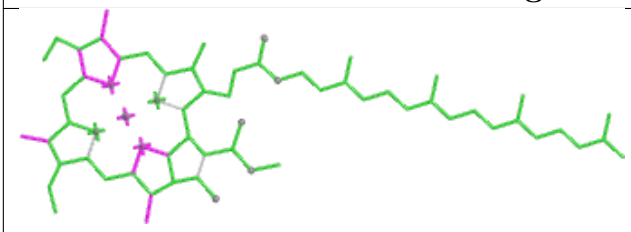


Rings

Ligand CLA P 601



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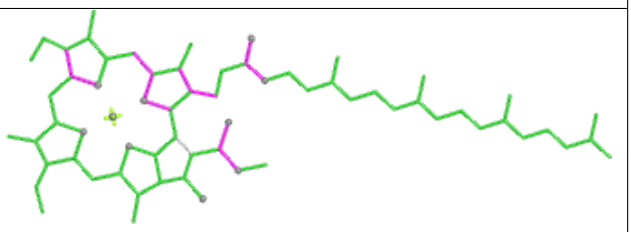

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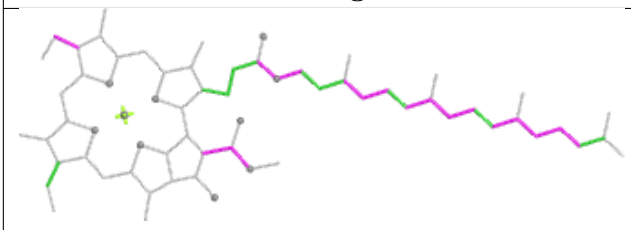

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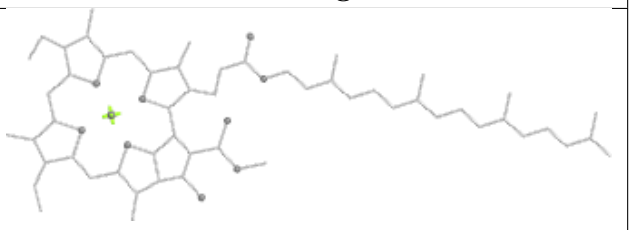
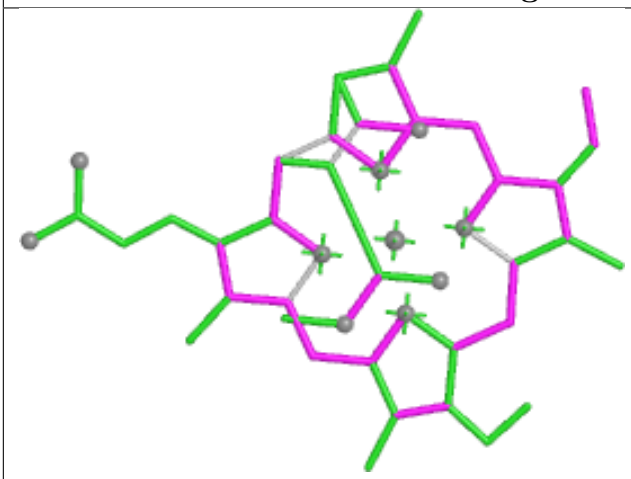


Rings

Ligand KC2 16 311



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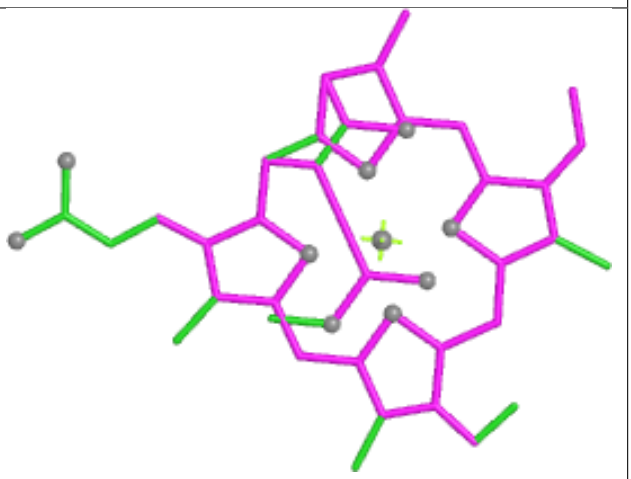

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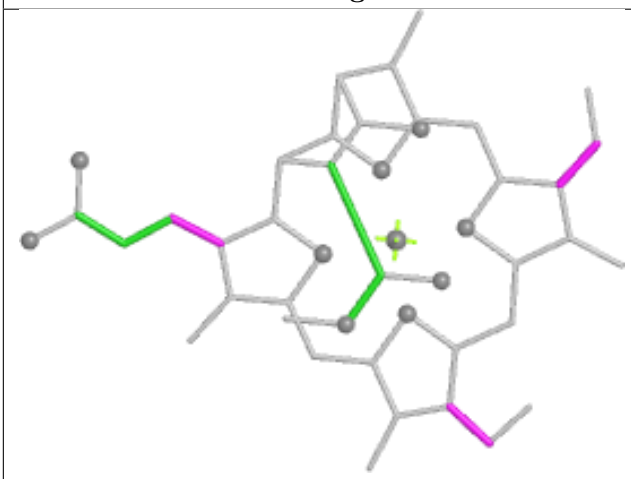

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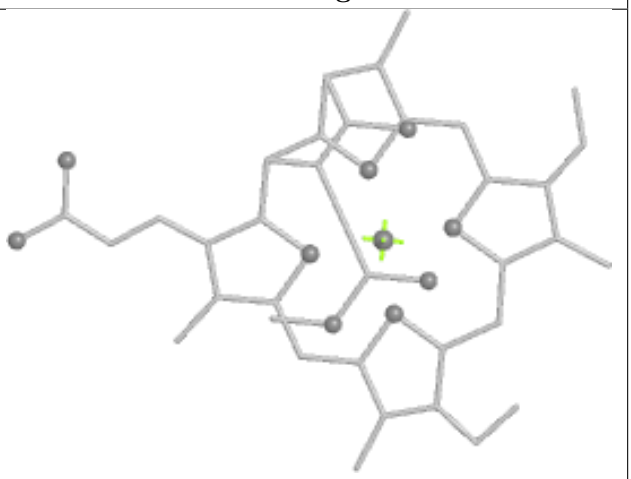
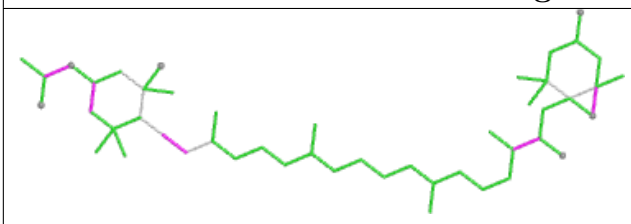


Rings

Ligand A86 4 306



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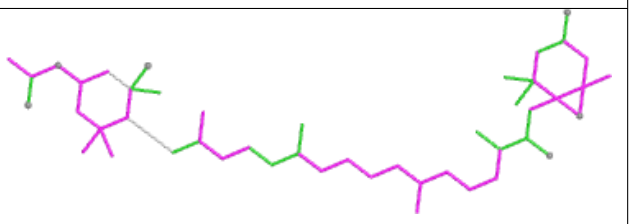
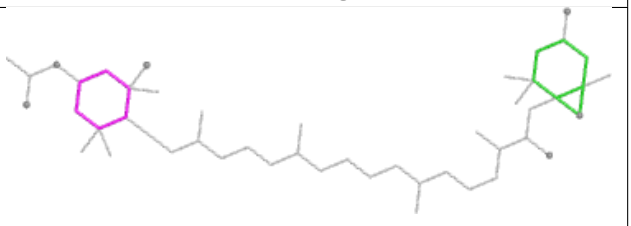


Bond angles

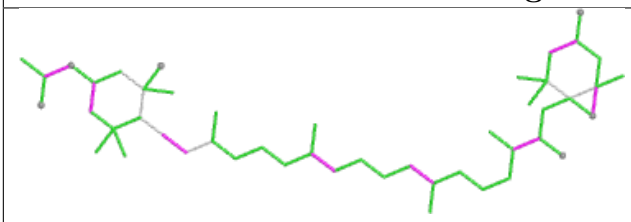


Torsions



Rings

Ligand A86 14 305



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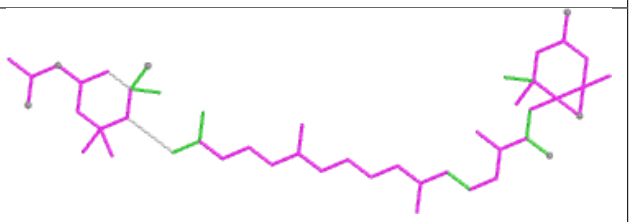
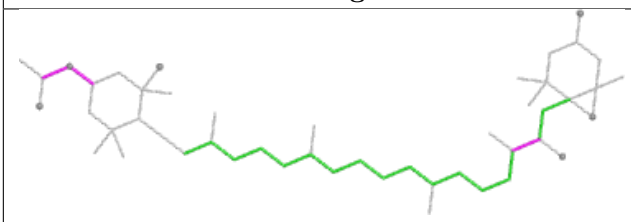


Bond angles



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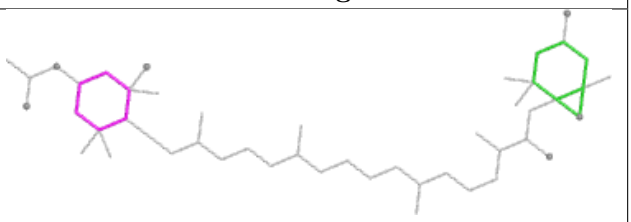
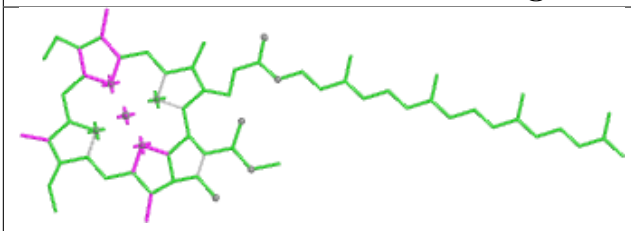


Rings

Ligand CLA b 615



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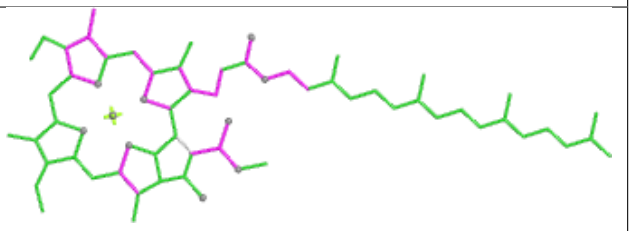
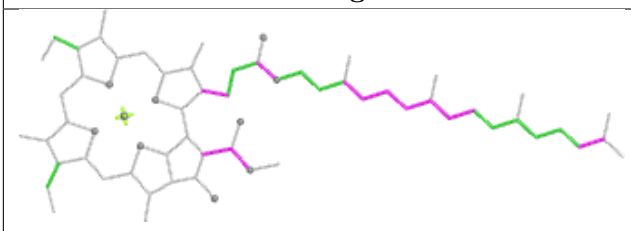


Bond angles



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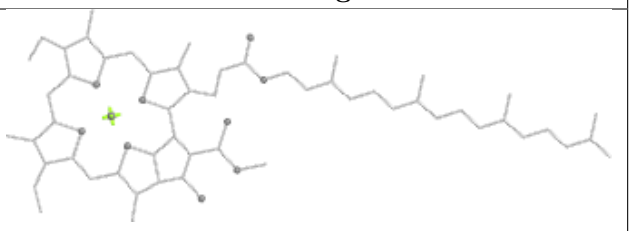
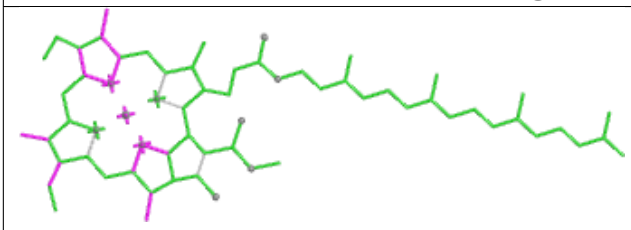


Rings

Ligand CLA c 505



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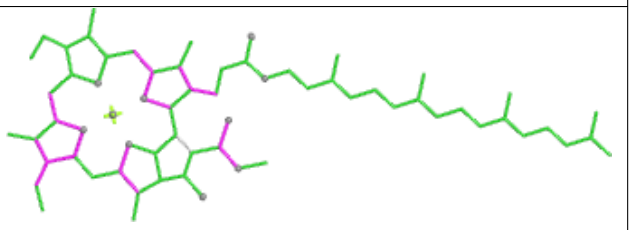
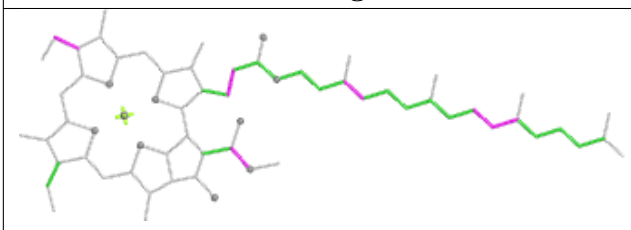


Bond angles



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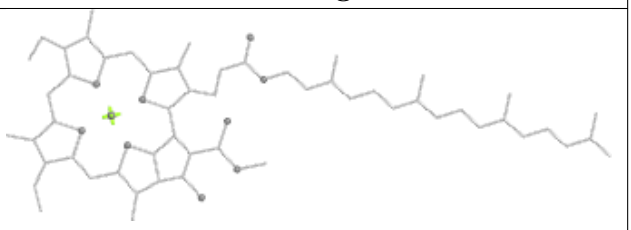
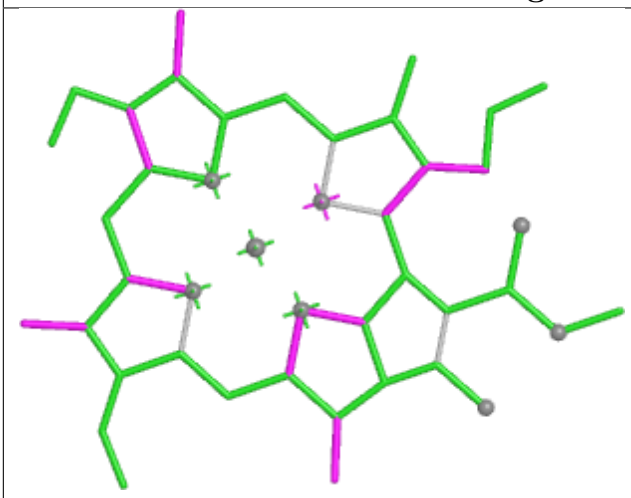


Rings

Ligand CLA p 606



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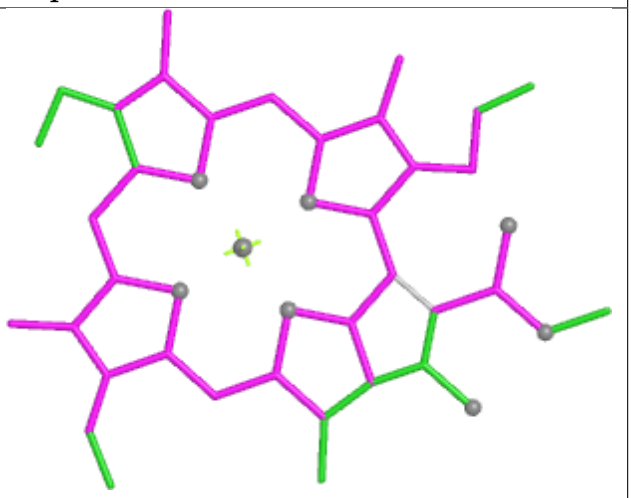
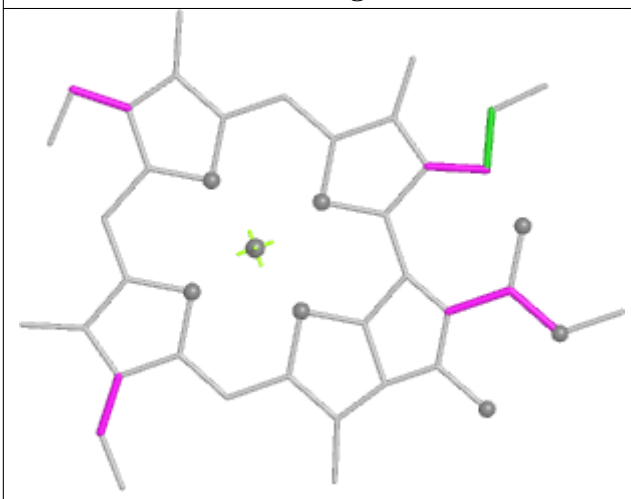


Bond angles



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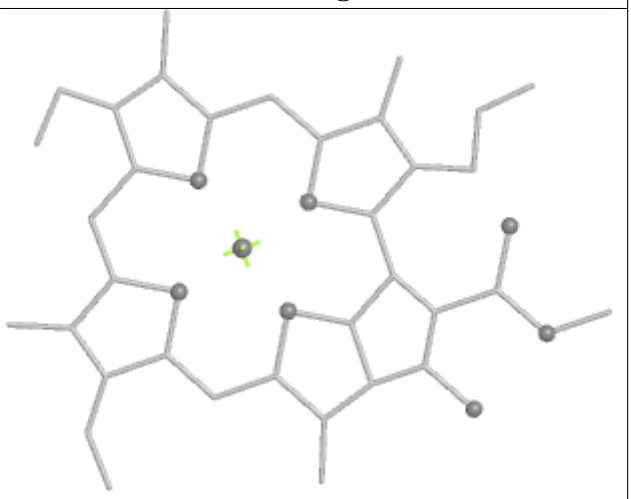
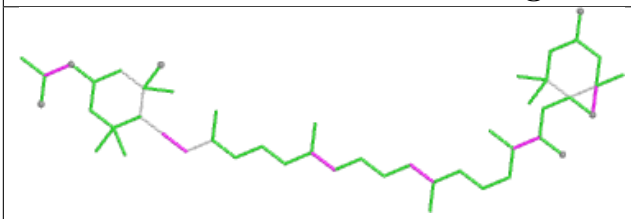


Rings

Ligand A86 16 304



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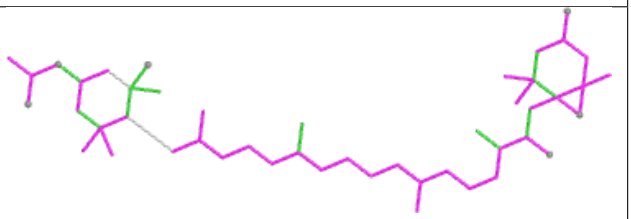
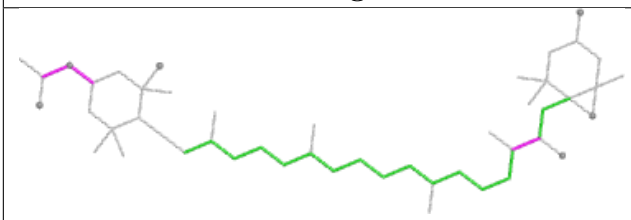


Bond angles



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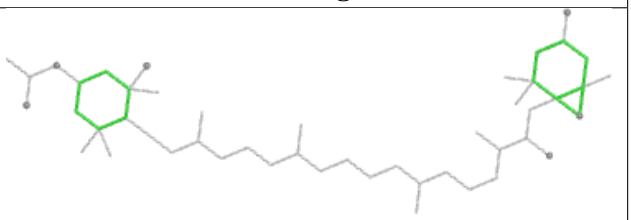
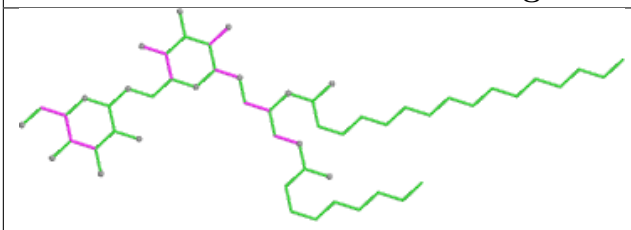
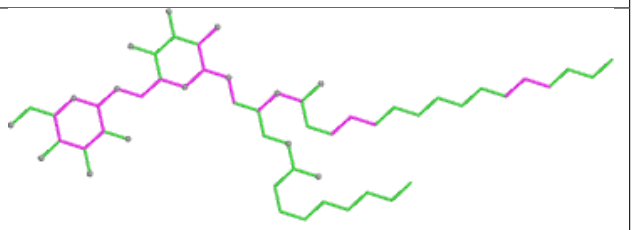


Rings

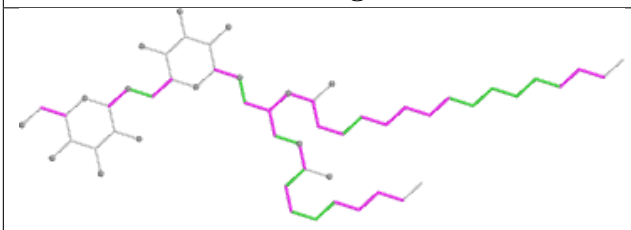
Ligand DGD b 622



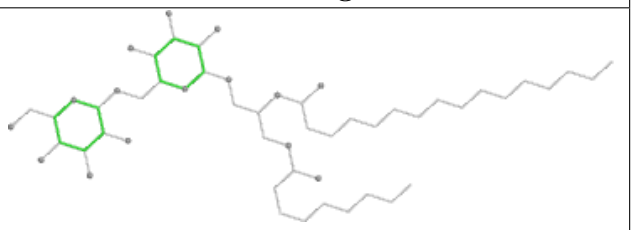
Bond lengths



Bond angles

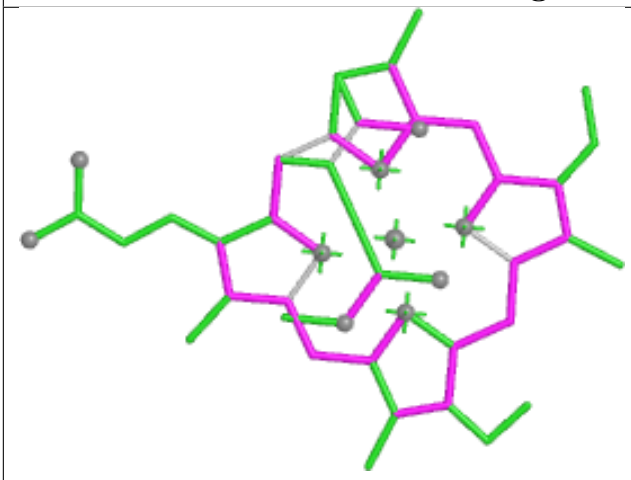


Torsions



Rings

Ligand KC1 9 314



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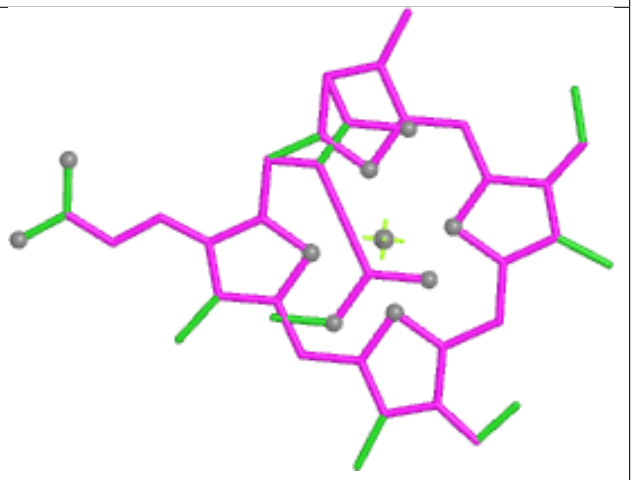

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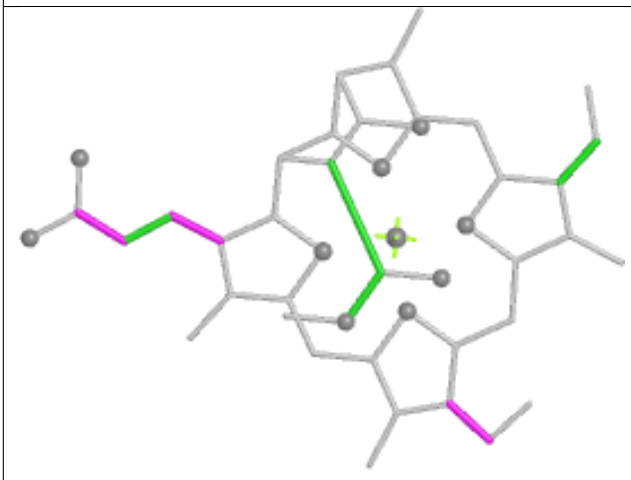

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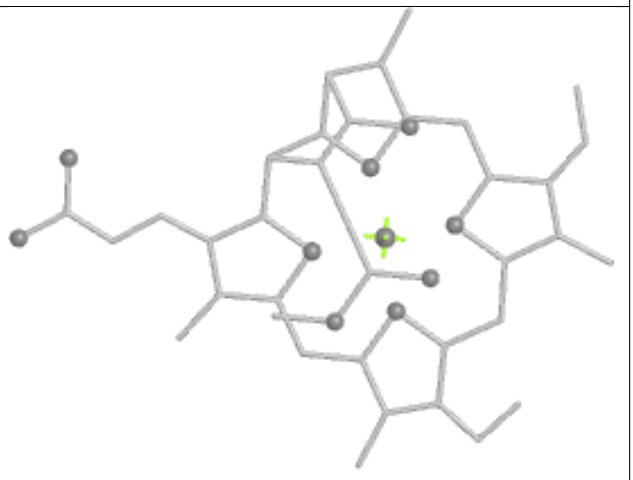

Rings

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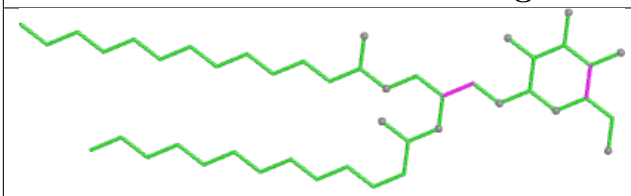
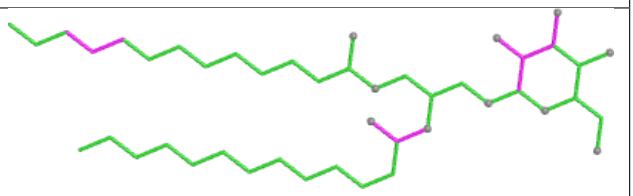
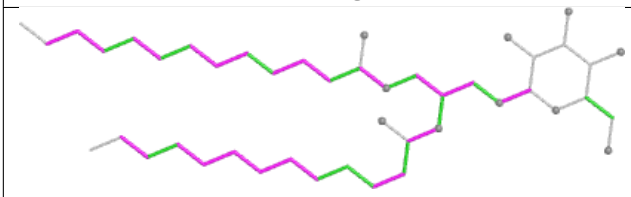
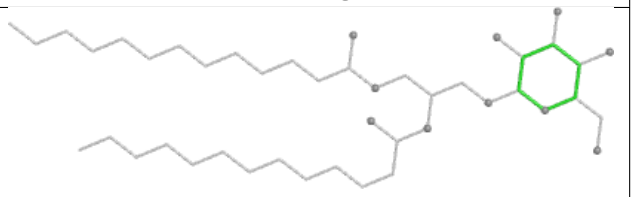
 Bond lengths	 Bond angles
 Torsions	 Rings

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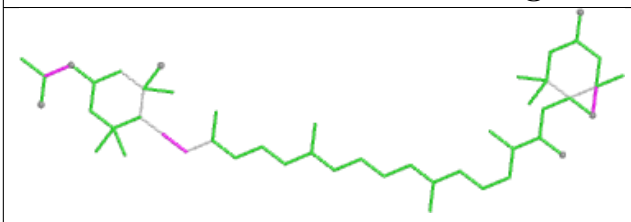
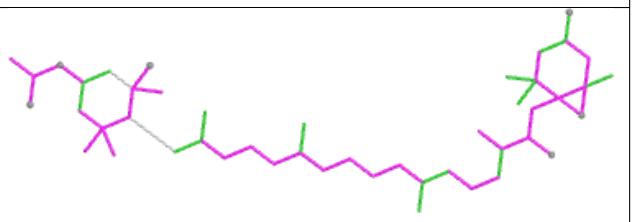
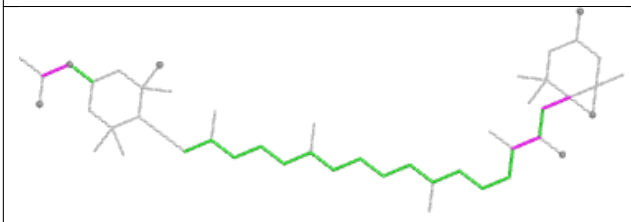
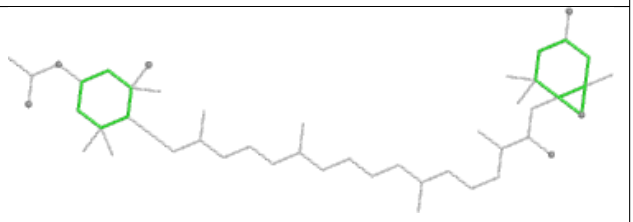
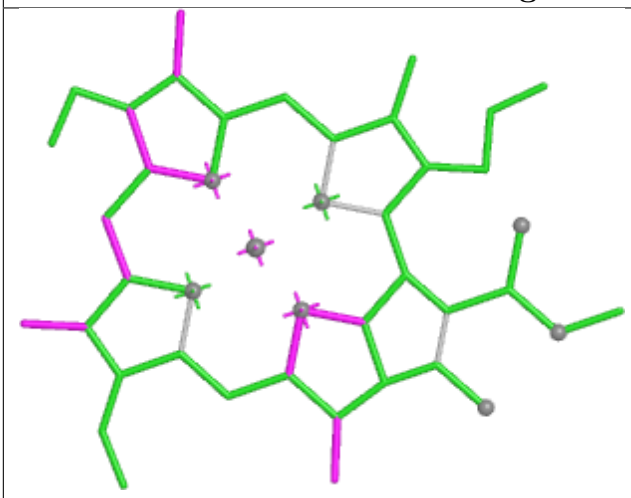
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 13 308



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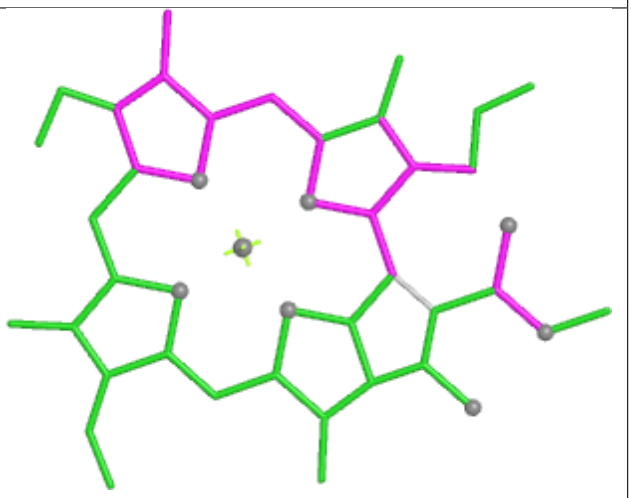
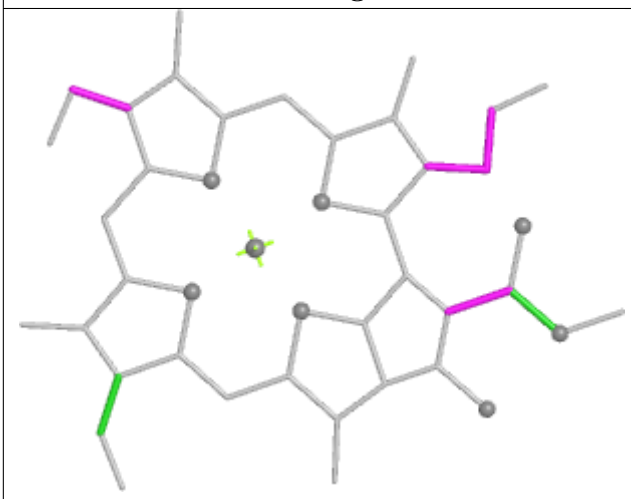


Bond angles



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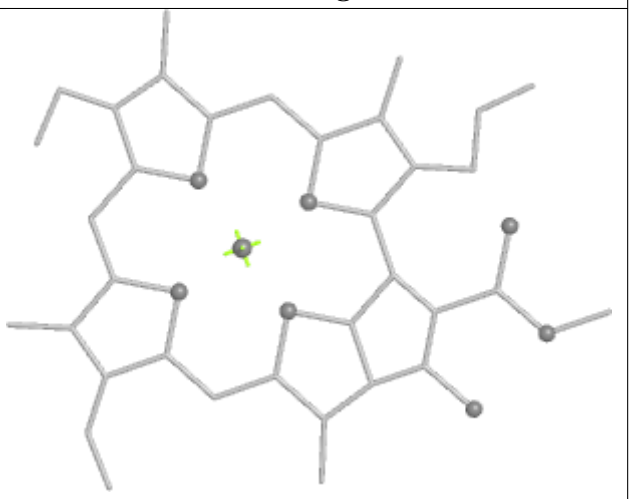
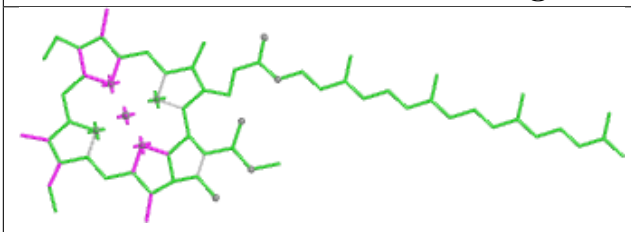


Rings

Ligand CLA c 511



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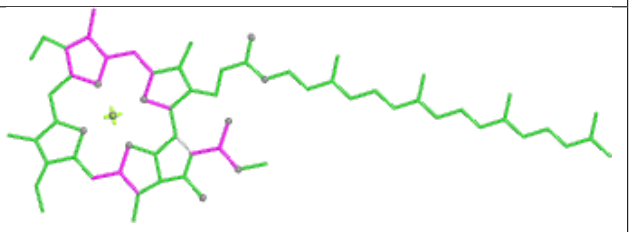

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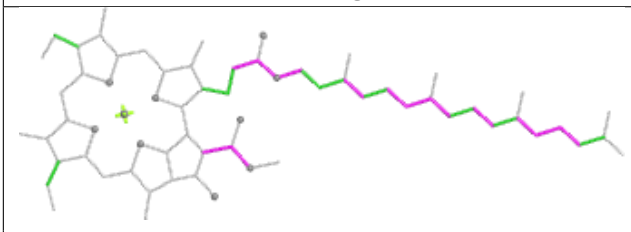

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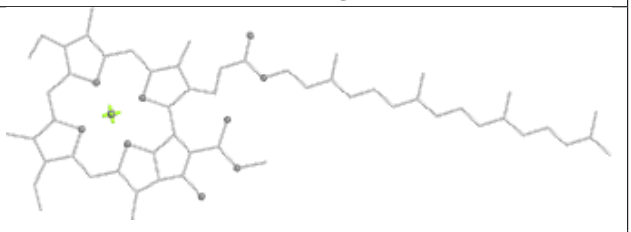

Rings

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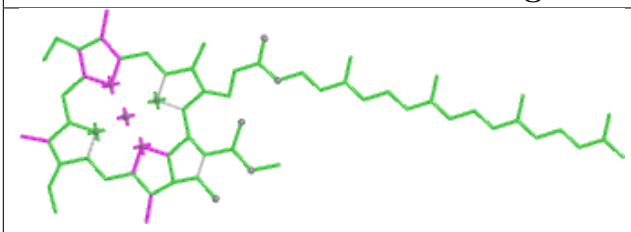

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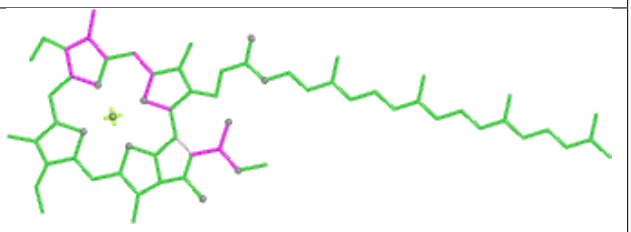

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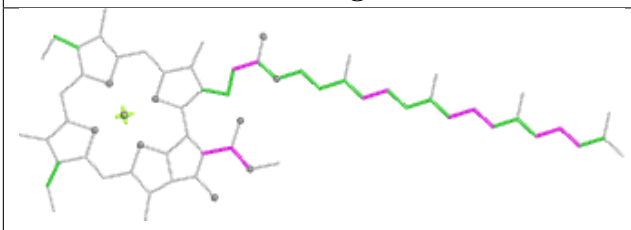

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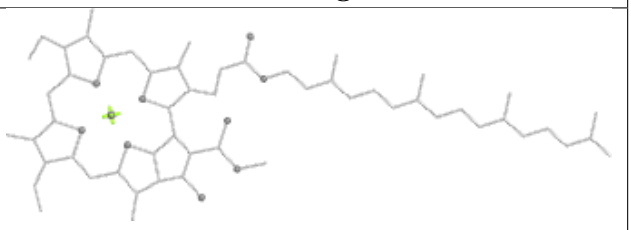
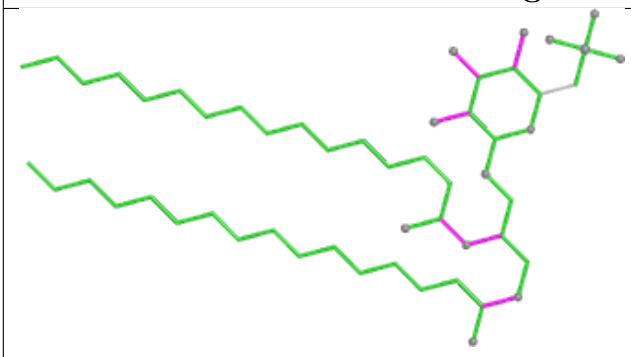


Rings

Ligand SQD A 408



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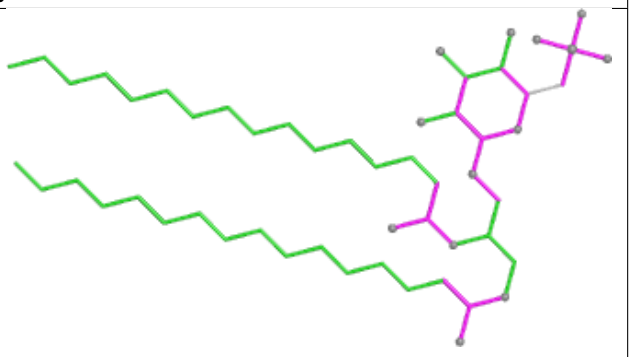

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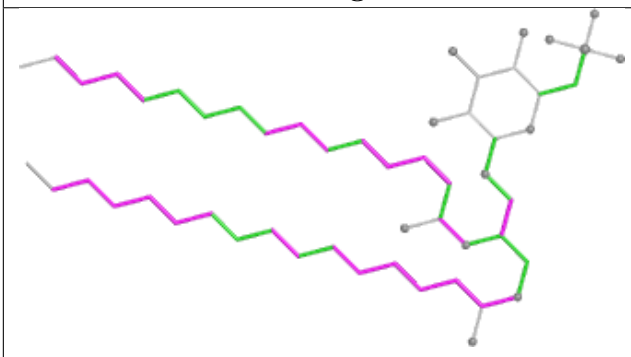

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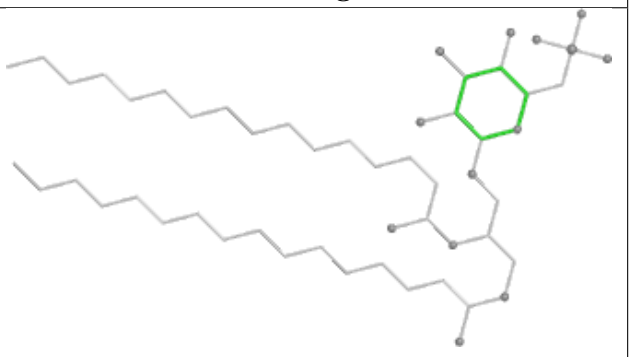
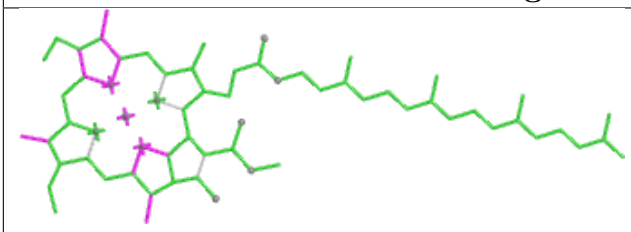


Rings

Ligand CLA C 510



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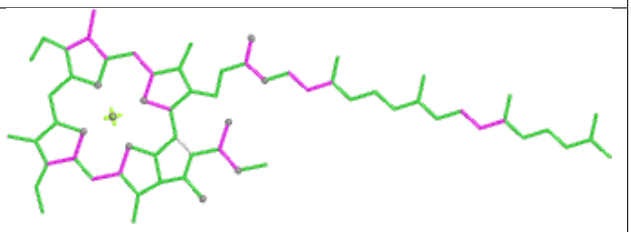

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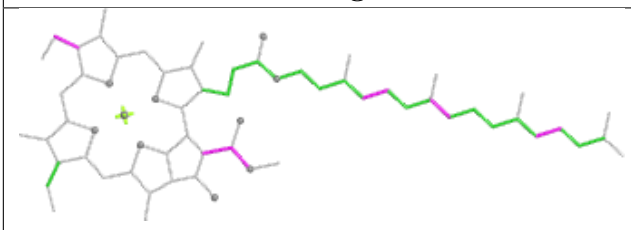

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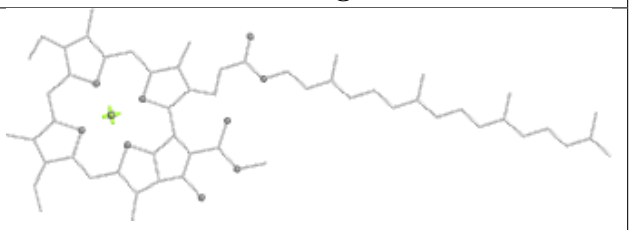
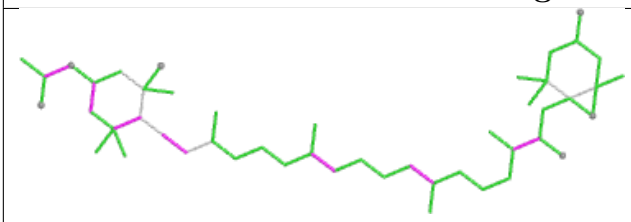


Rings

Ligand A86 8 302



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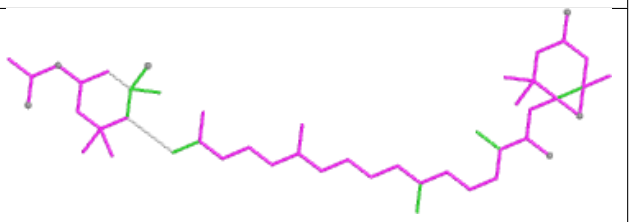

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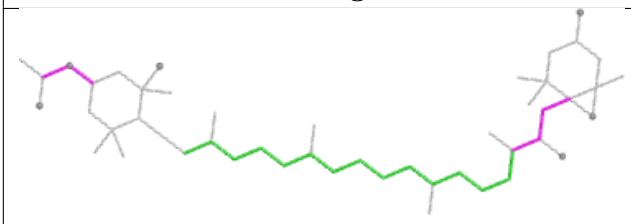

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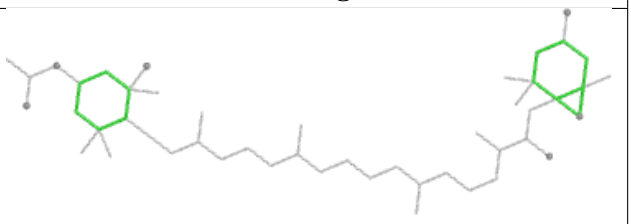
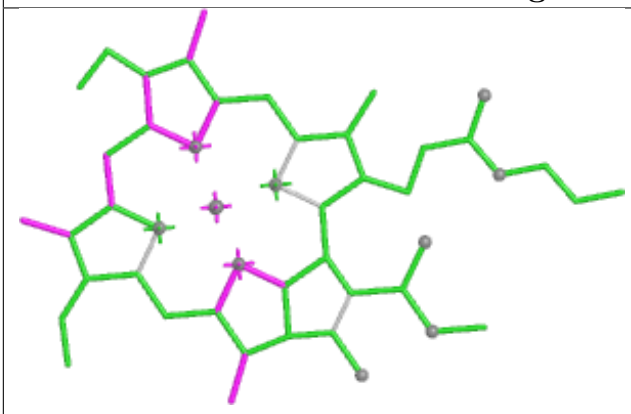


Rings

Ligand CLA 0 307



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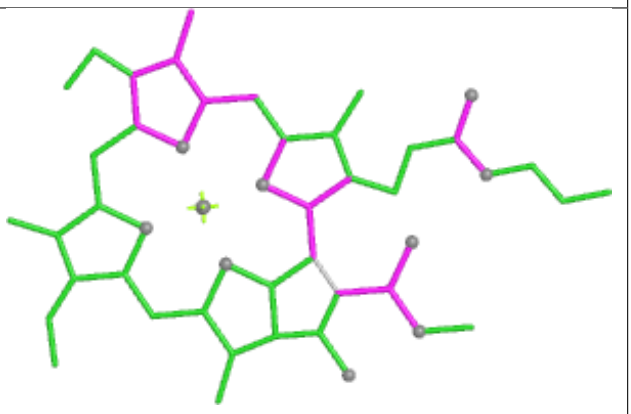

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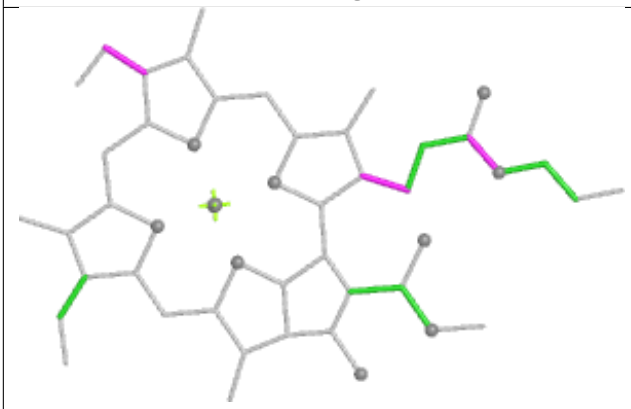

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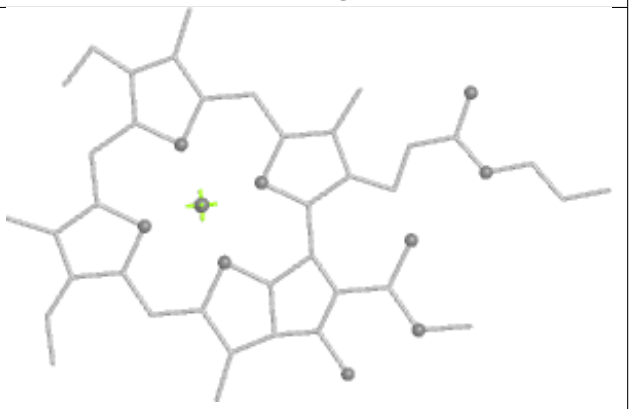
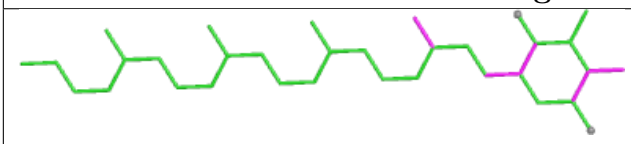


Rings

Ligand PL9 a 409



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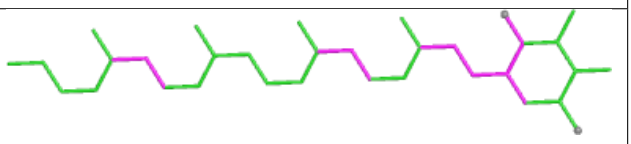

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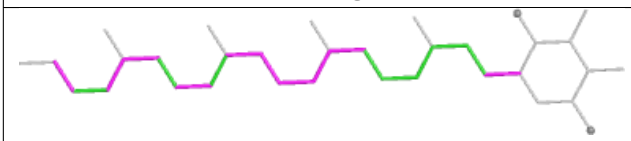

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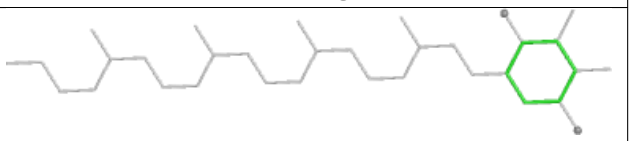
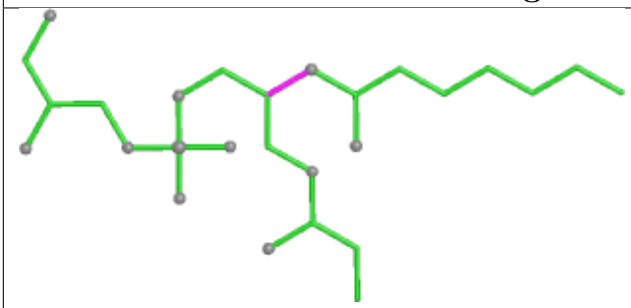


Rings

Ligand LHG P 615



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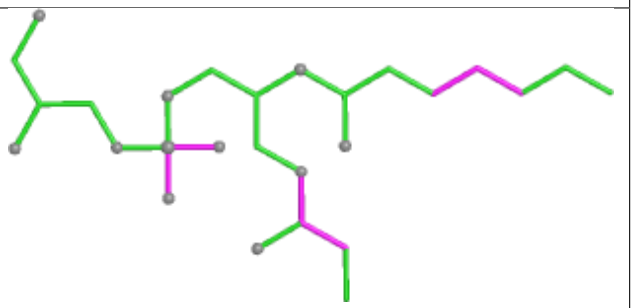

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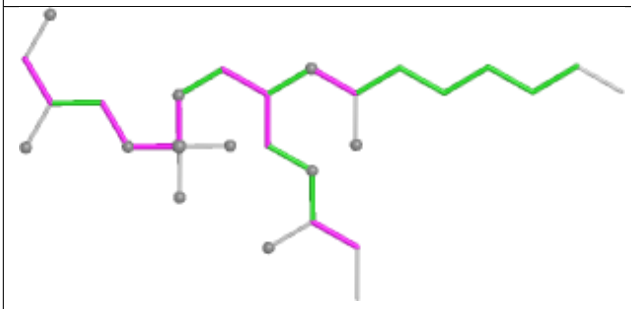

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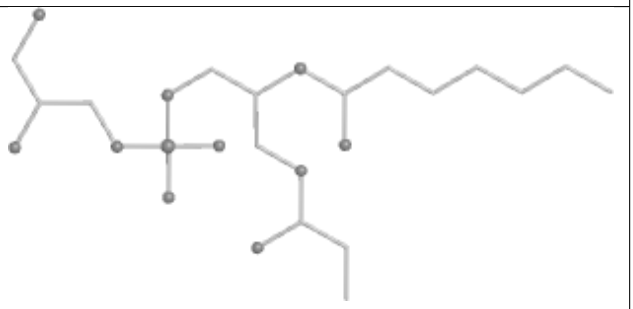
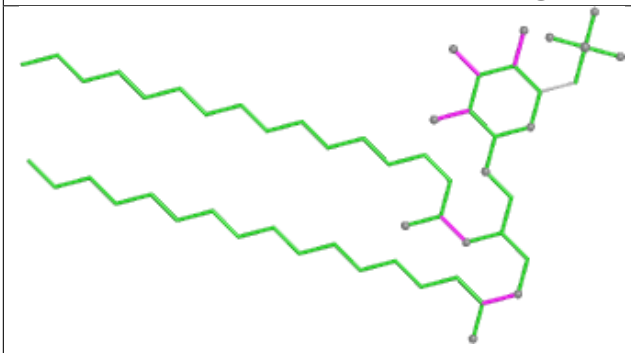


Rings

Ligand SQD l 101



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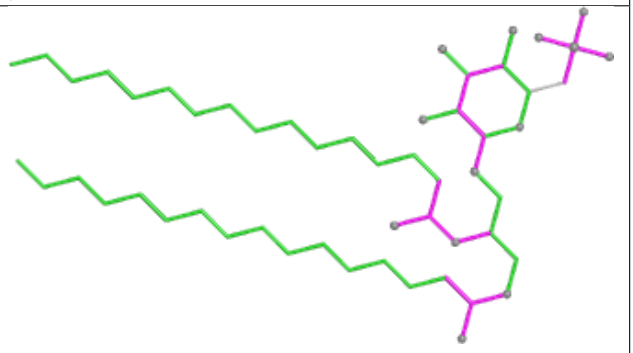
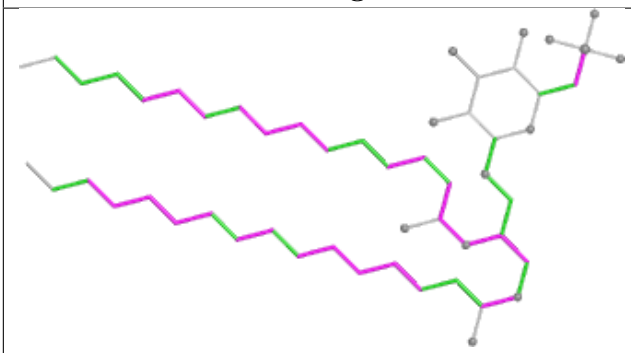


Bond angles



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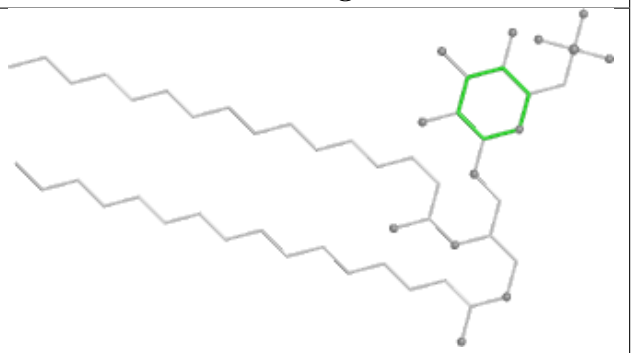
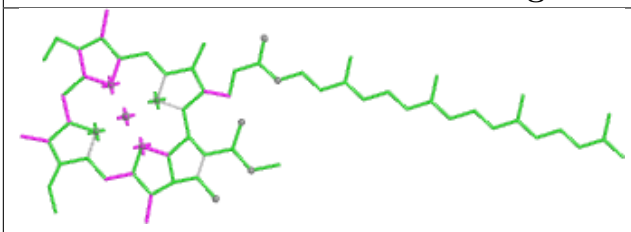


Rings

Ligand CLA d 405



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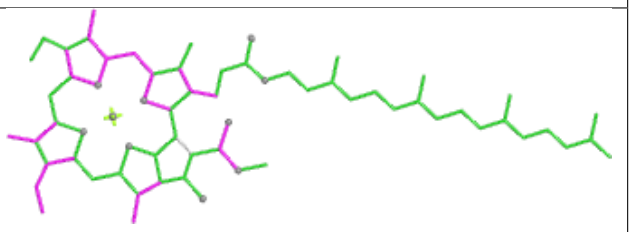
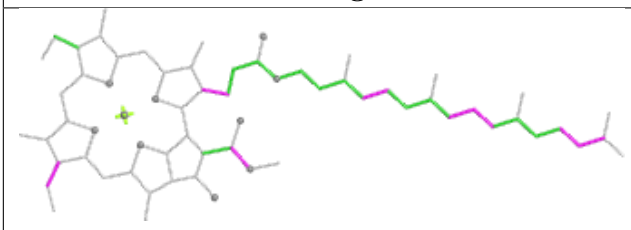


Bond angles



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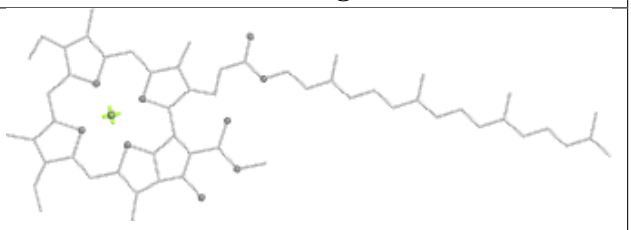
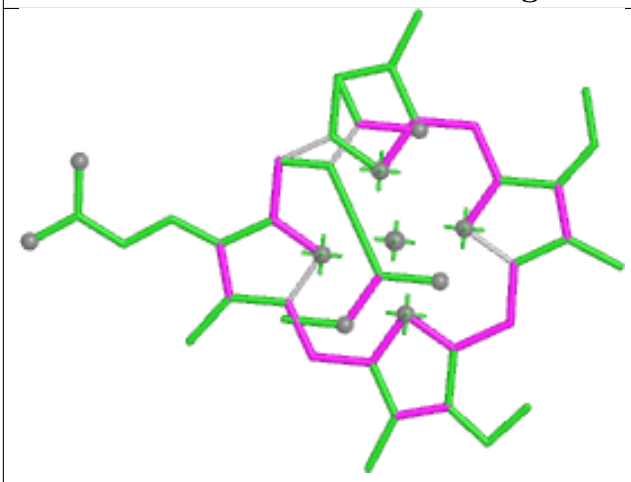
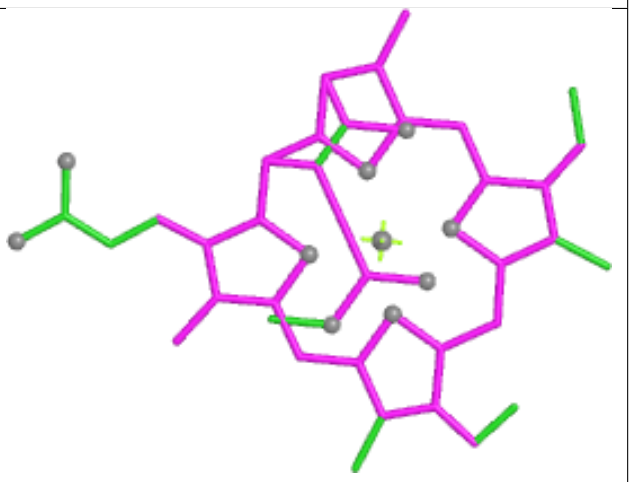


Rings

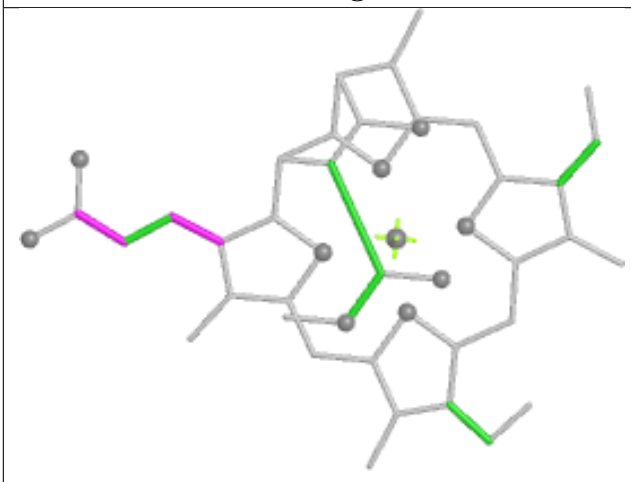
Ligand KC1 10 315



Bond lengths



Bond angles



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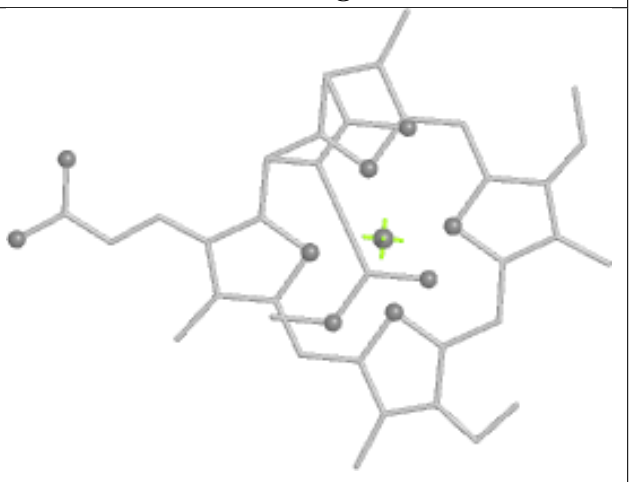
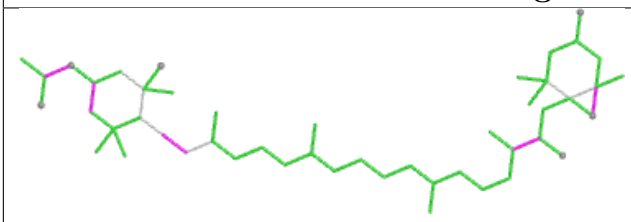


Rings

Ligand A86 3 302



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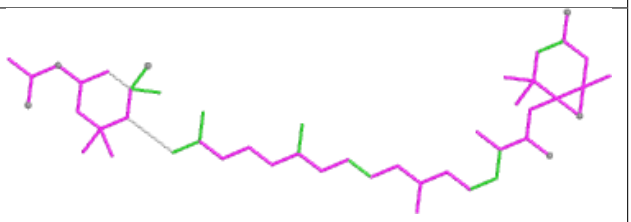

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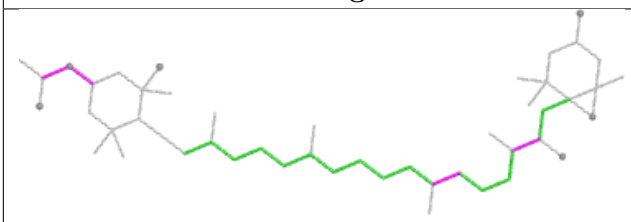

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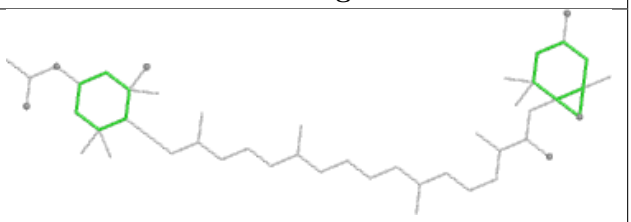

Rings

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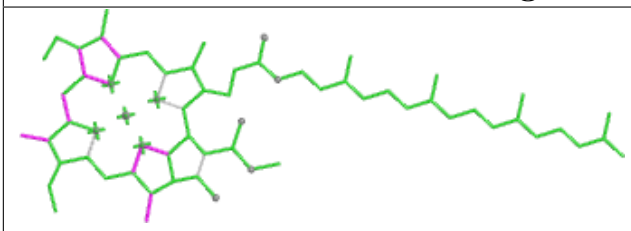

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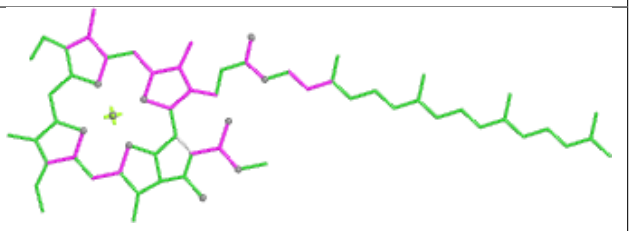

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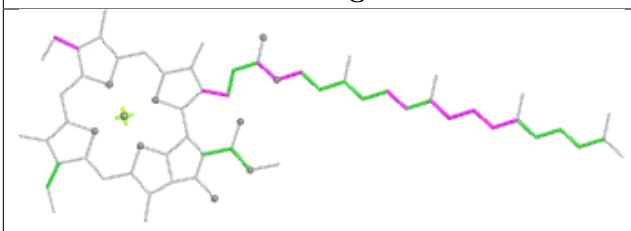

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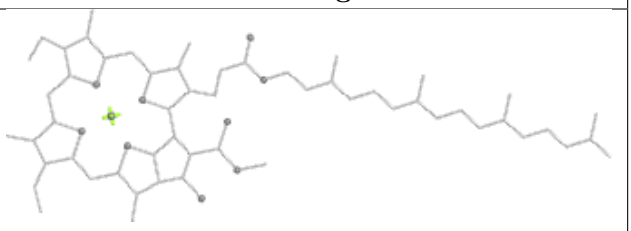
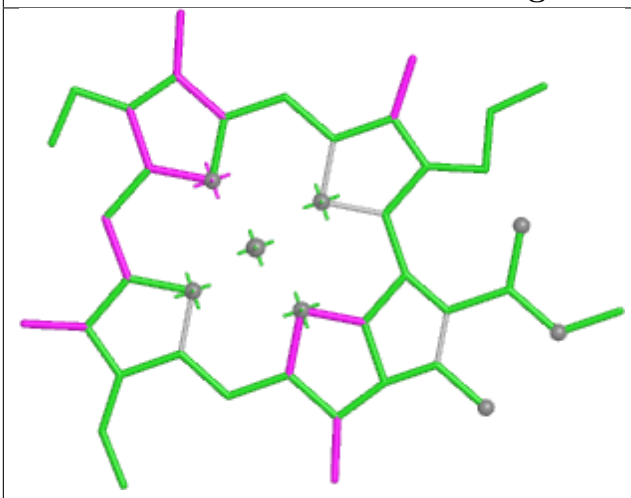


Rings

Ligand CLA 4 315



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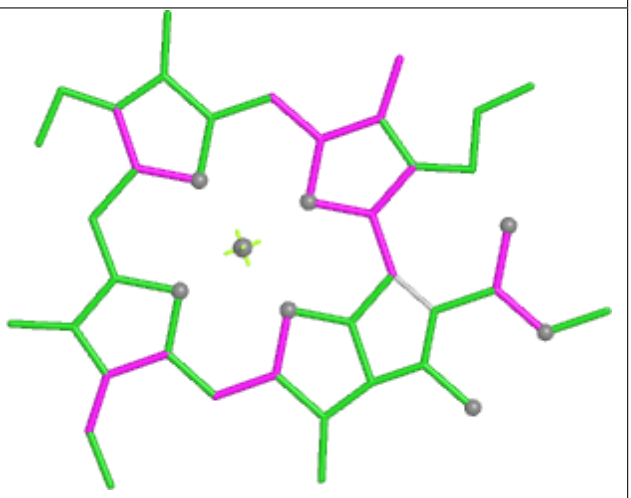

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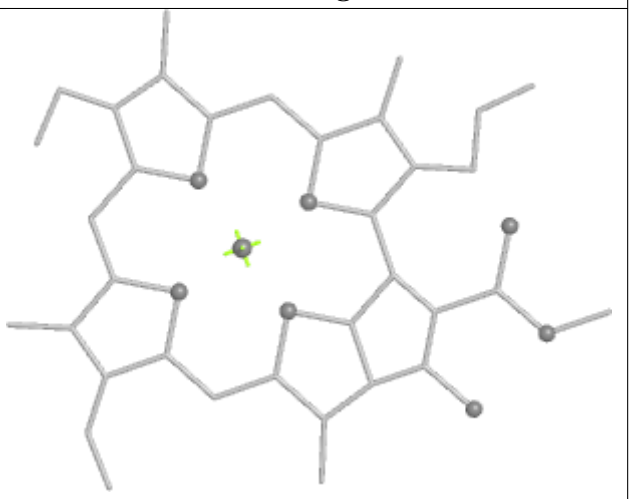
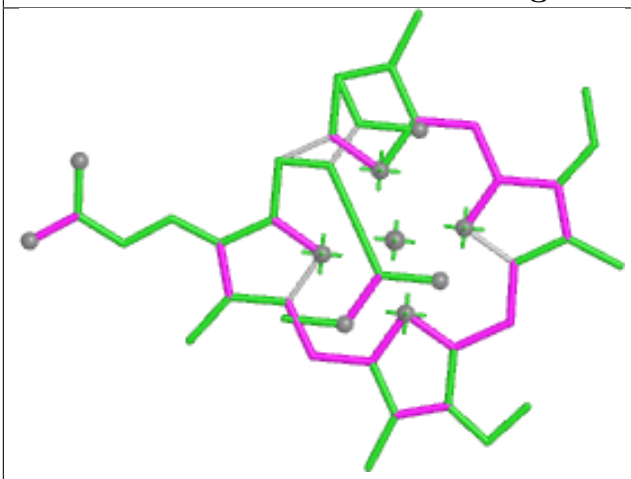


Rings

Ligand KC1 4 313



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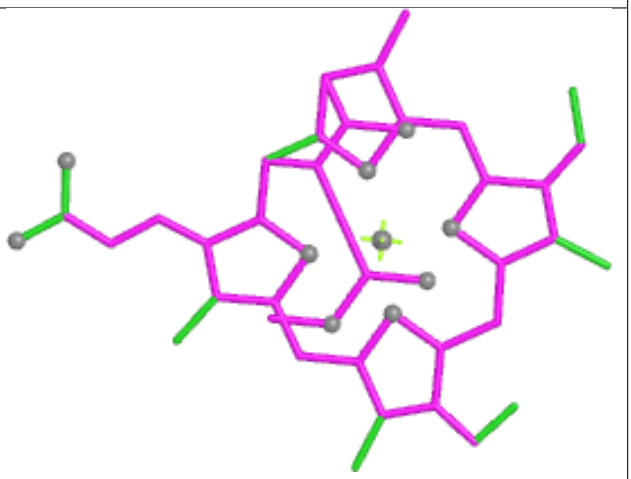

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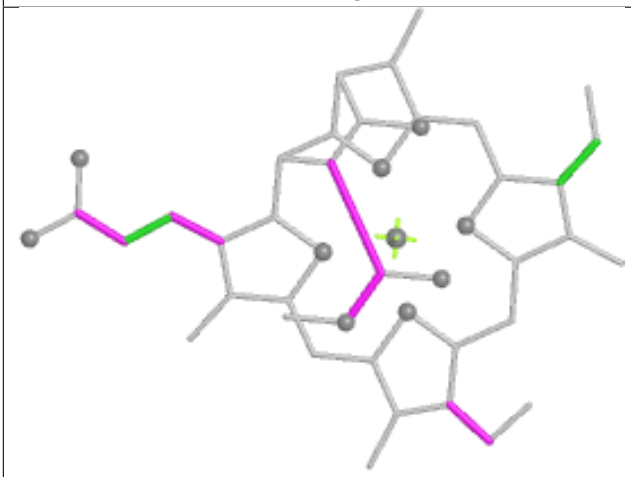

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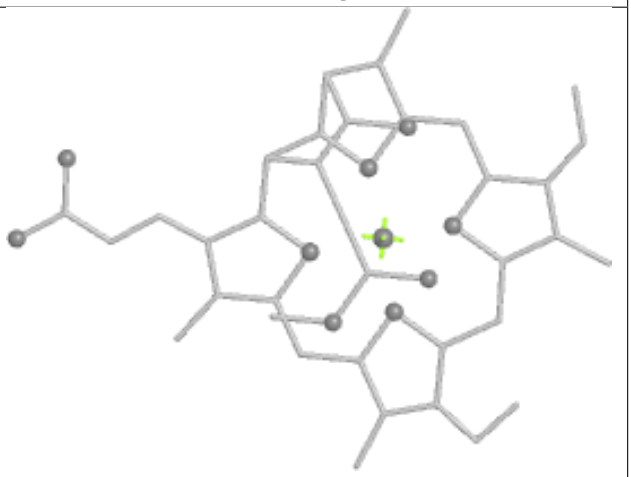
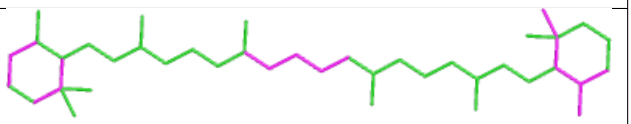


Rings

Ligand BCR H 101



Bond lengths



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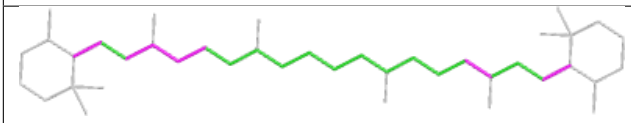

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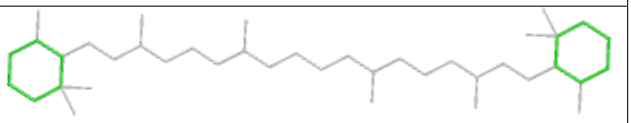
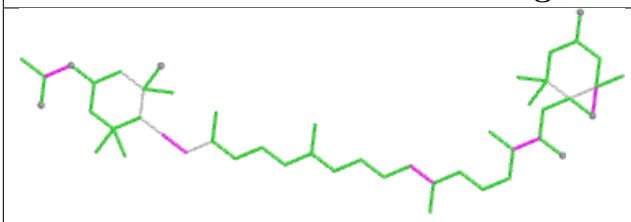


Rings

Ligand A86 1 304



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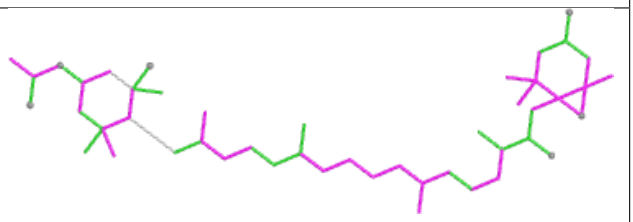

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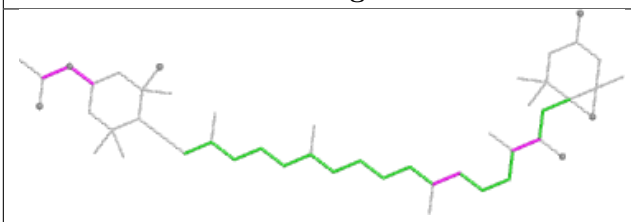

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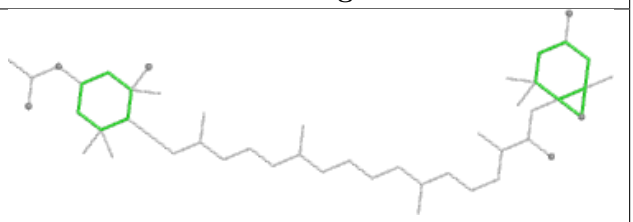
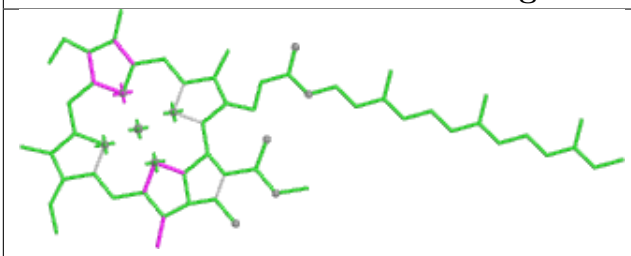


Rings

Ligand CLA 19 307



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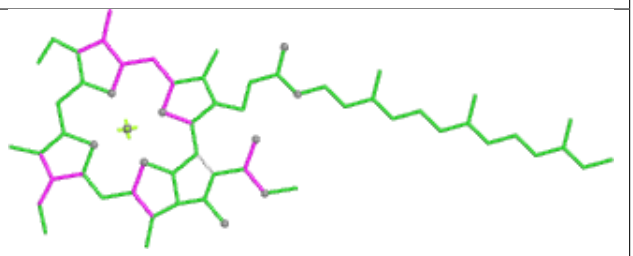

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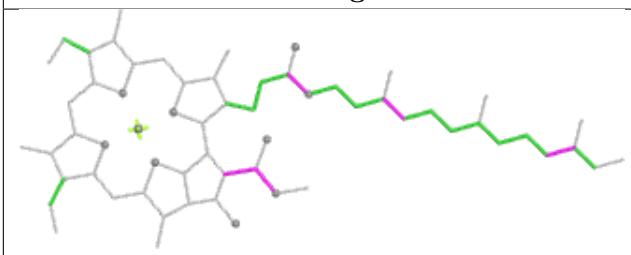

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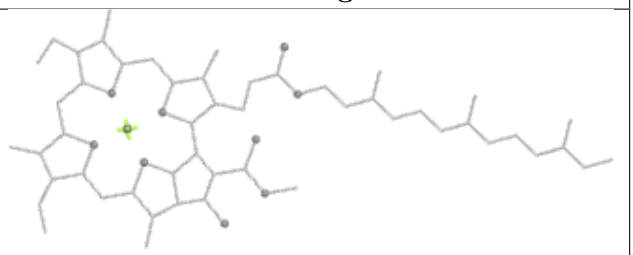
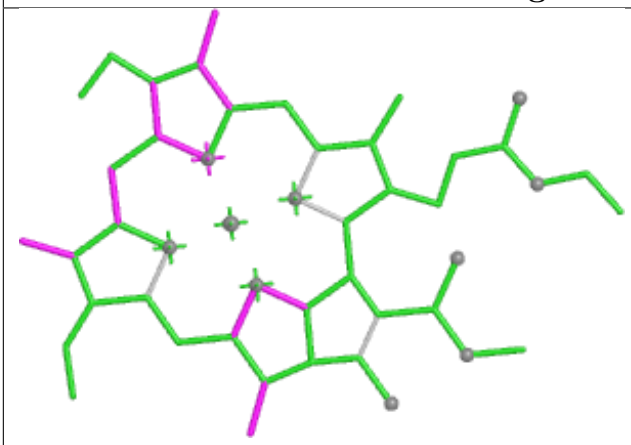


Rings

Ligand CLA 7 312



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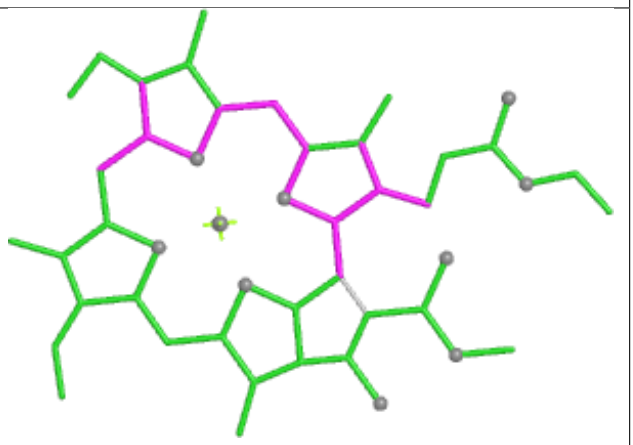

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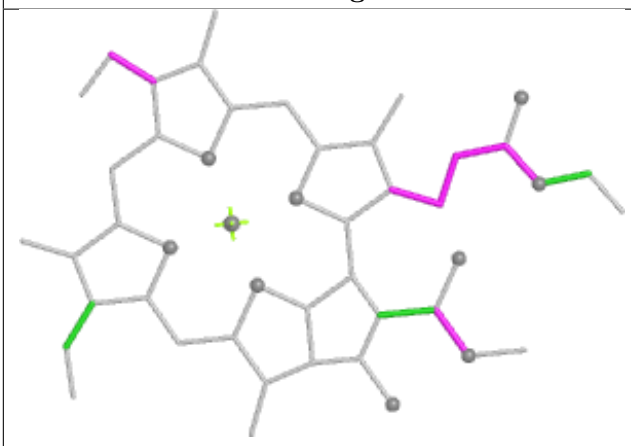

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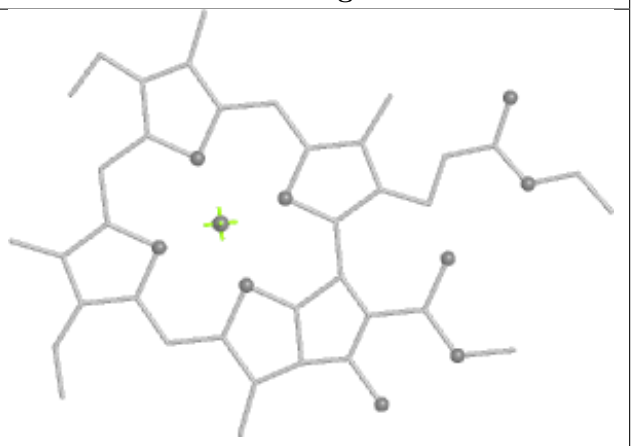

Rings

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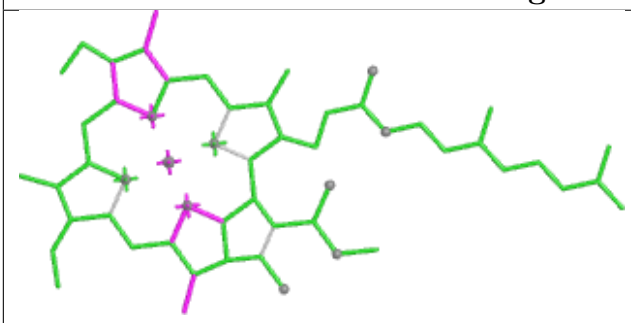

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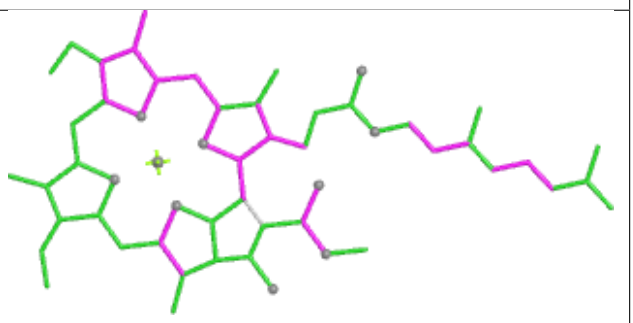
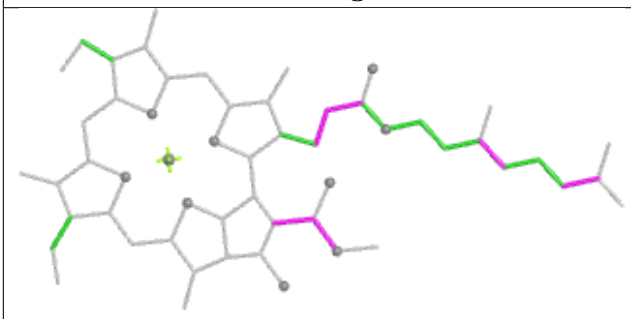


Bond angles



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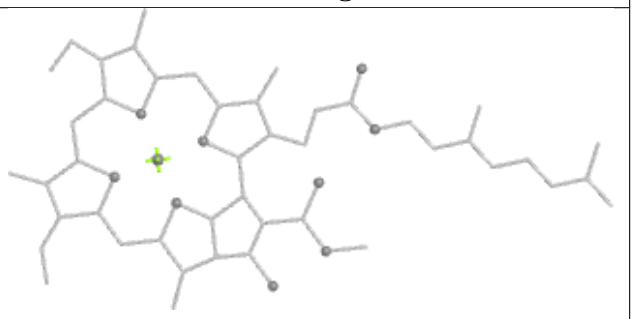

Rings

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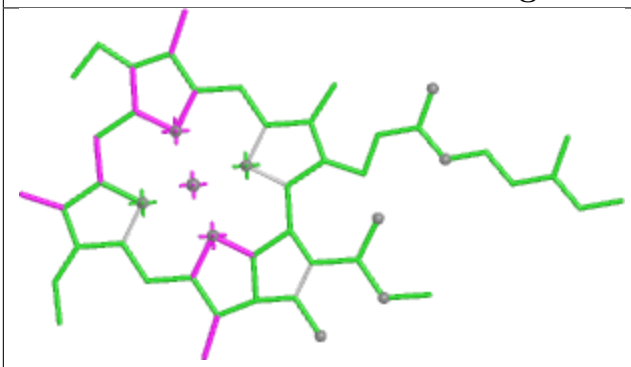

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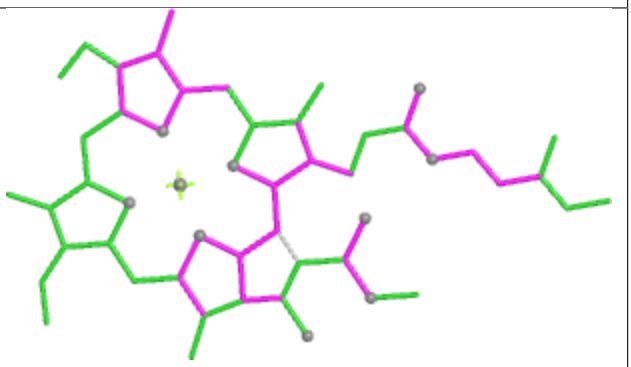

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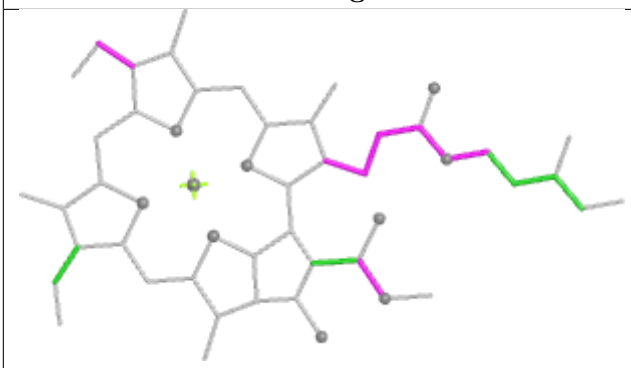

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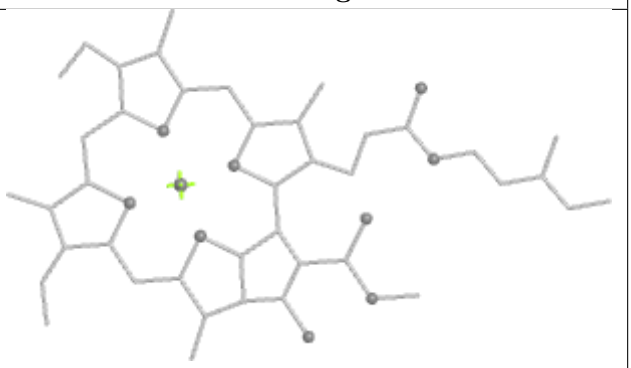
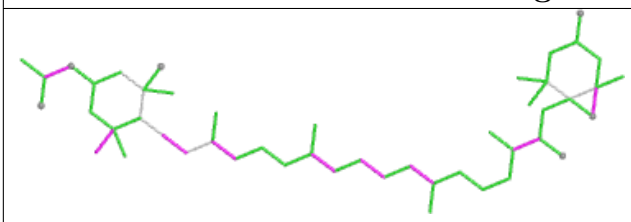


Rings

Ligand A86 3 301



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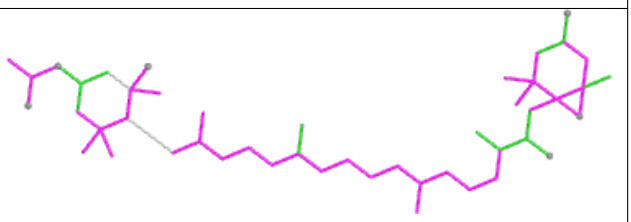

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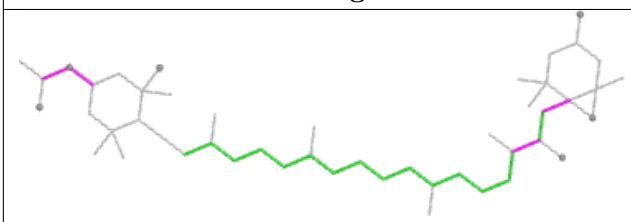

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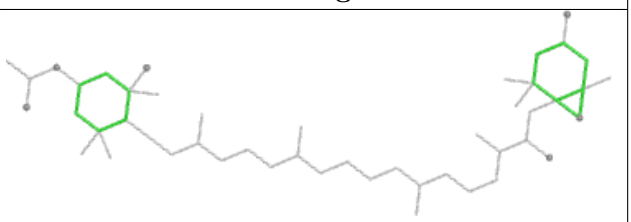
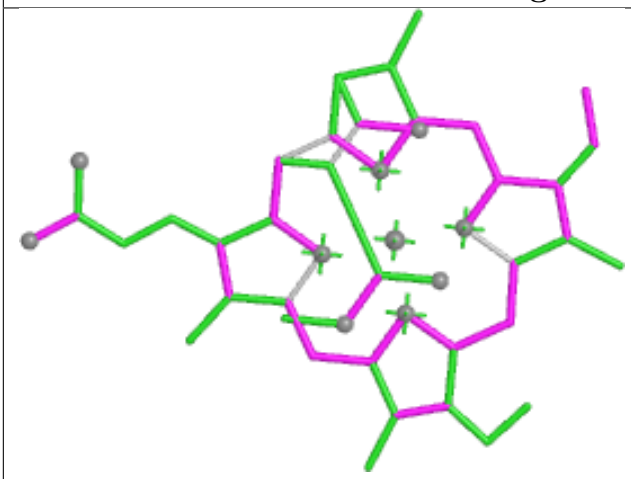


Rings

Ligand KC2 8 309



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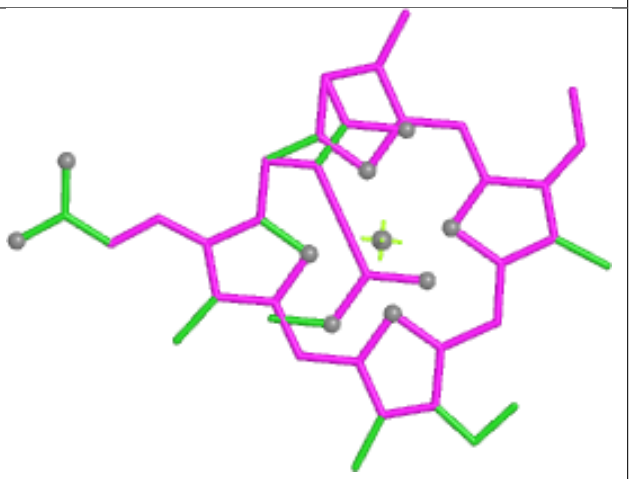

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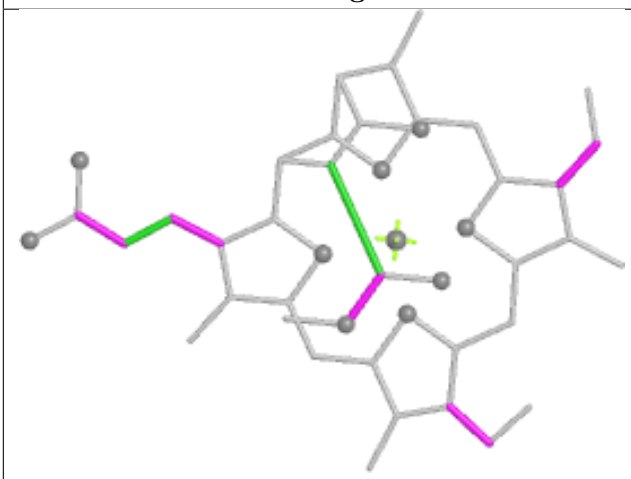

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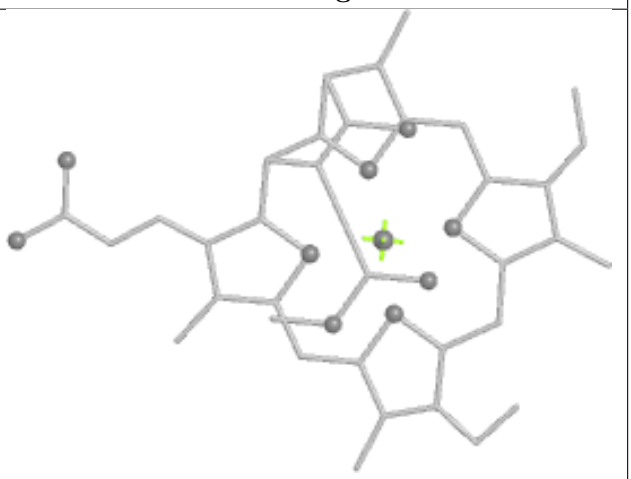
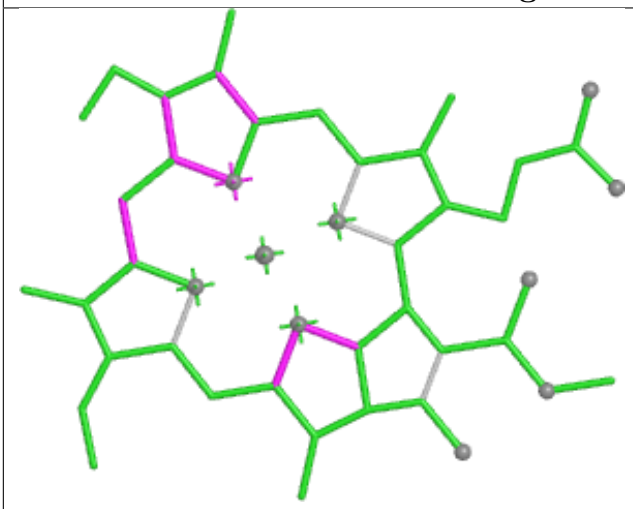


Rings

Ligand CLA 17 310



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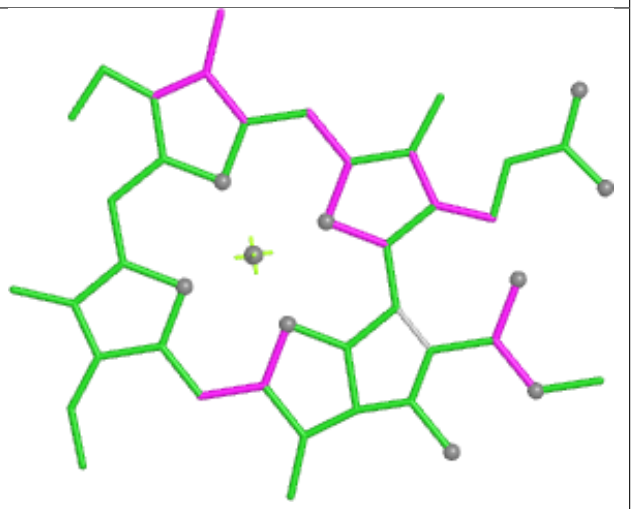

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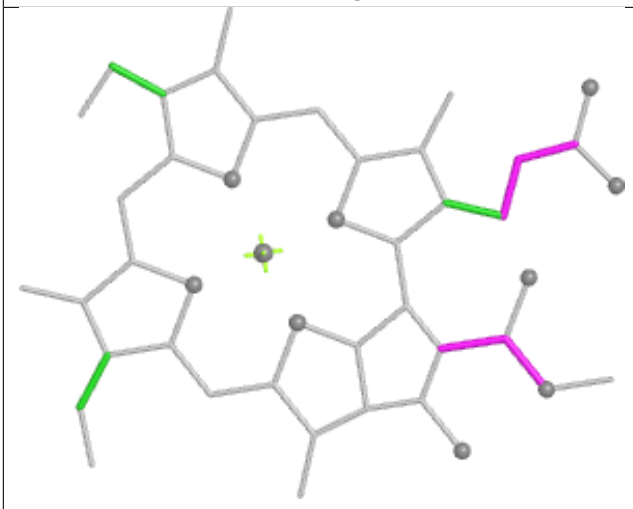
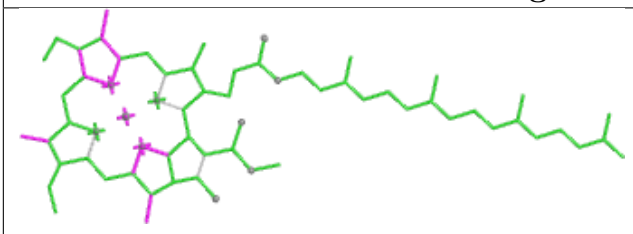


Torsions



Rings

Ligand CLA c 508



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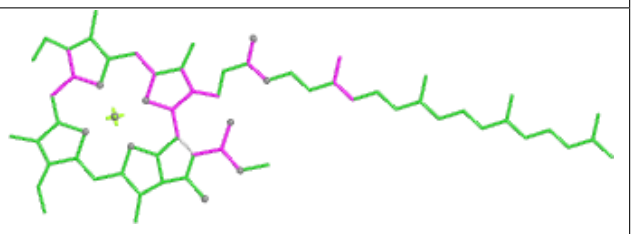
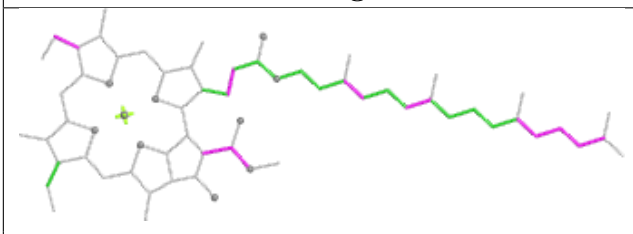


Bond angles



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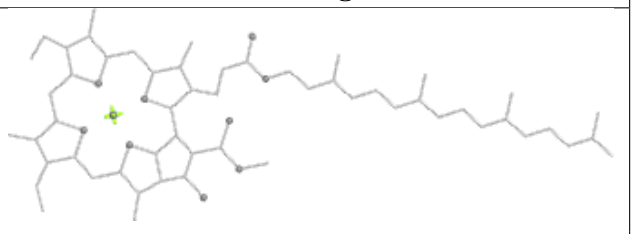
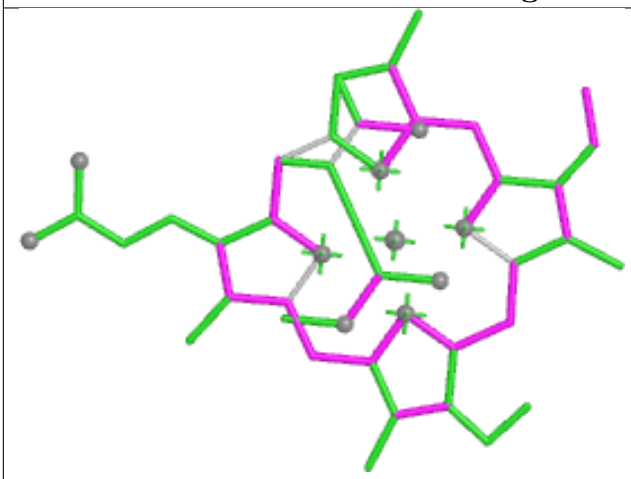


Rings

Ligand KC2 10 310



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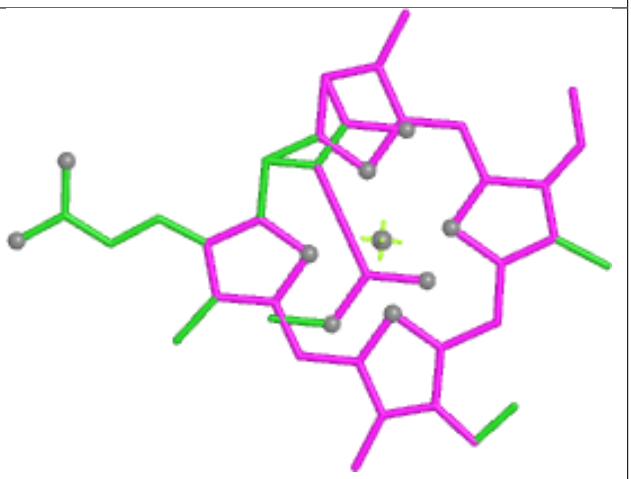
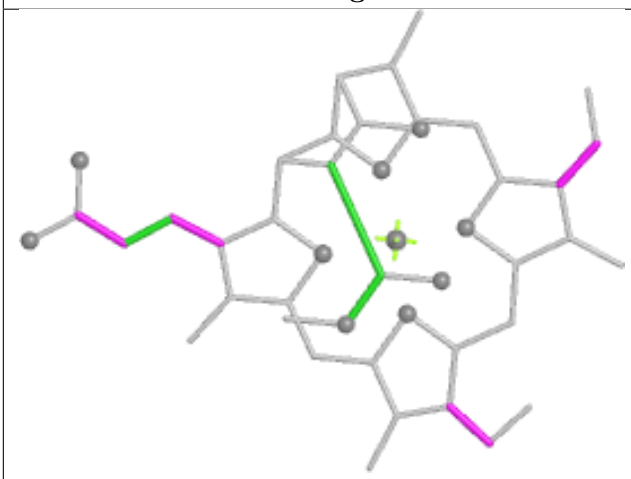
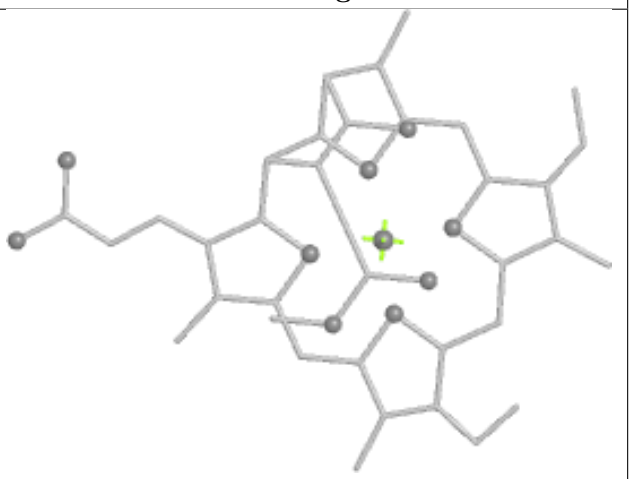


Bond angles

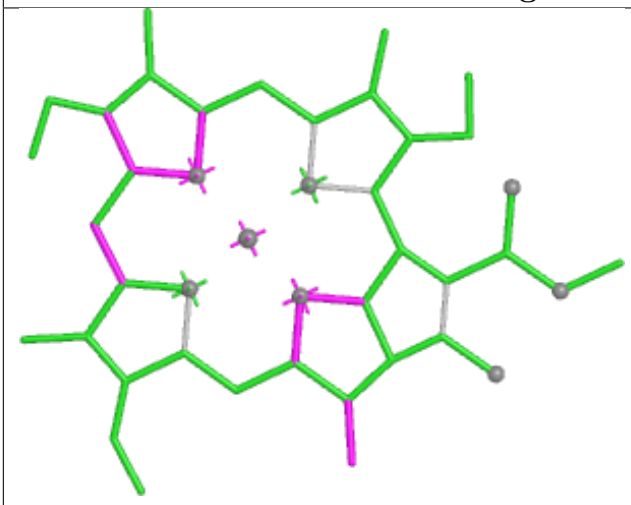


Torsions



Rings

Ligand CLA 12 307



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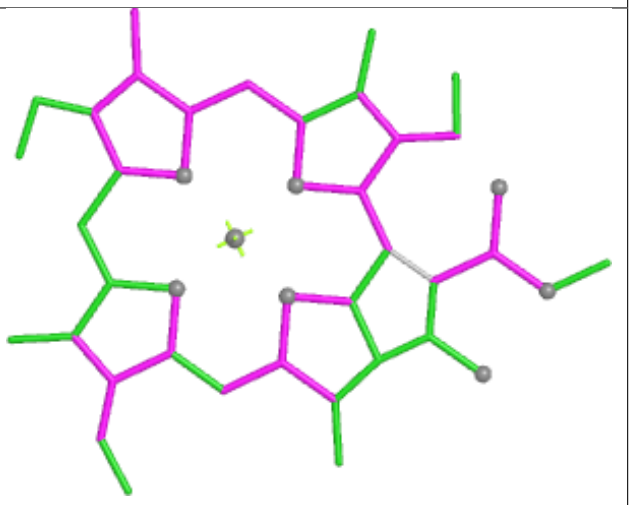

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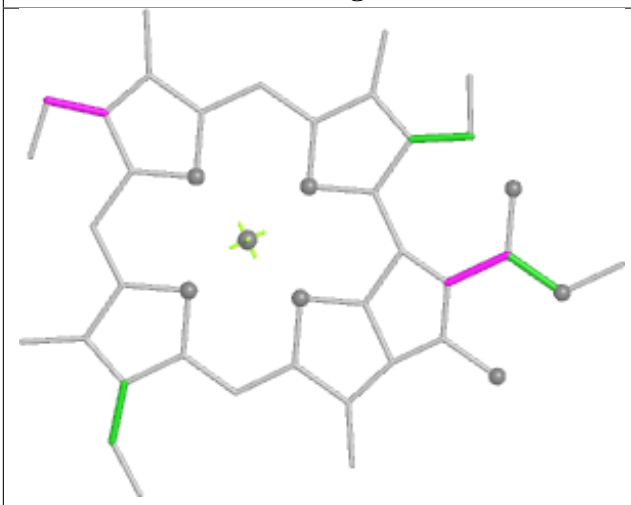
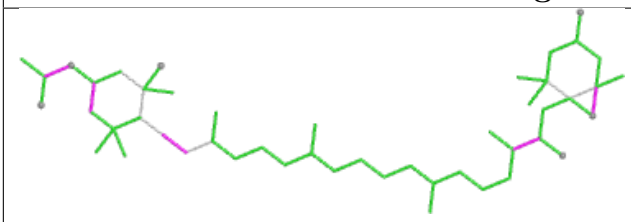


Torsions



Rings

Ligand A86 7 301



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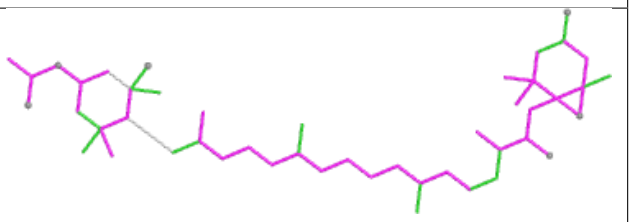
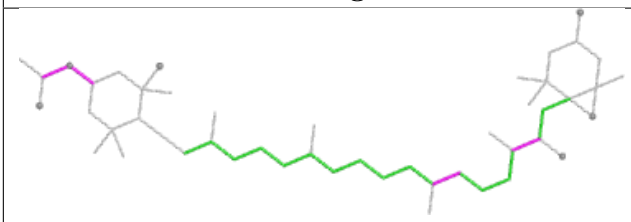


Bond angles



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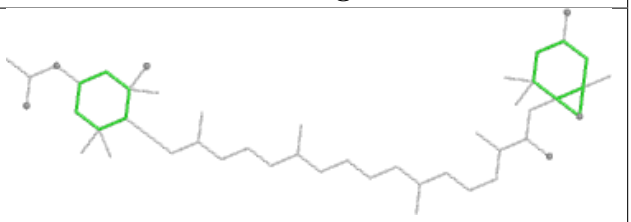
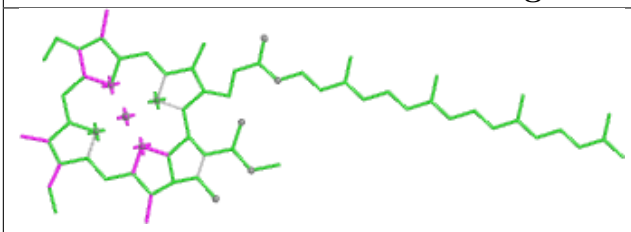


Rings

Ligand CLA B 606



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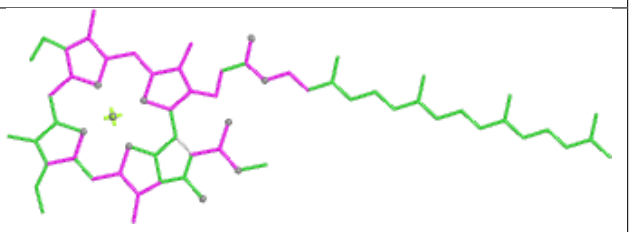

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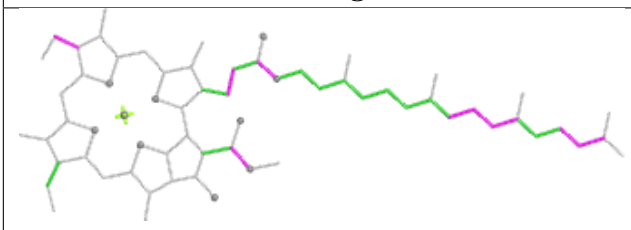

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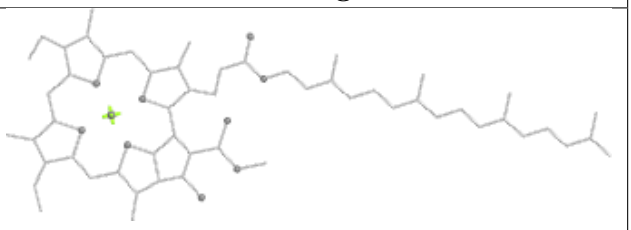
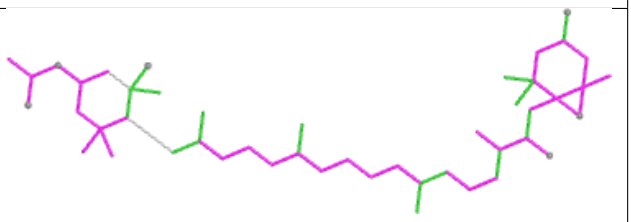


Rings

Ligand A86 8 303



Bond lengths



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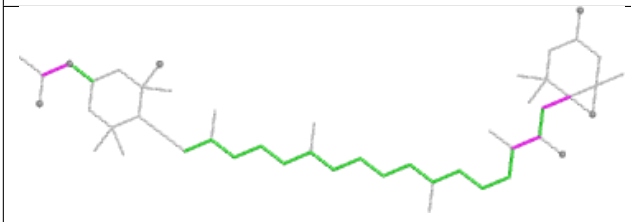

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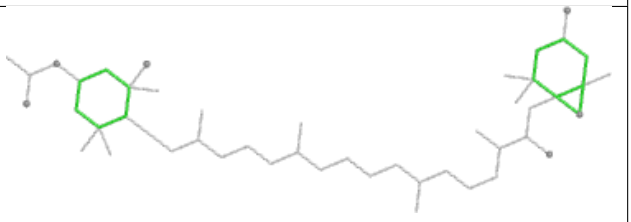
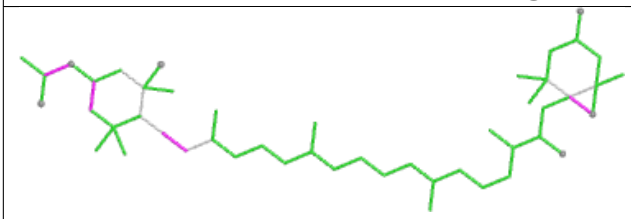


Rings

Ligand A86 19 301



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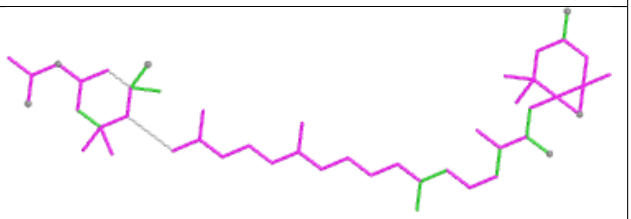

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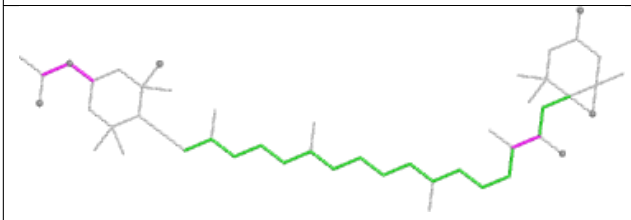

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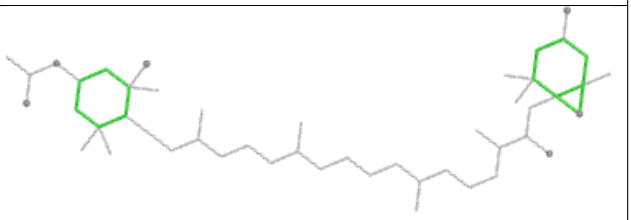
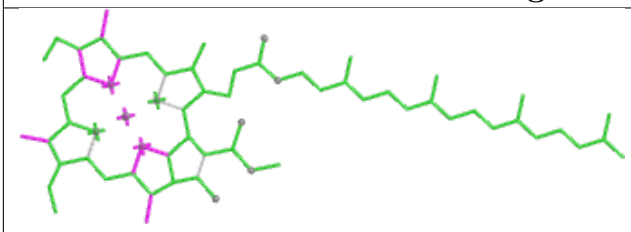


Rings

Ligand CLA b 608



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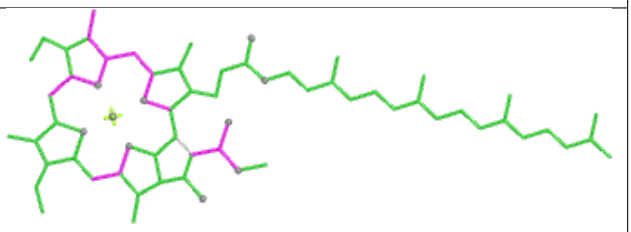
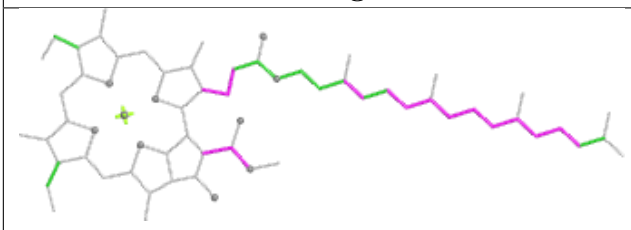


Bond angles



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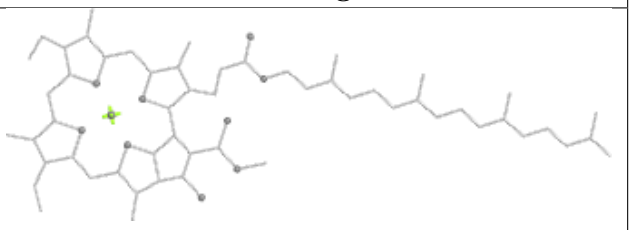
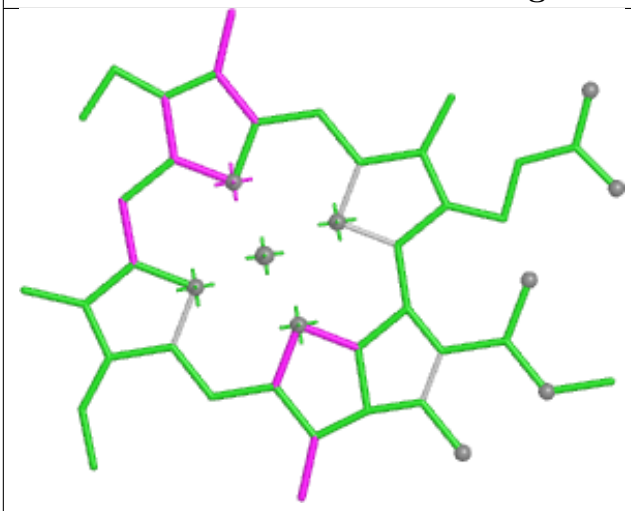


Rings

Ligand CLA 3 312



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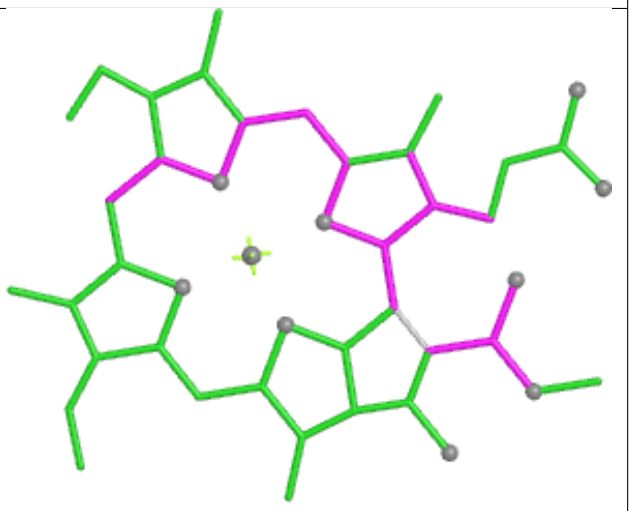
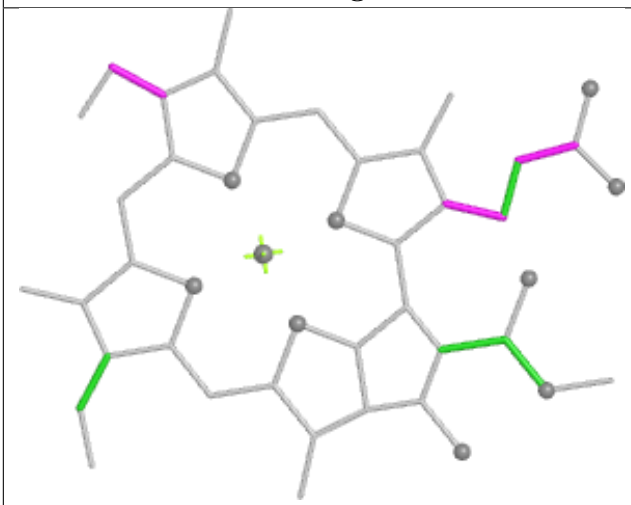


Bond angles



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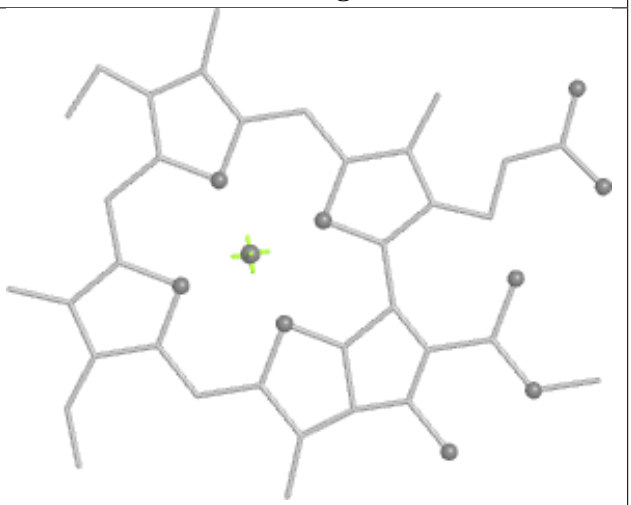
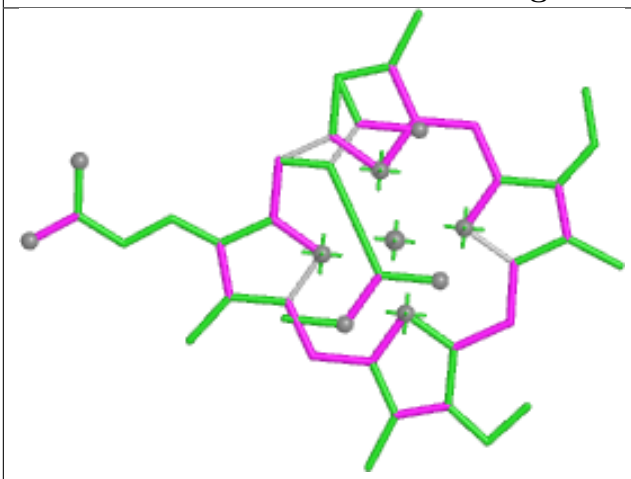


Rings

Ligand KC1 8 314



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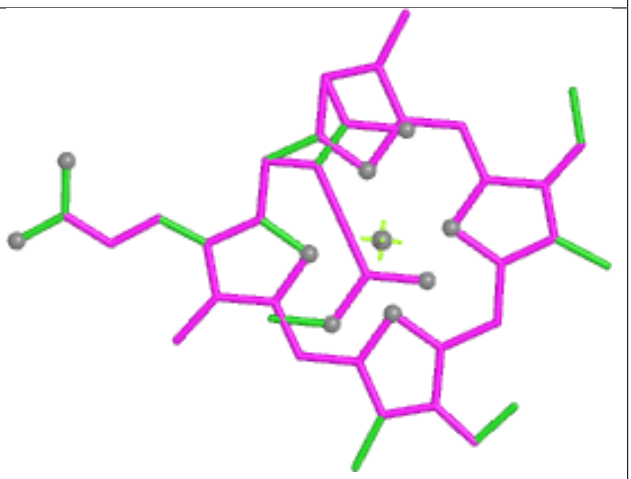
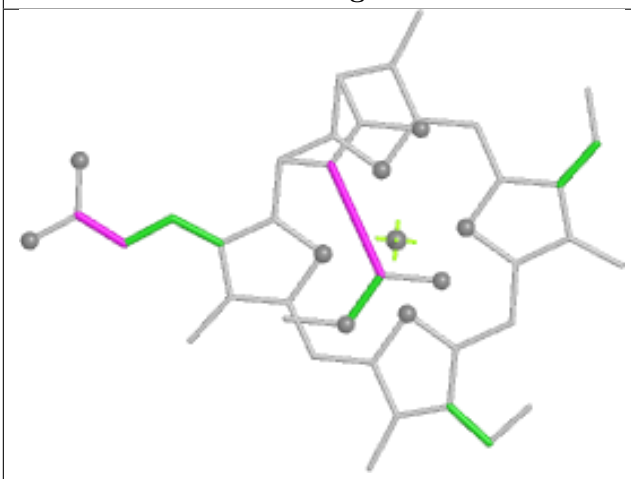


Bond angles



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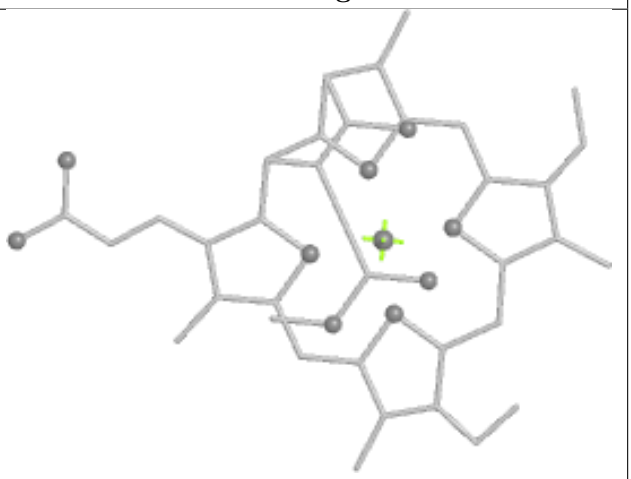
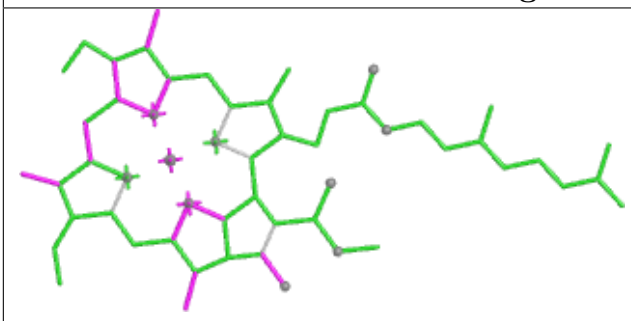


Rings

Ligand CLA 18 312



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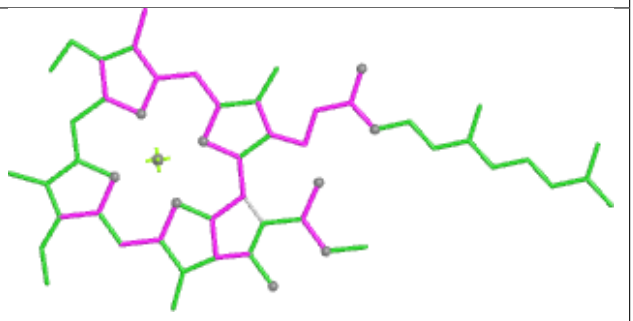
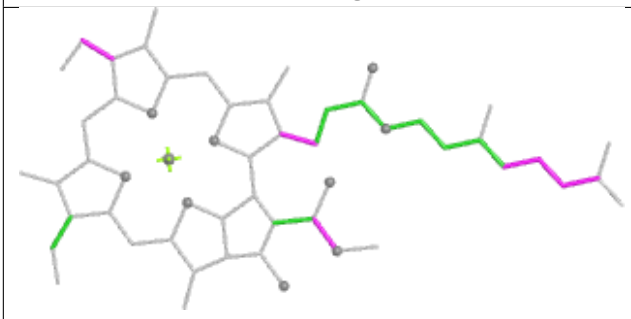


Bond angles



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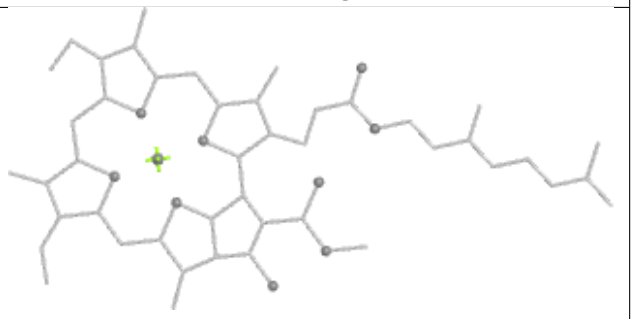
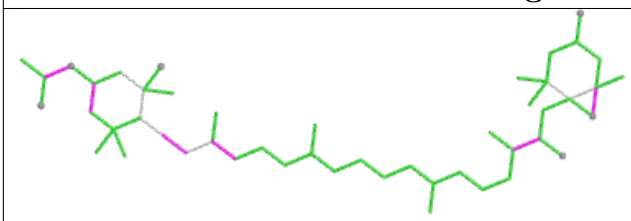


Rings

Ligand A86 16 302



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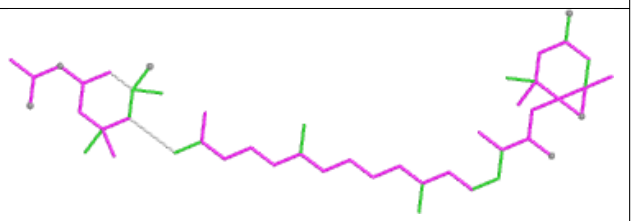
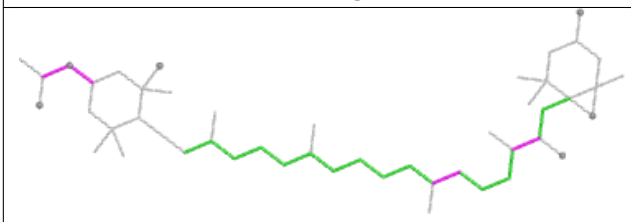


Bond angles



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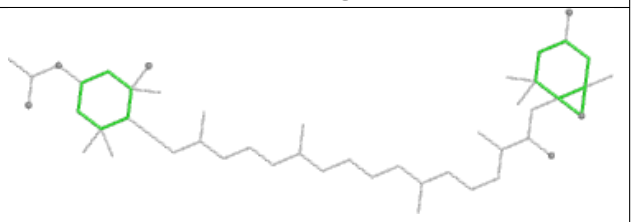
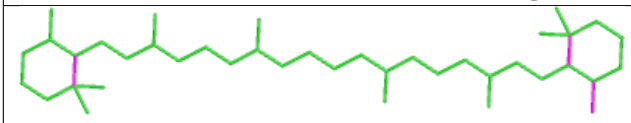


Rings

Ligand BCR b 620



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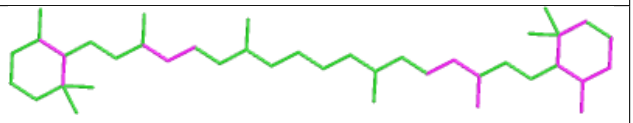
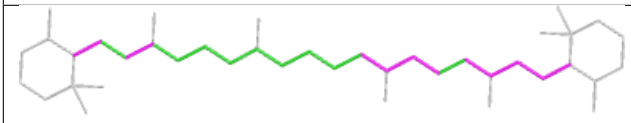


Bond angles



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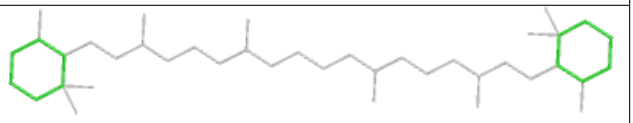
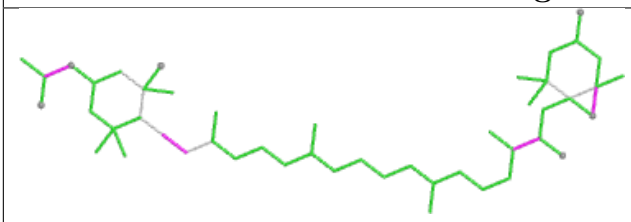


Rings

Ligand A86 3 303



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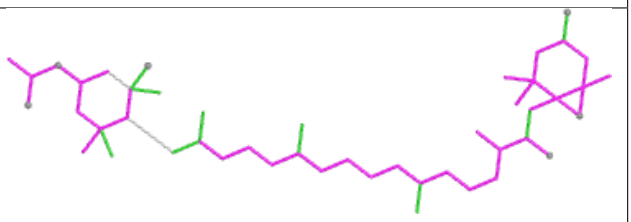
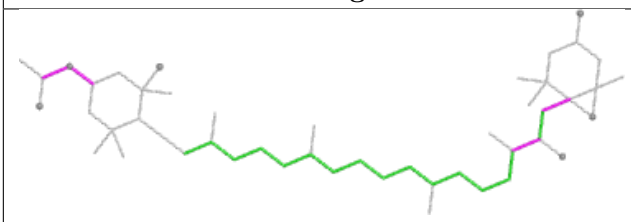


Bond angles



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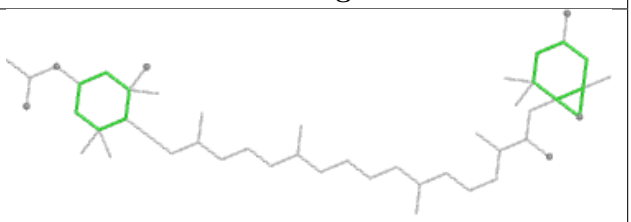
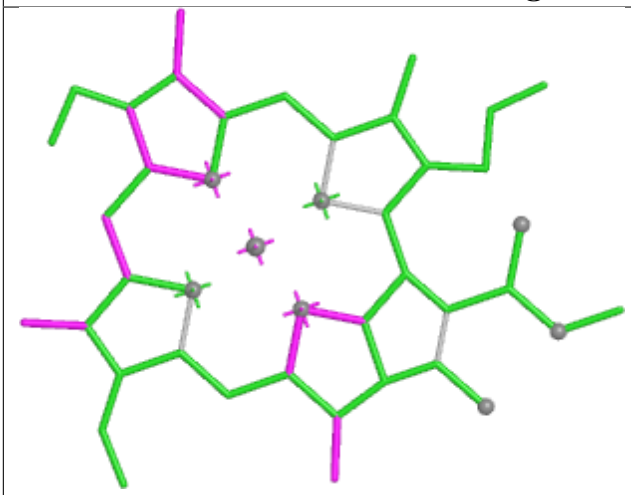


Rings

Ligand CLA P 607



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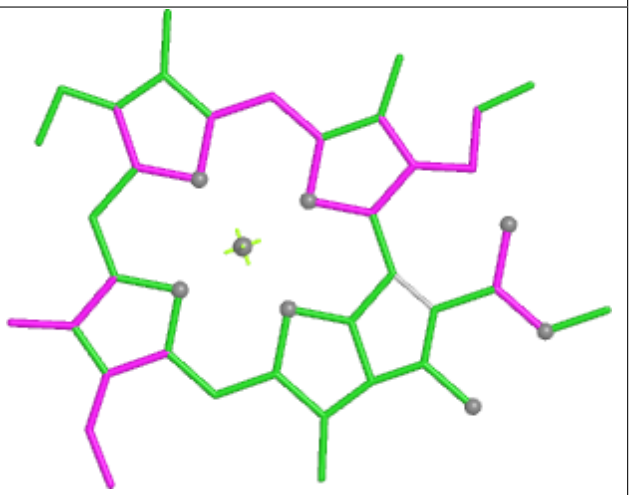
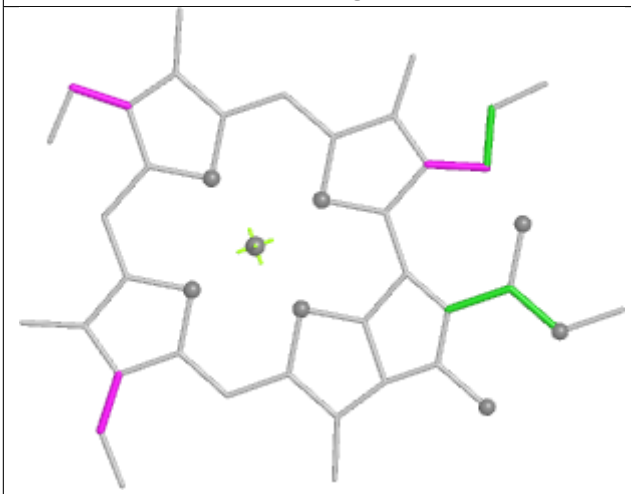


Bond angles



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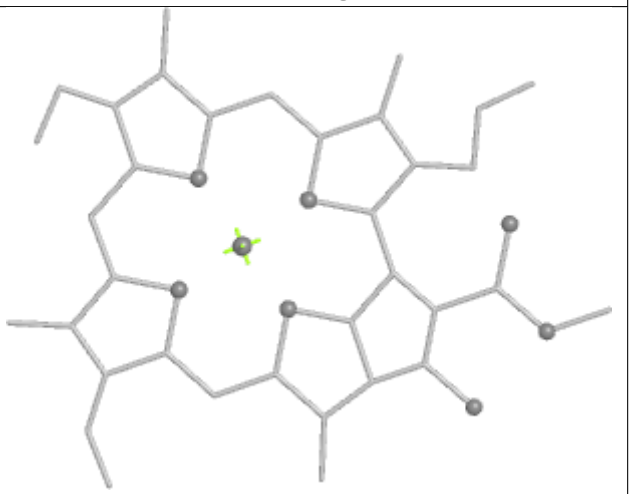
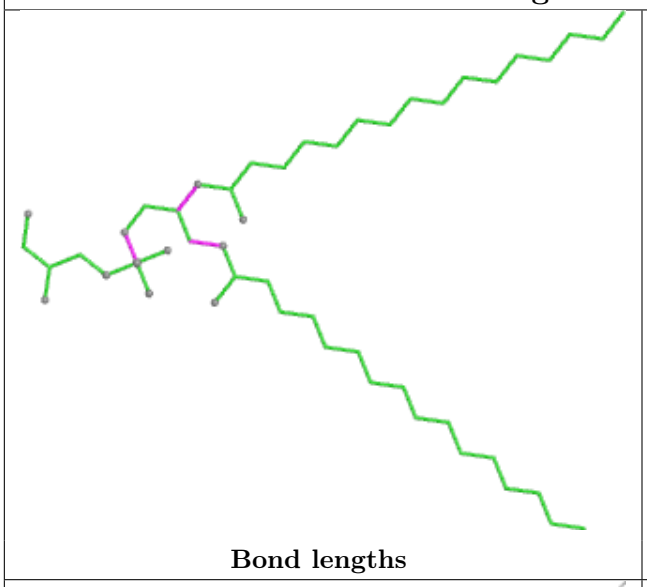


Rings

Ligand LHG l 102



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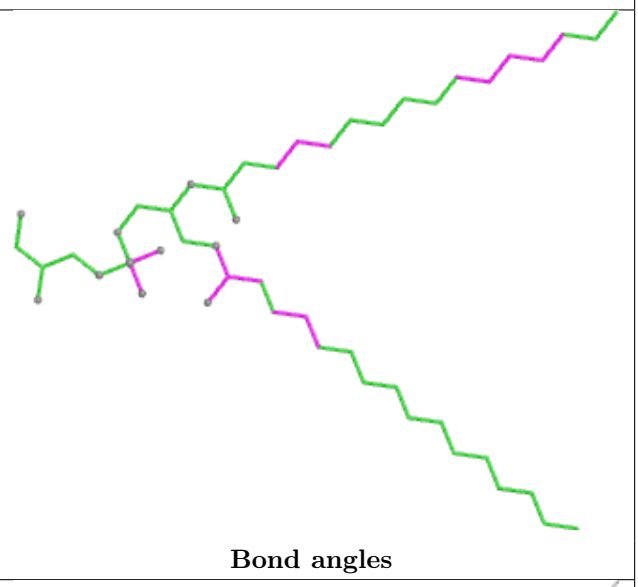
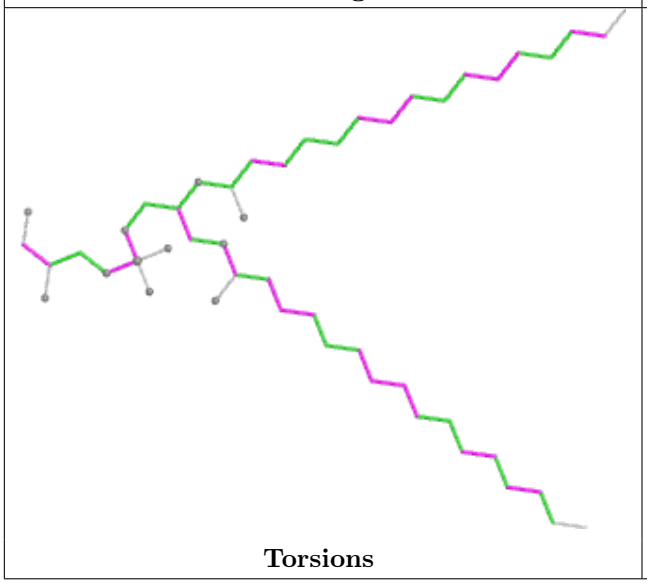


Bond angles



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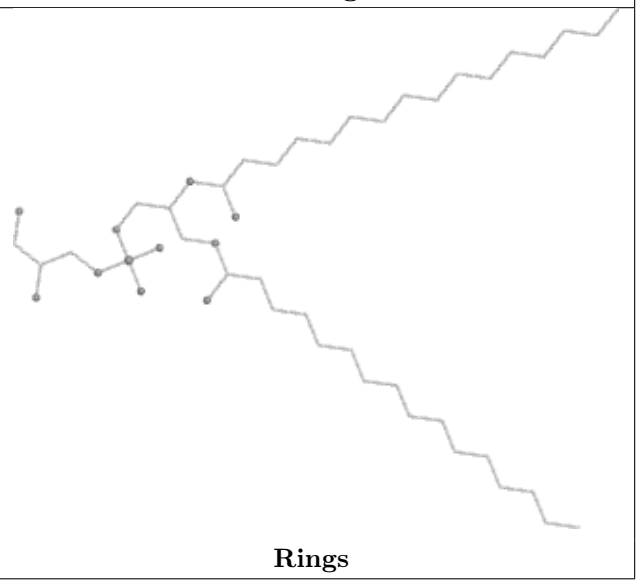
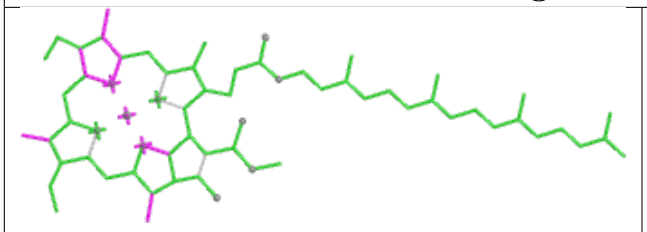
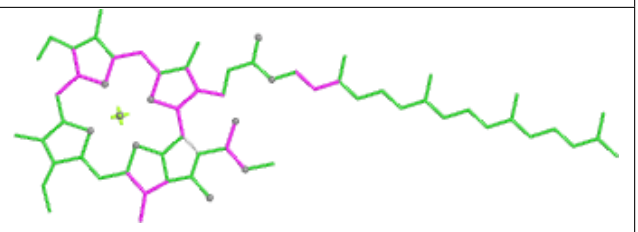


Rings

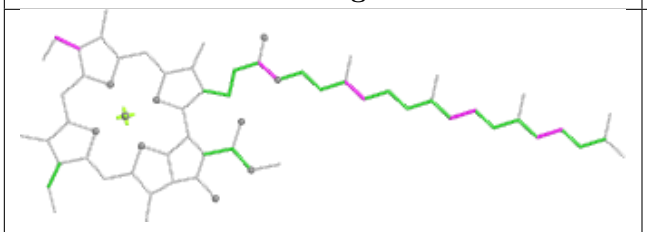
Ligand CLA c 512



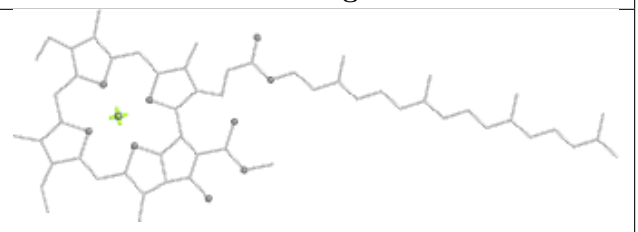
Bond lengths



Bond angles

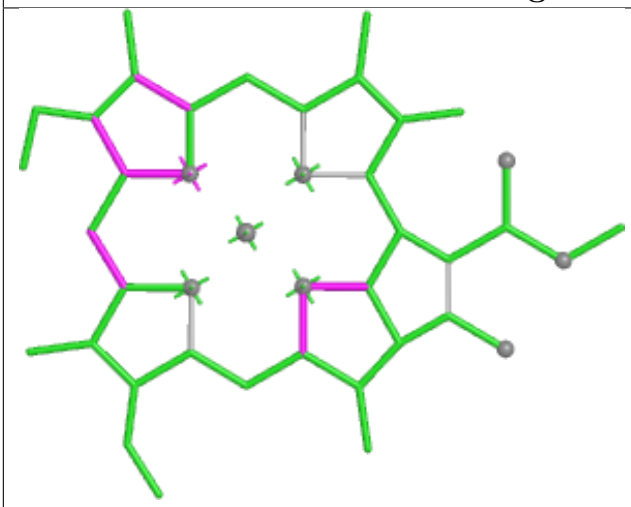


Torsions



Rings

Ligand CLA 3 310



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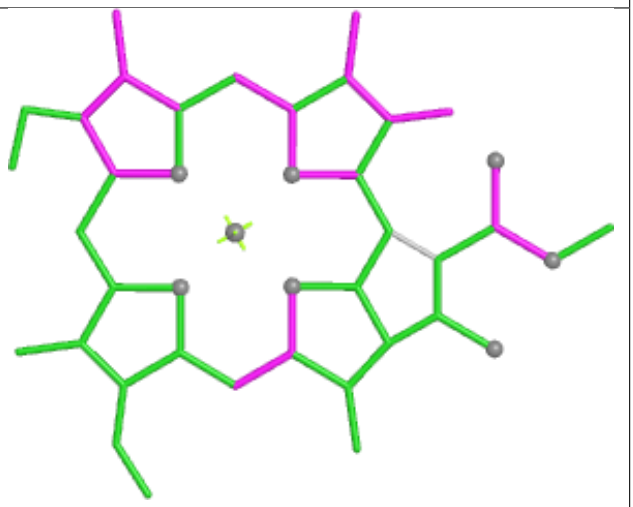

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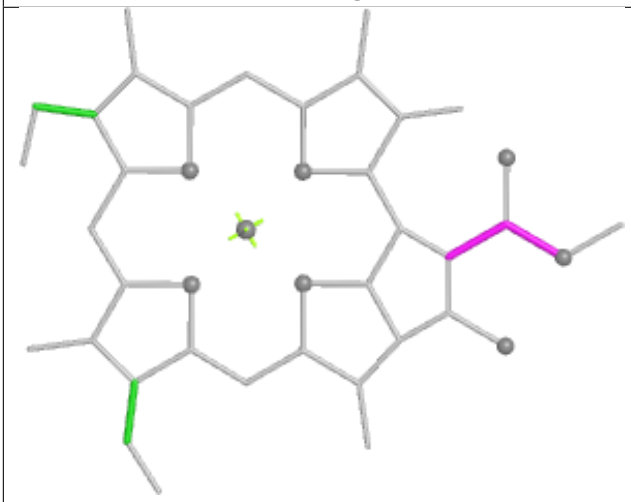

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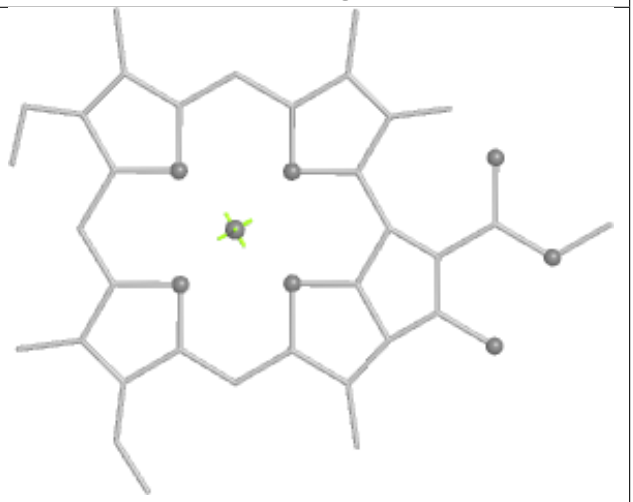
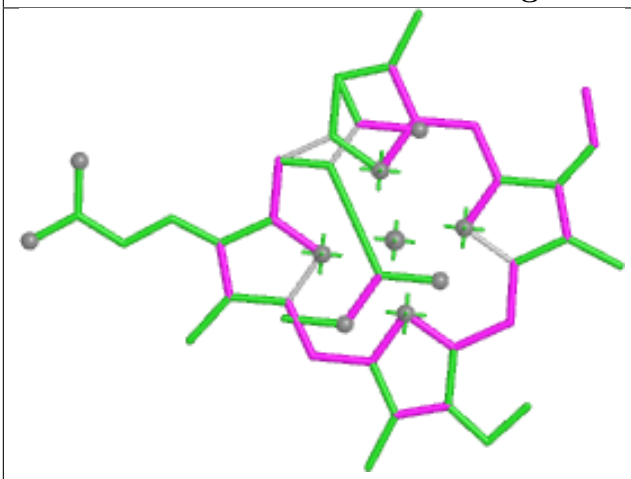


Rings

Ligand KC2 14 310



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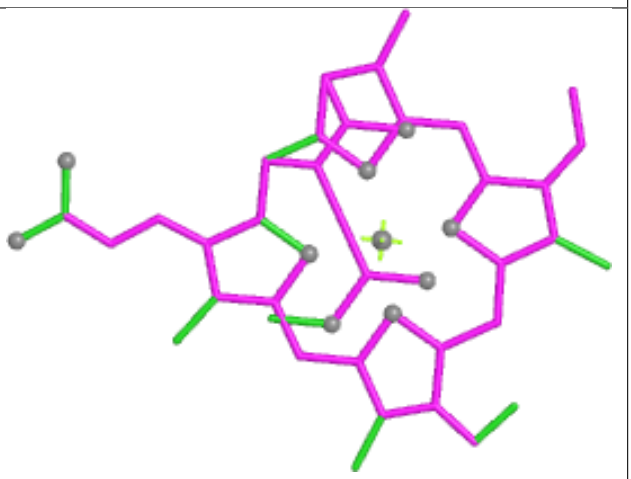

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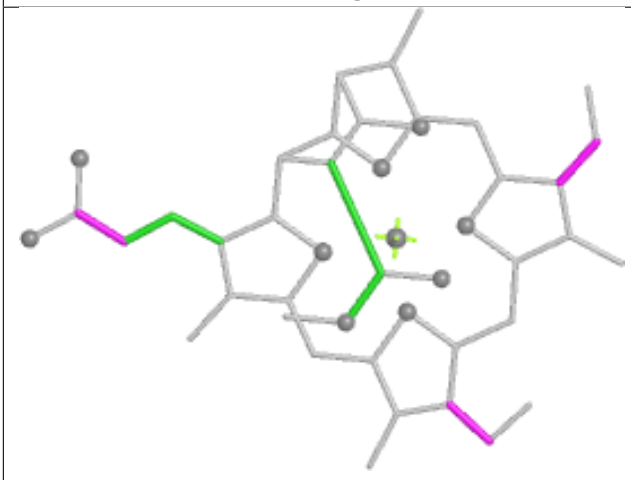

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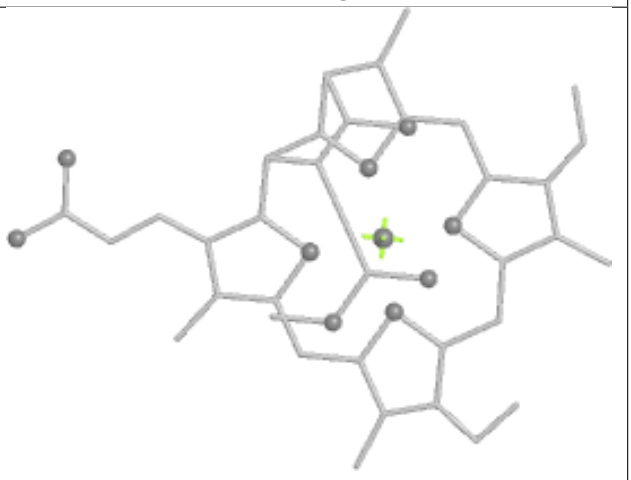
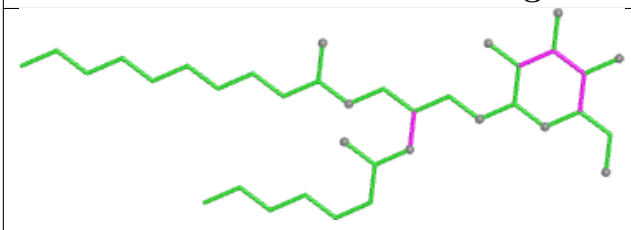


Rings

Ligand LMG 1 301



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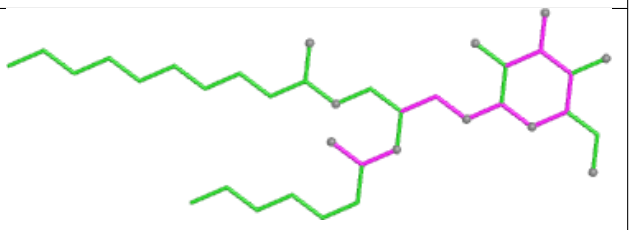

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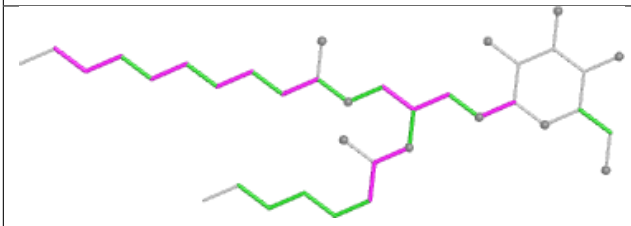

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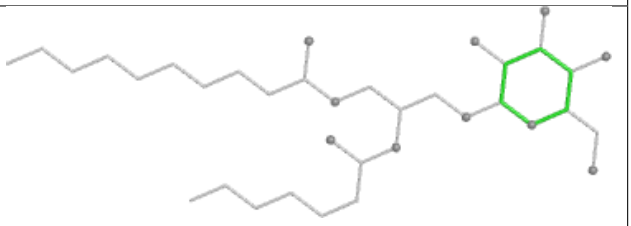
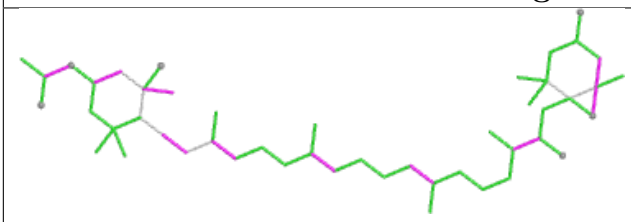


Rings

Ligand A86 p 611



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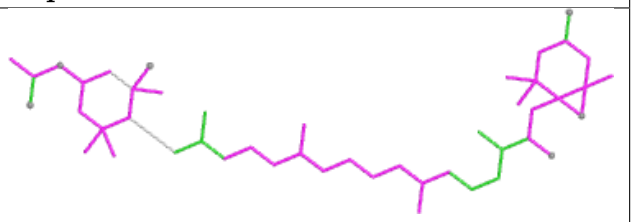

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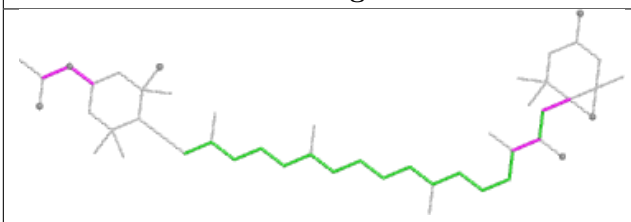

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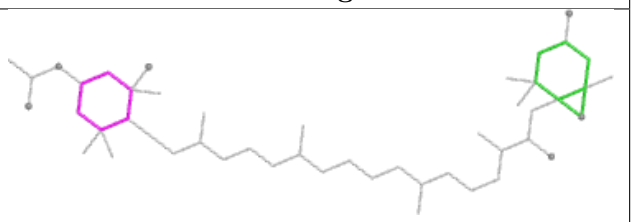
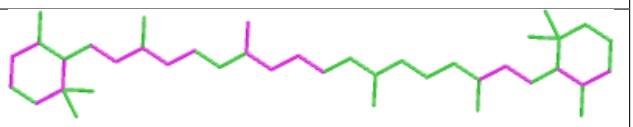


Rings

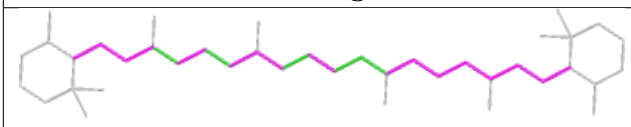
Ligand BCR F 101



Bond lengths



Bond angles



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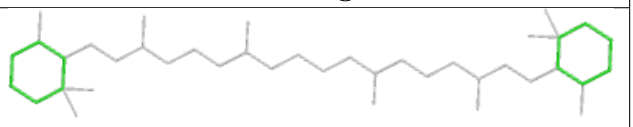
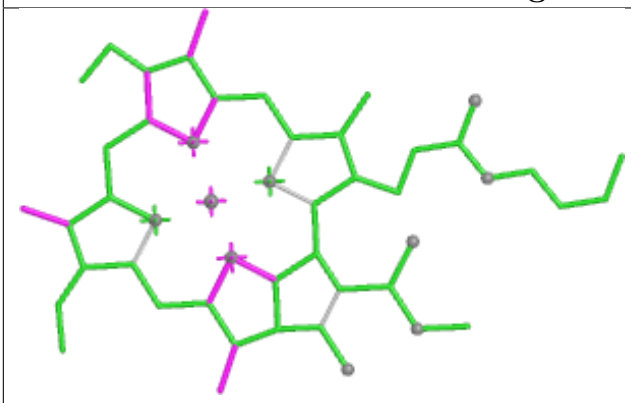


Rings

Ligand CLA a 404



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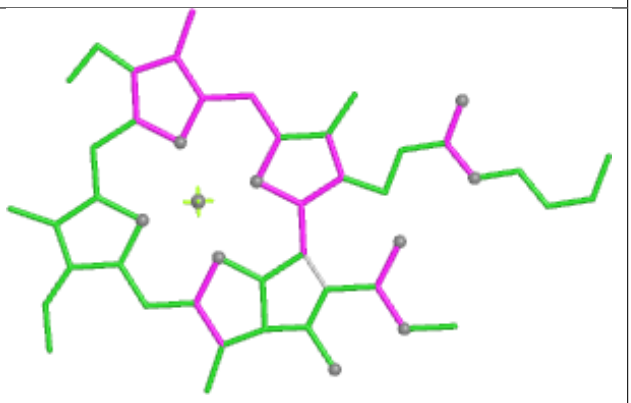
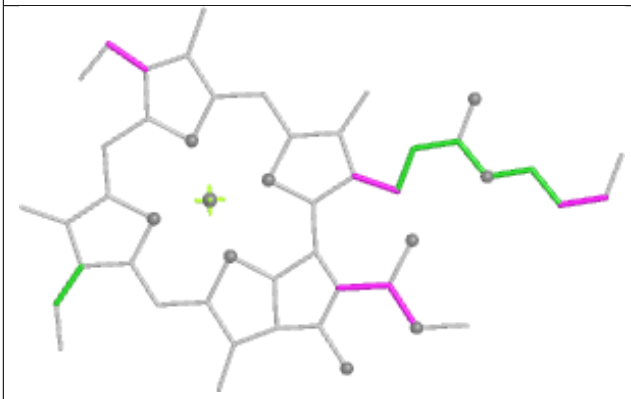


Bond angles



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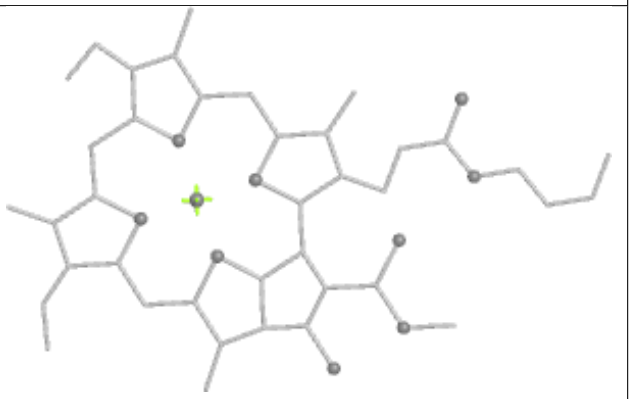
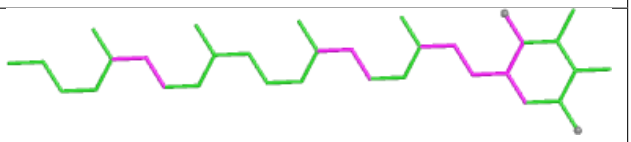


Rings

Ligand PL9 A 409



Bond lengths



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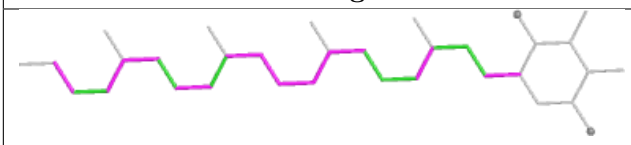

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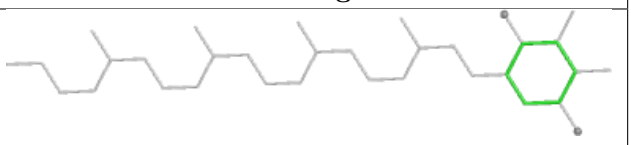
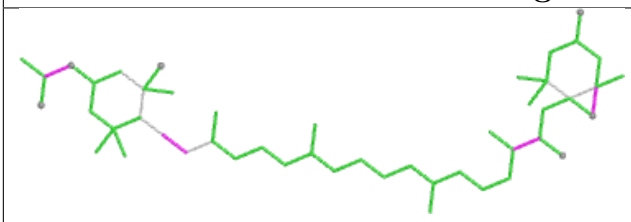


Rings

Ligand A86 9 302



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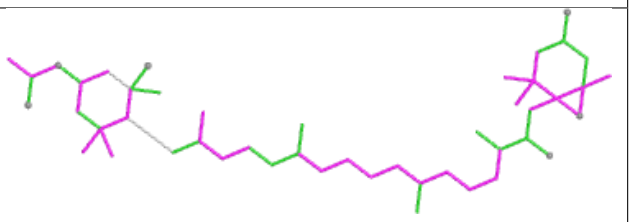
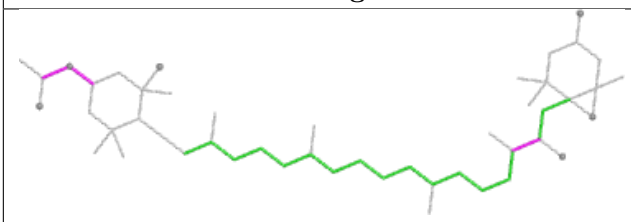


Bond angles



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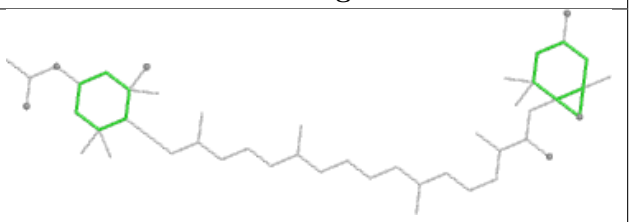
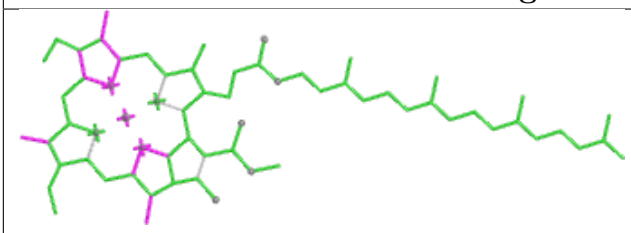


Rings

Ligand CLA 15 307



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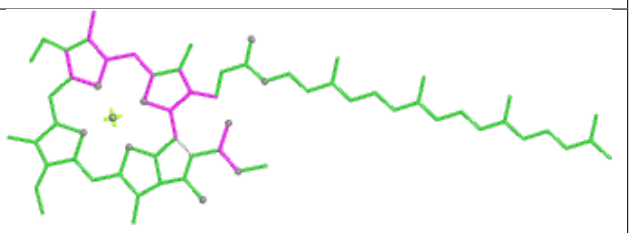

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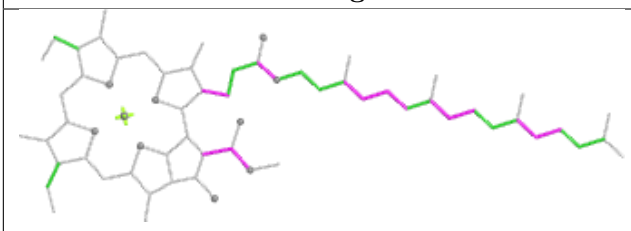

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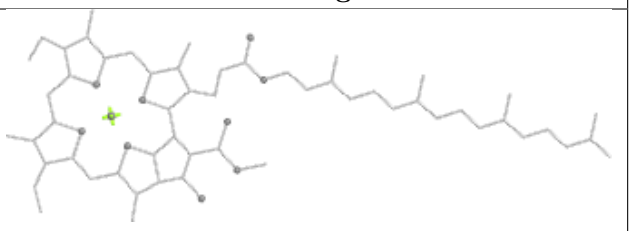
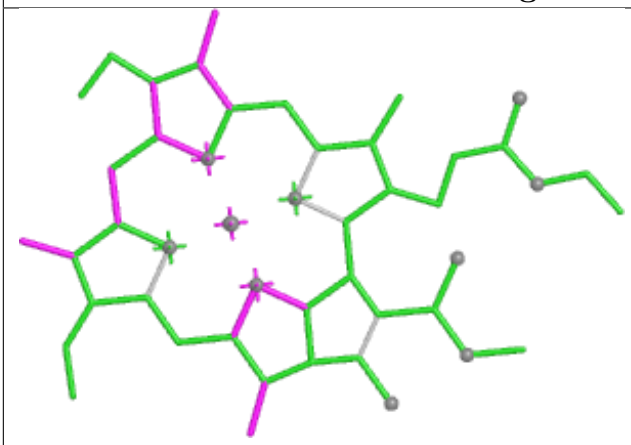


Rings

Ligand CLA 17 312



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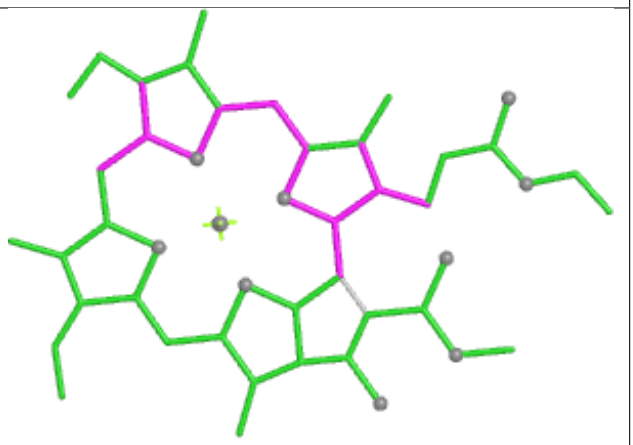

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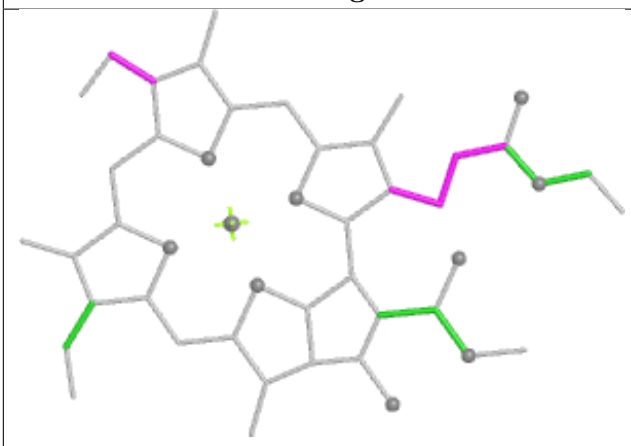

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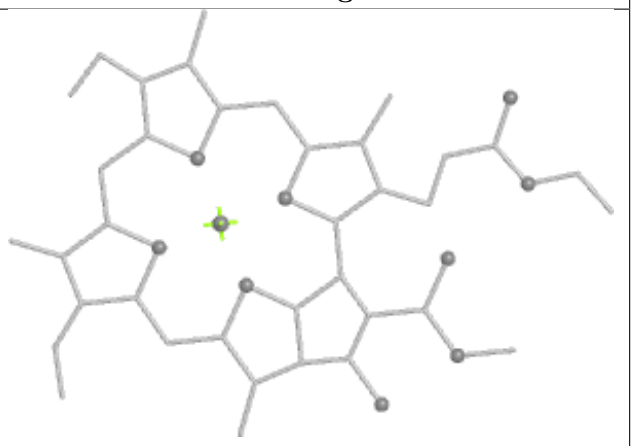
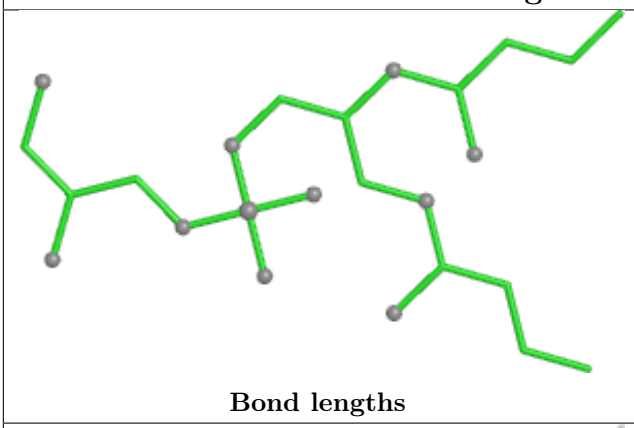


Rings

Ligand LHG Z 103



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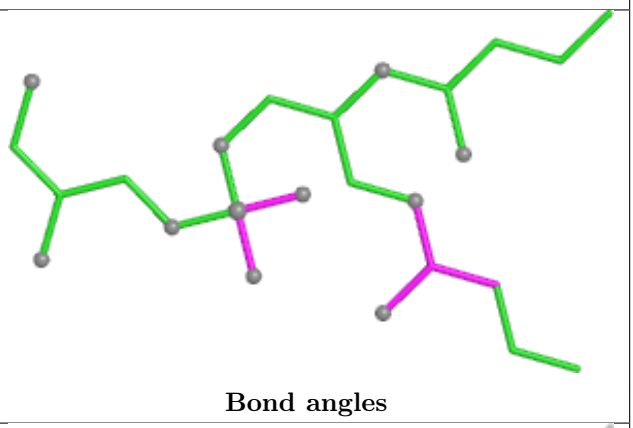
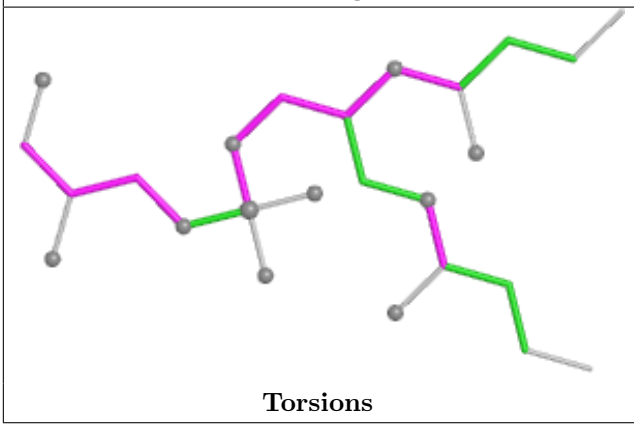


Bond angles



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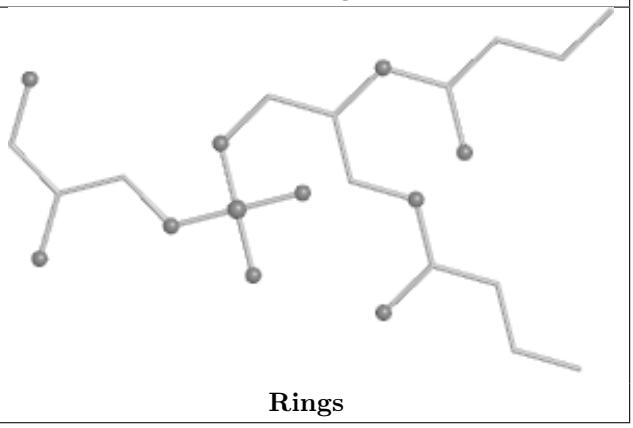
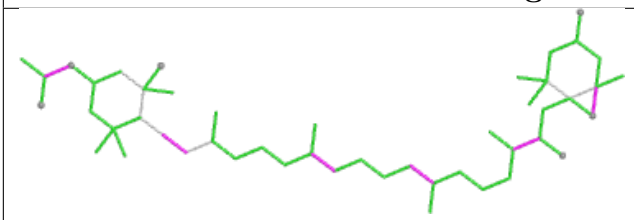


Rings

Ligand A86 11 304



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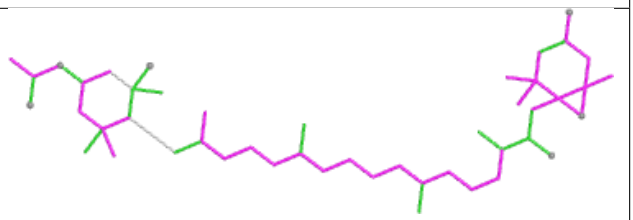

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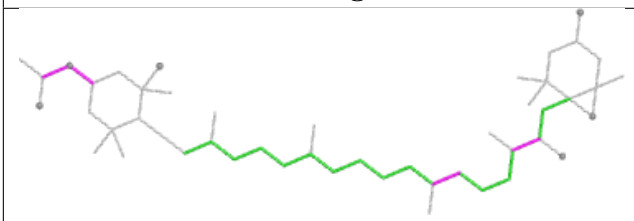

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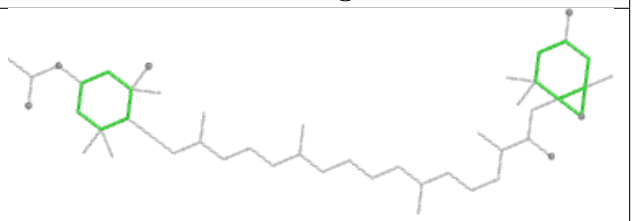
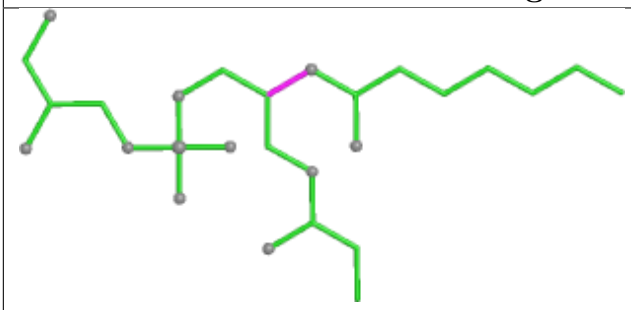


Rings

Ligand LHG p 615



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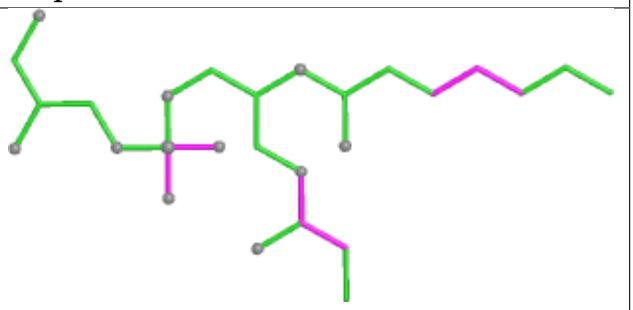

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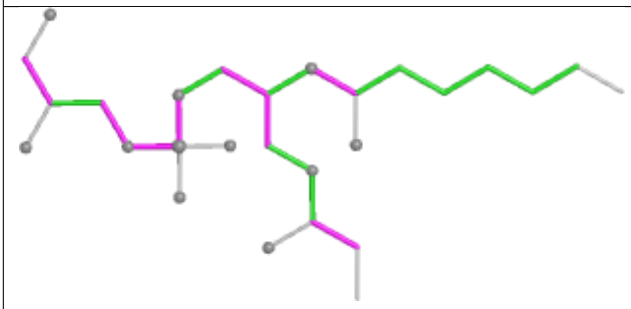

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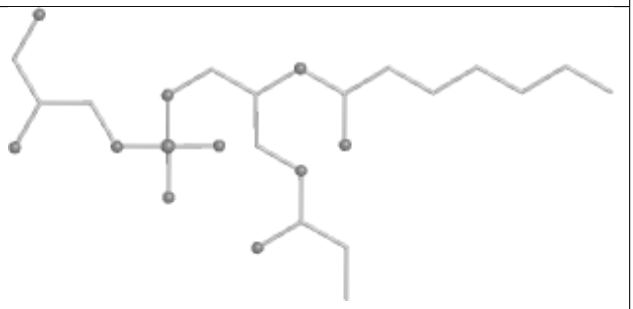
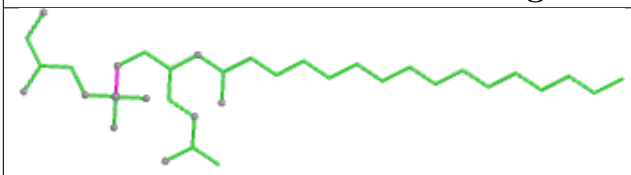


Rings

Ligand LHG 4 317



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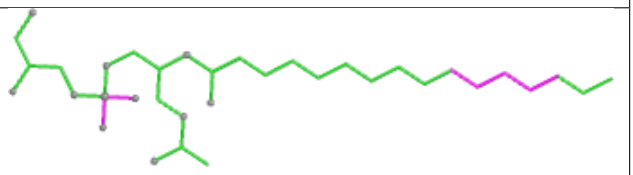
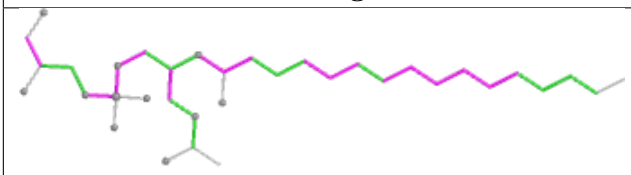


Bond angles



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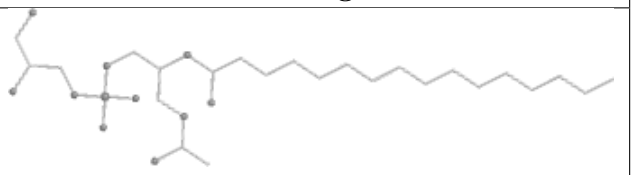
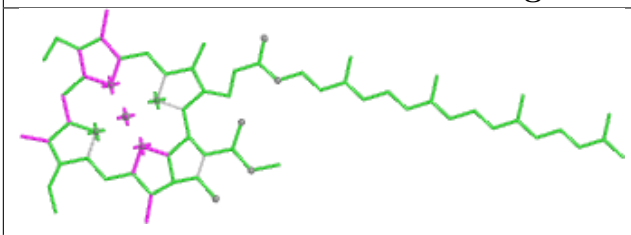


Rings

Ligand CLA C 506



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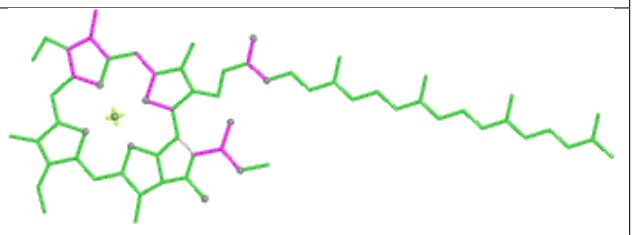
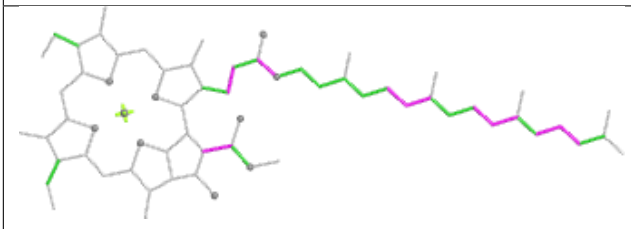
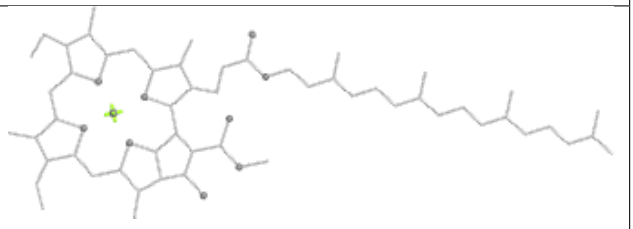


Bond angles

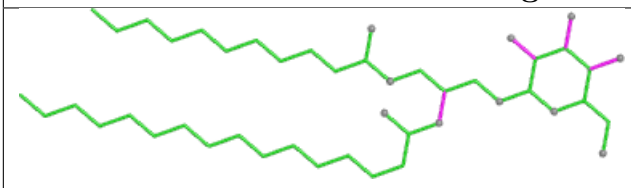


Torsions

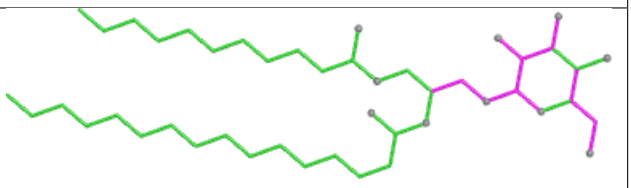


Rings

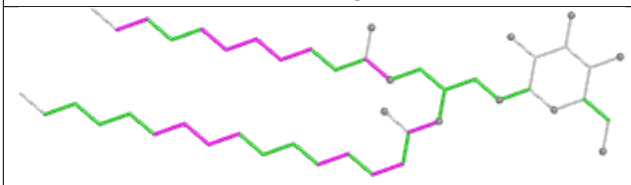
Ligand LMG F 102



Bond lengths



Bond angles



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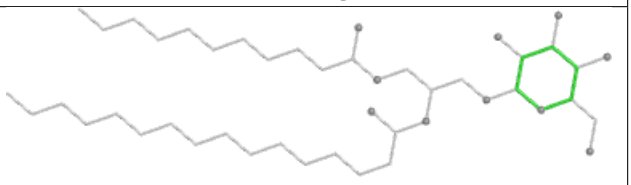
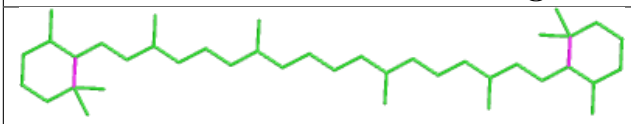


Rings

Ligand BCR c 515



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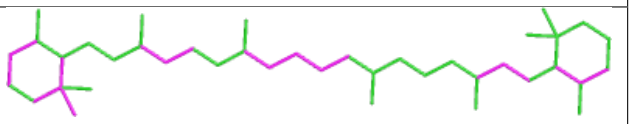

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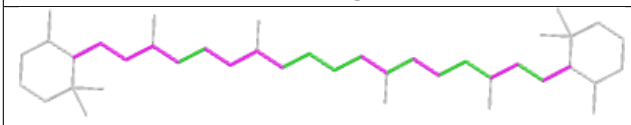

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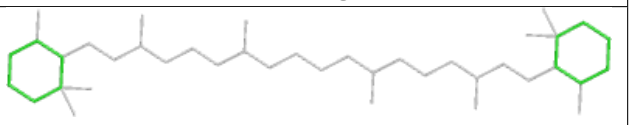
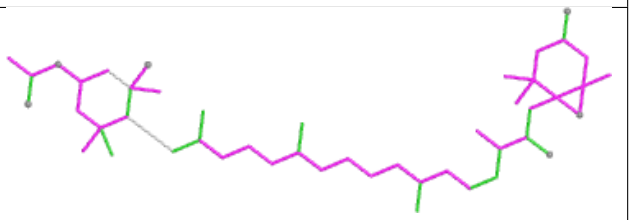


Rings

Ligand A86 4 301



Bond lengths



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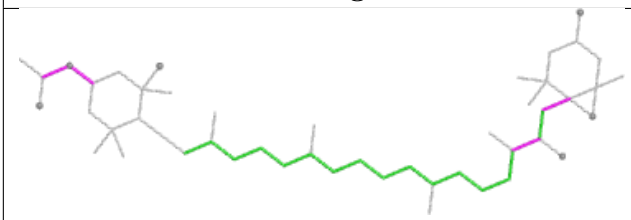

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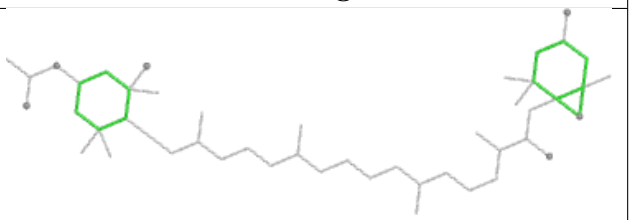
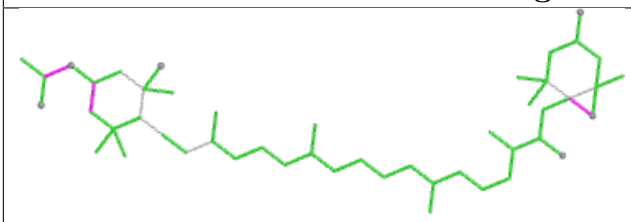


Rings

Ligand A86 9 301



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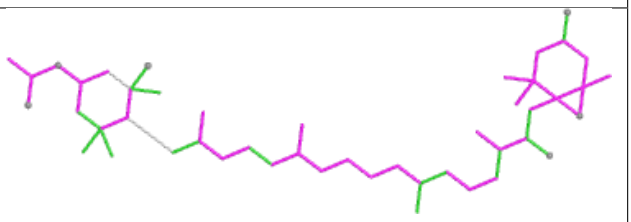
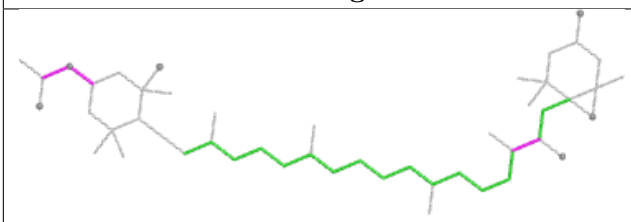


Bond angles



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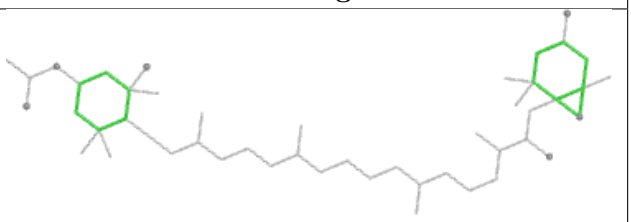
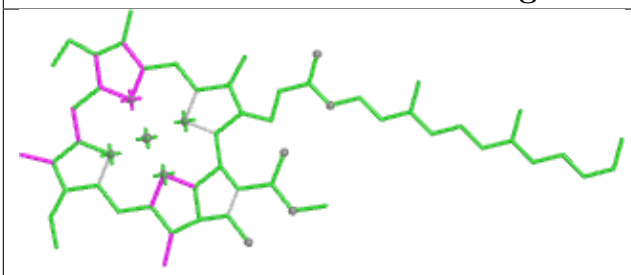


Rings

Ligand CLA 10 309



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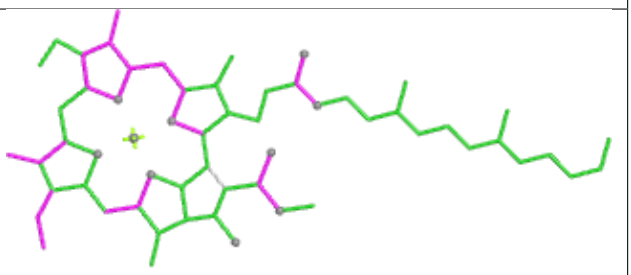

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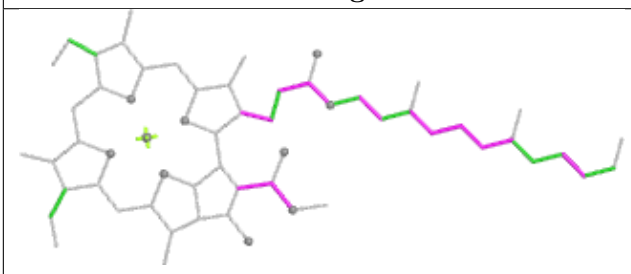

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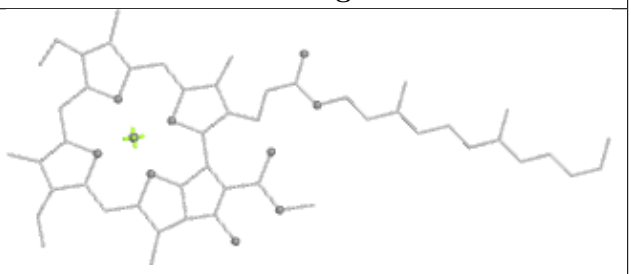
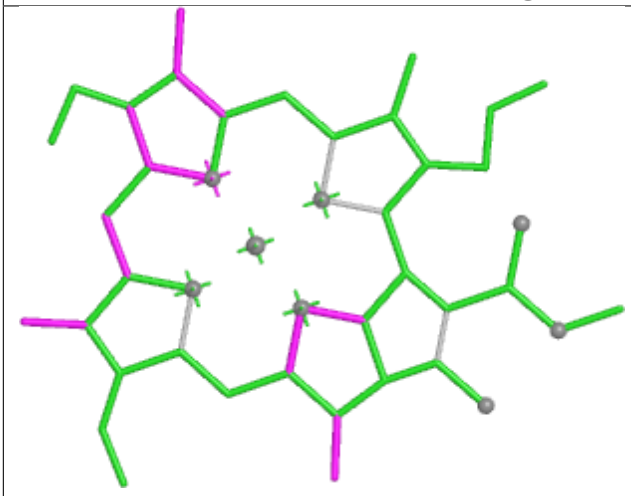


Rings

Ligand CLA 14 314



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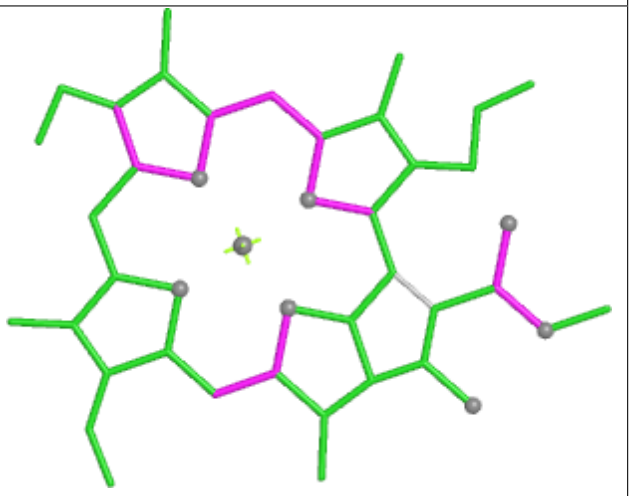
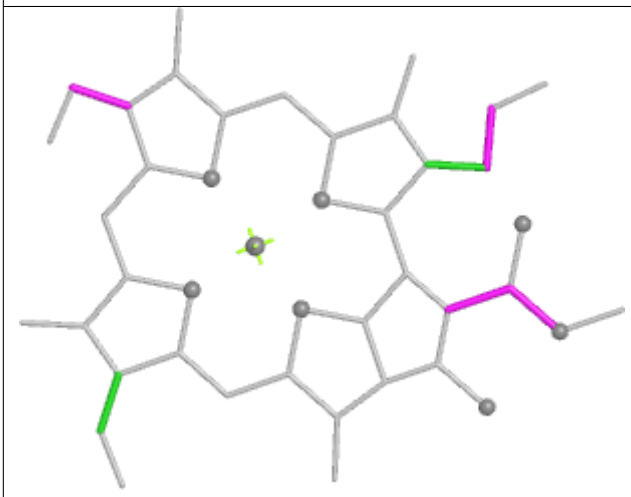


Bond angles



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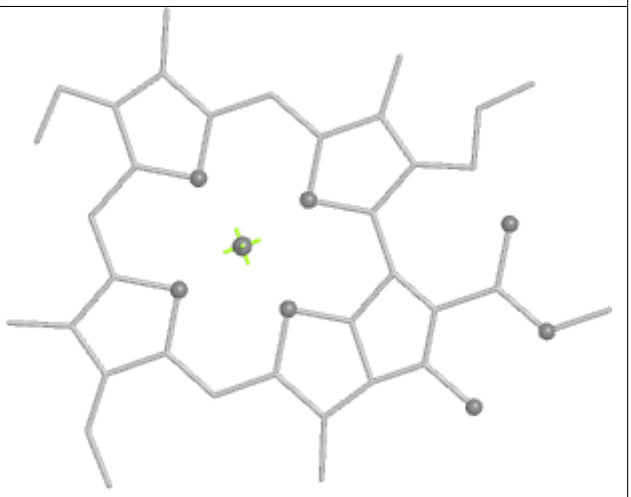
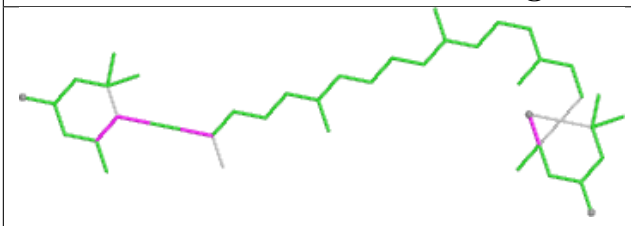


Rings

Ligand DD6 P 612



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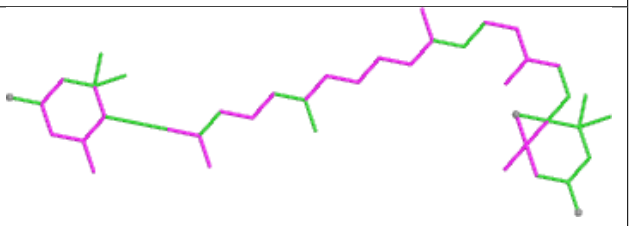
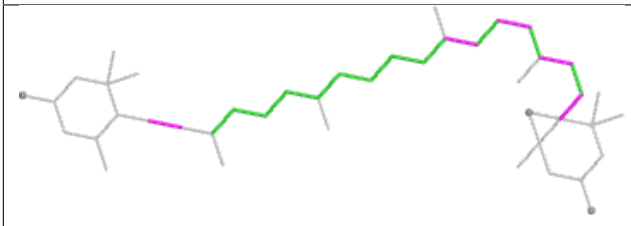


Bond angles



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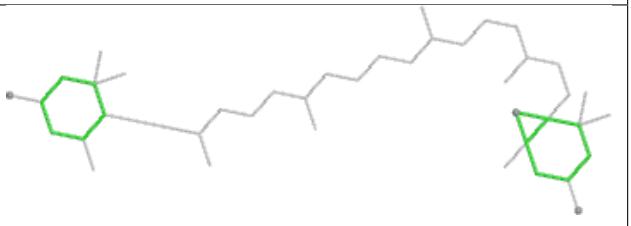
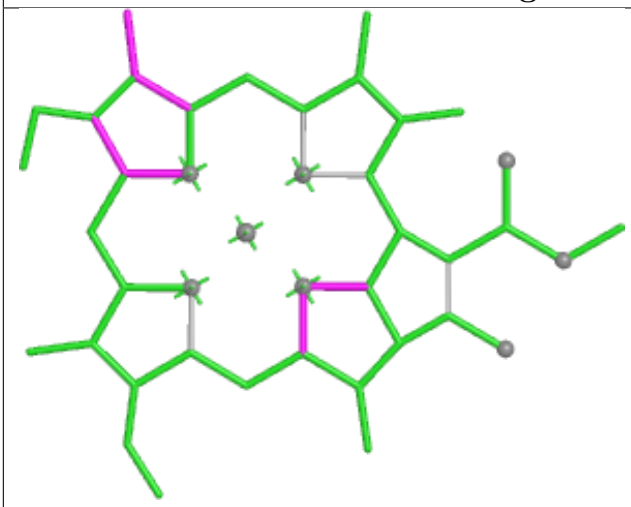


Rings

Ligand CLA 17 307



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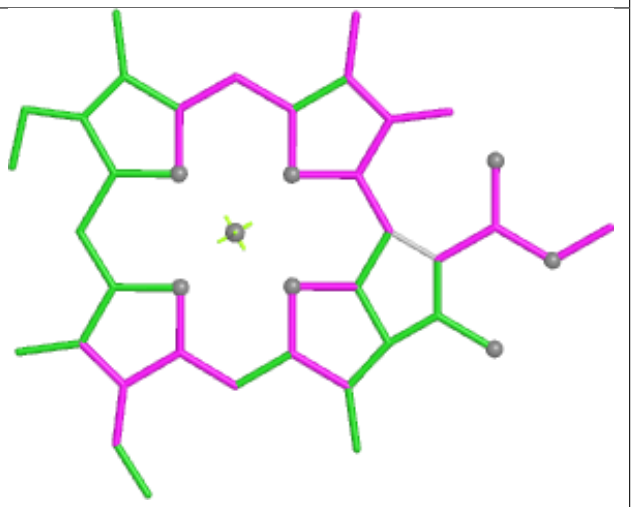

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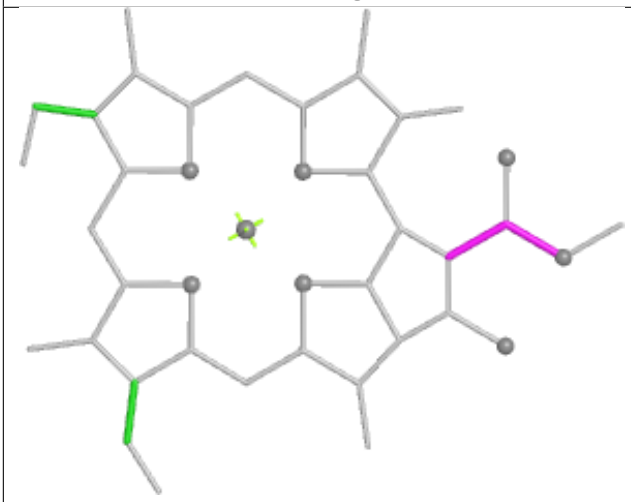

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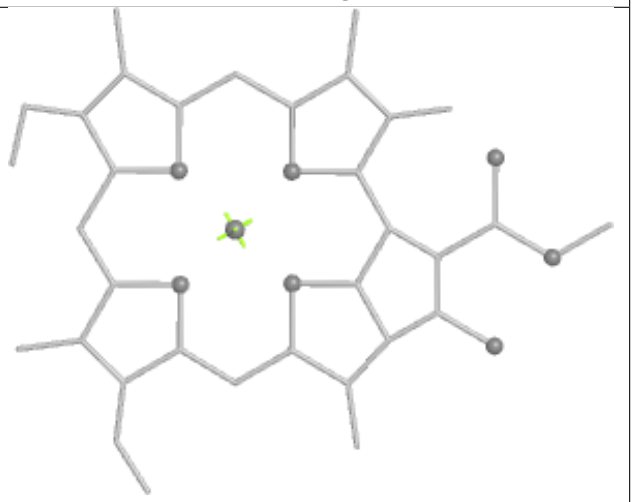
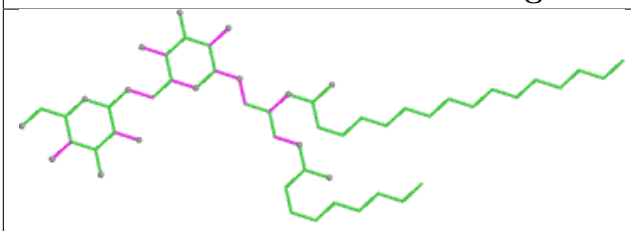


Rings

Ligand DGD c 518



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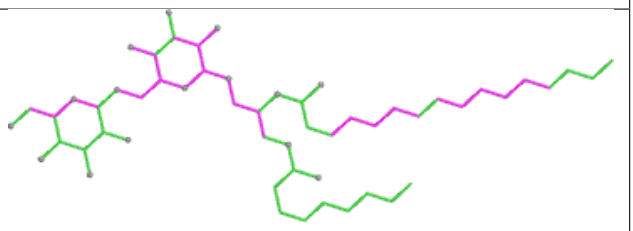
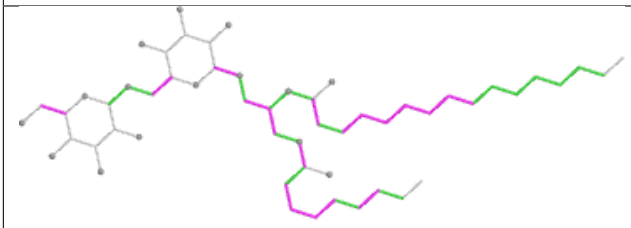


Bond angles



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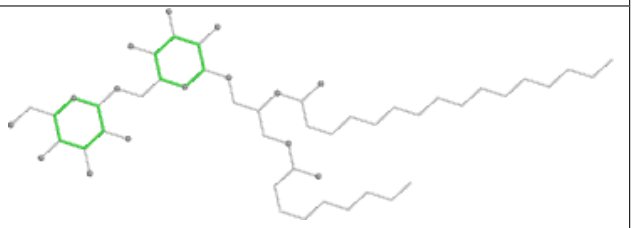
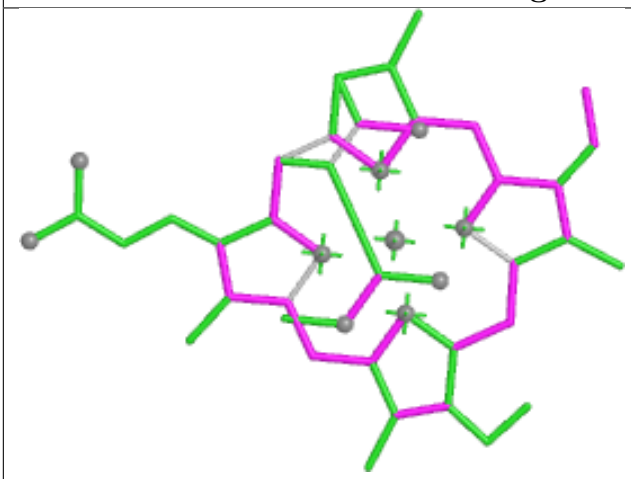


Rings

Ligand KC2 3 311



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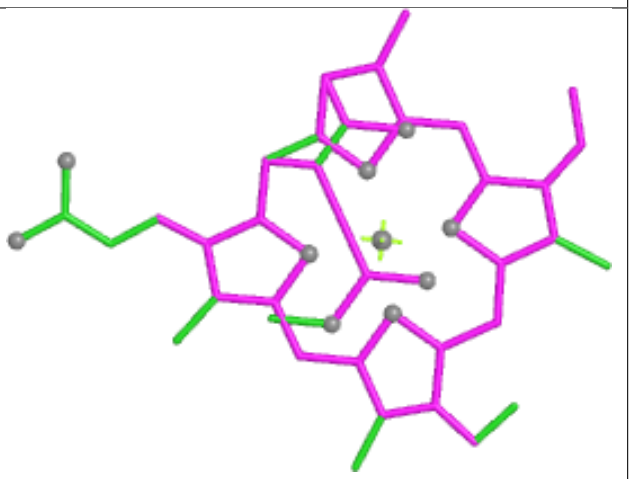
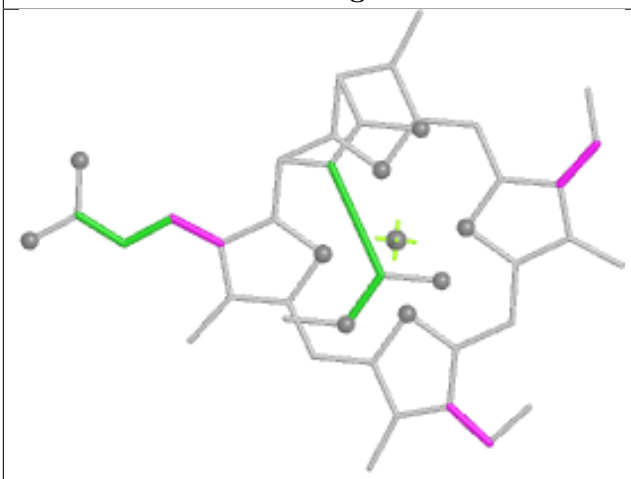


Bond angles



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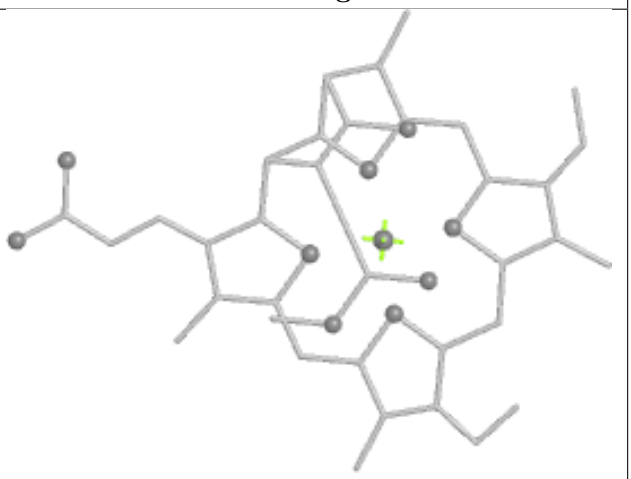
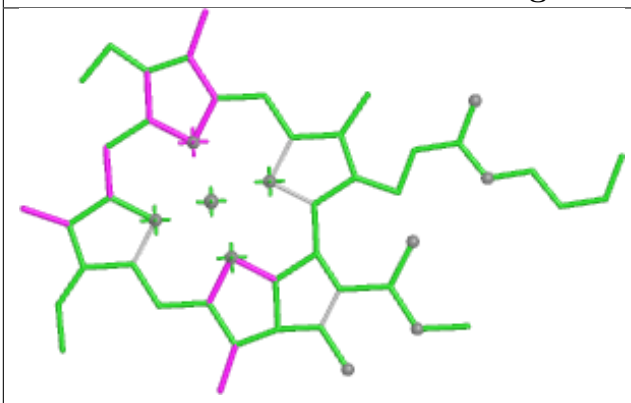


Rings

Ligand CLA c 514



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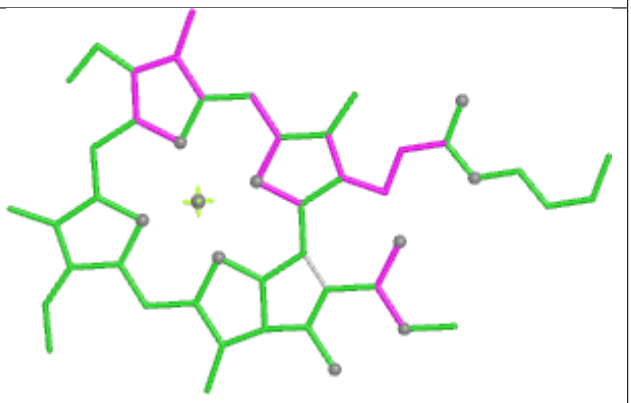
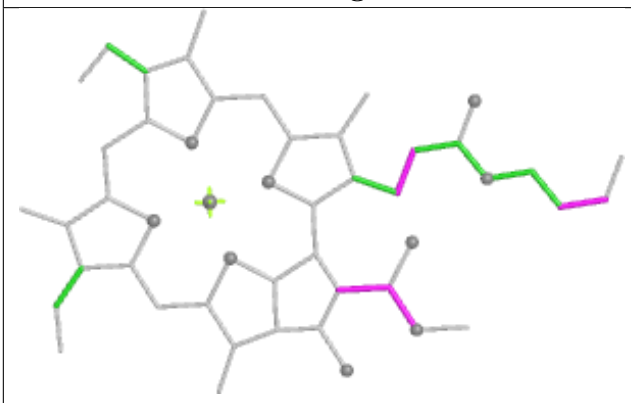


Bond angles



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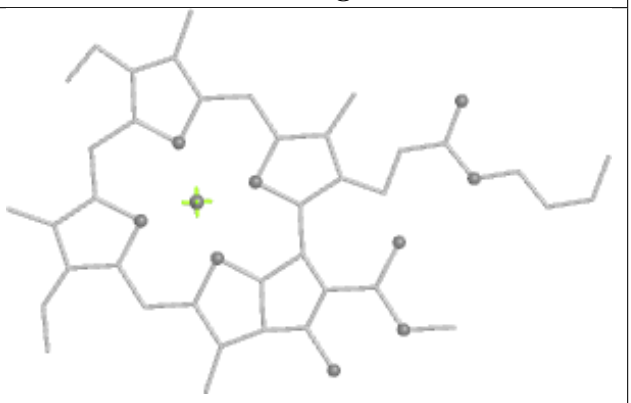
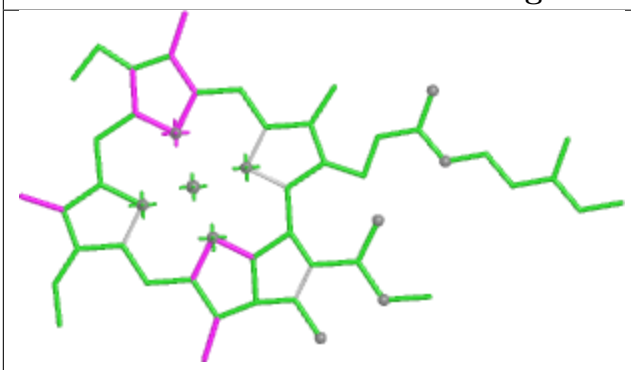


Rings

Ligand CLA P 608



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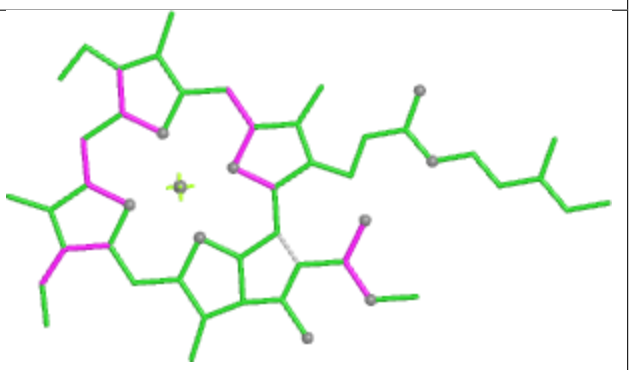
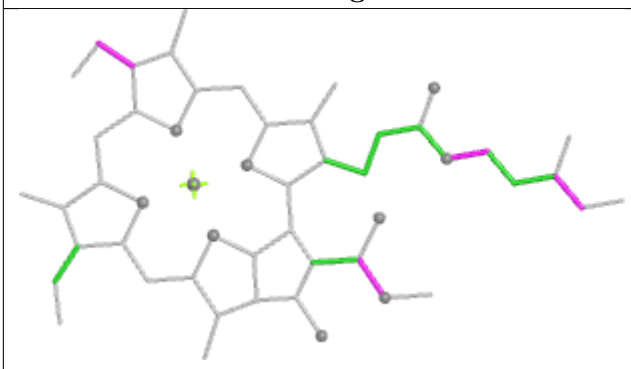


Bond angles



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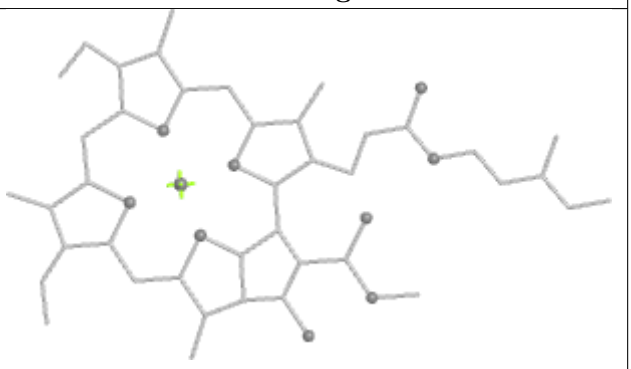
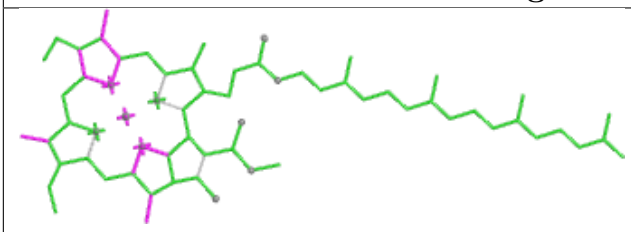
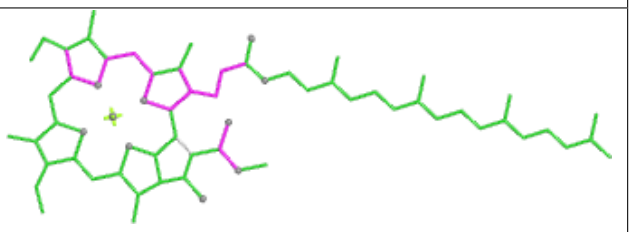


Rings

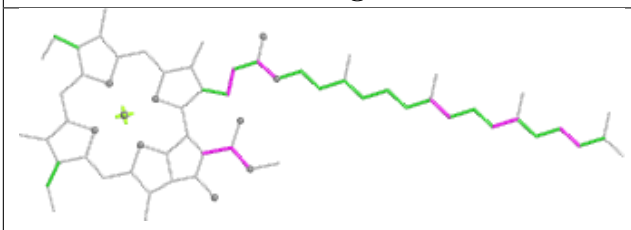
Ligand CLA b 611



Bond lengths



Bond angles



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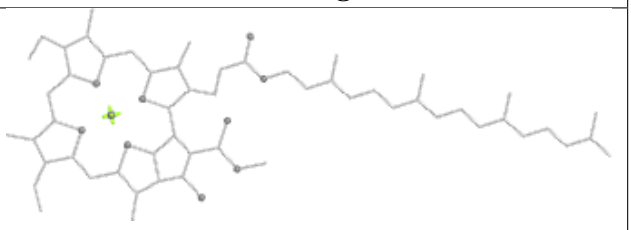
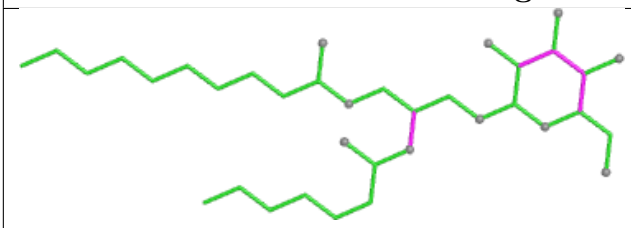


Rings

Ligand LMG 11 301



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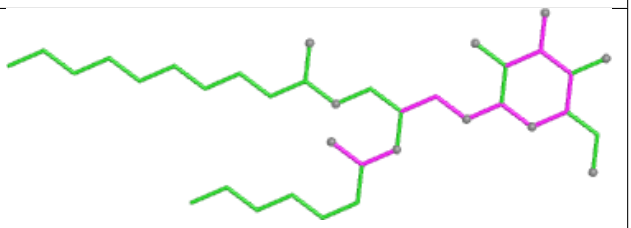
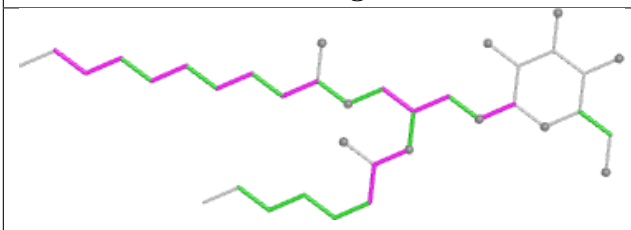


Bond angles



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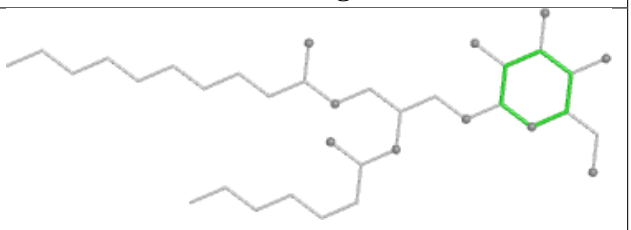
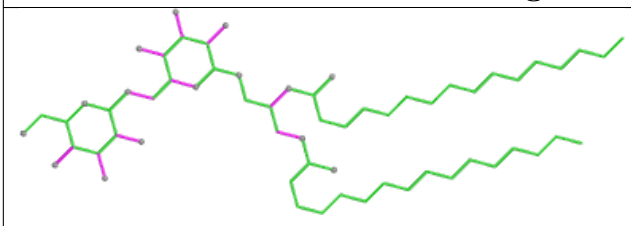
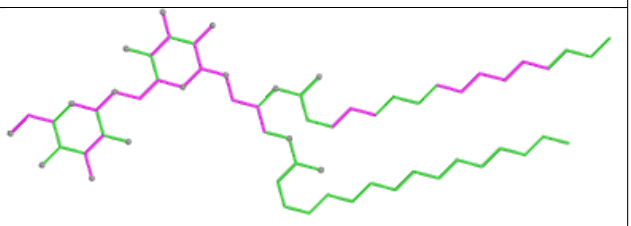


Rings

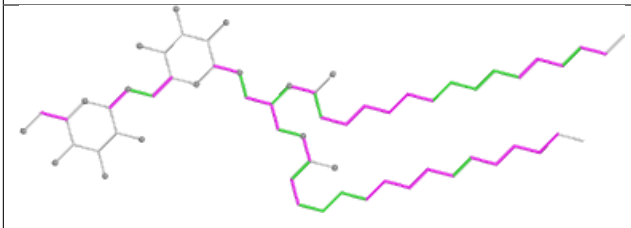
Ligand DGD c 520



Bond lengths



Bond angles



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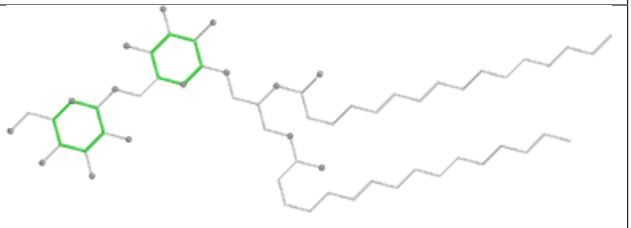
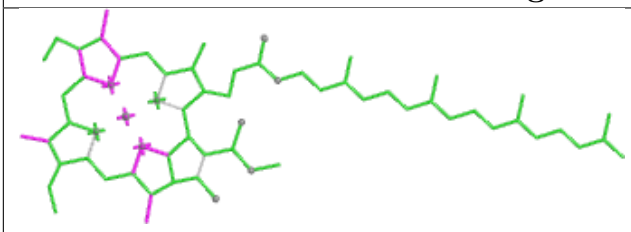


Rings

Ligand CLA b 614



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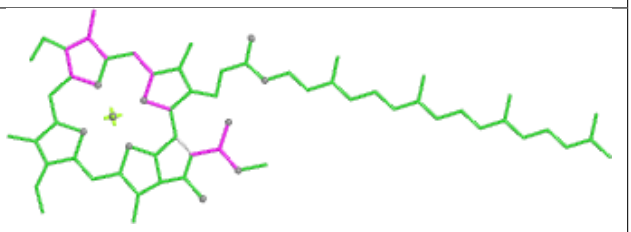

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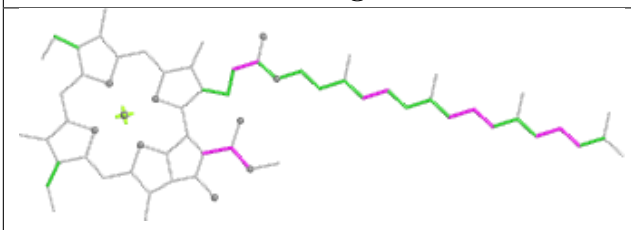

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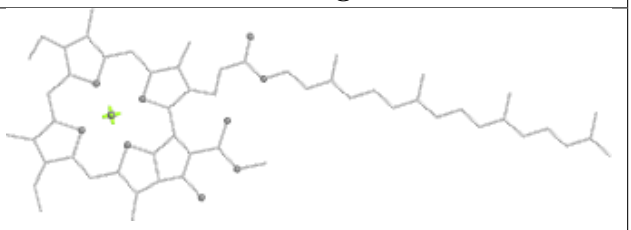

Rings

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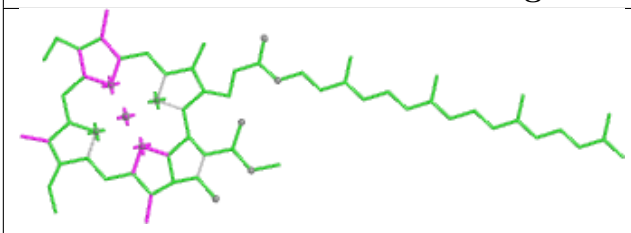

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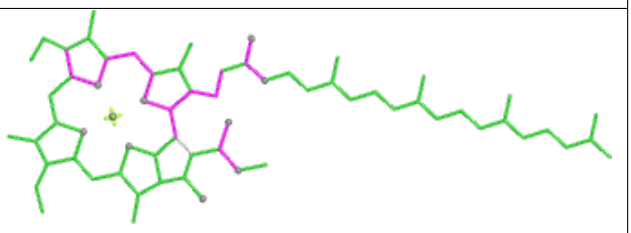

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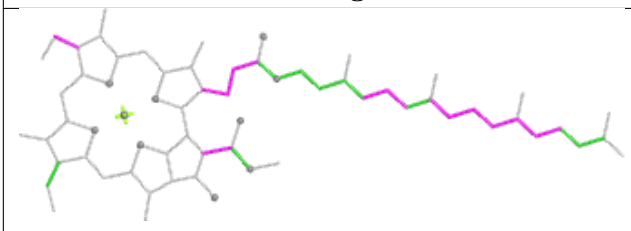

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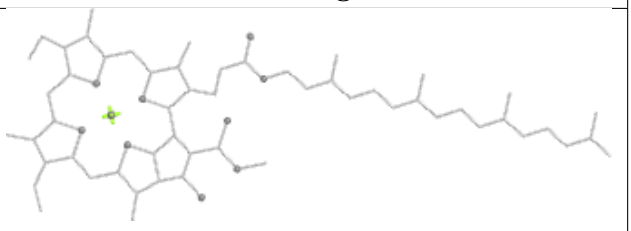
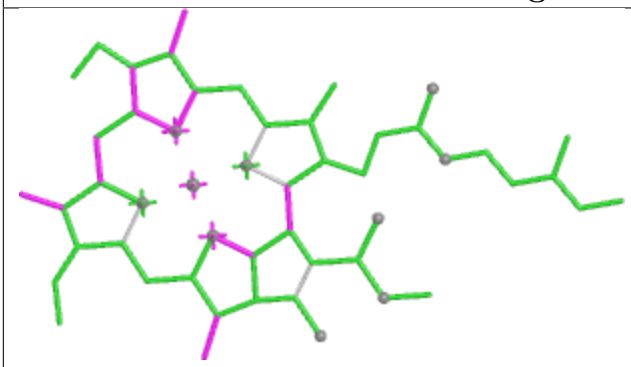


Rings

Ligand CLA 4 312



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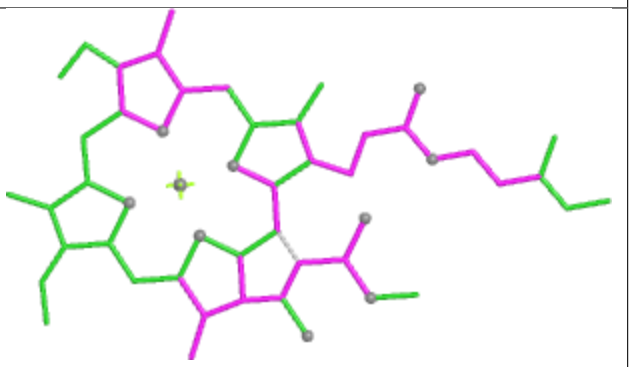

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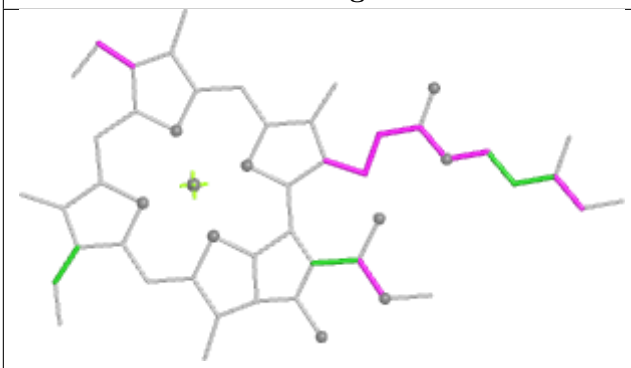

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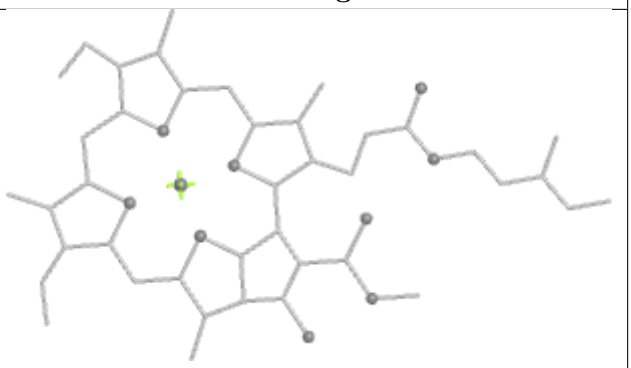
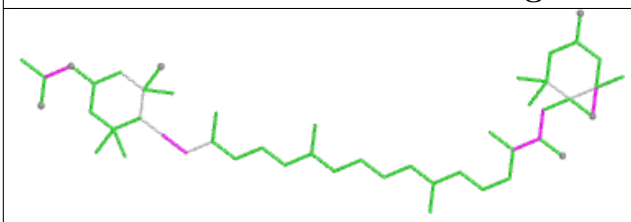


Rings

Ligand A86 18 303



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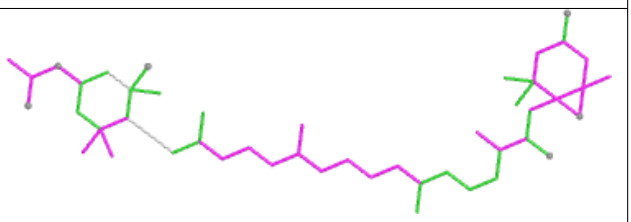

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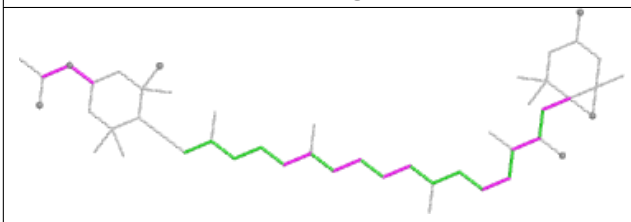

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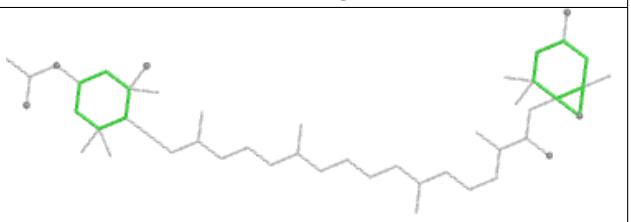
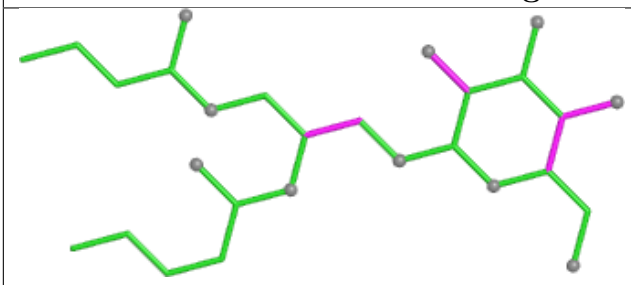


Rings

Ligand LMG n 701



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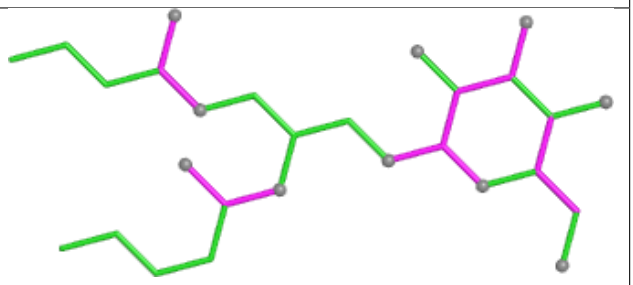

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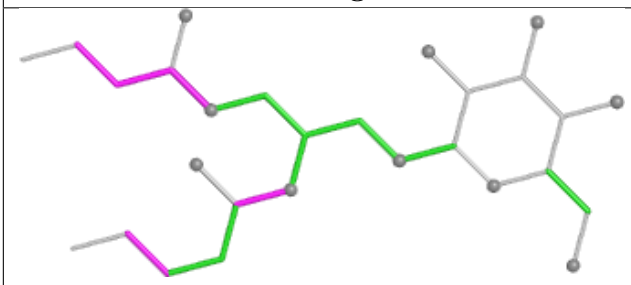

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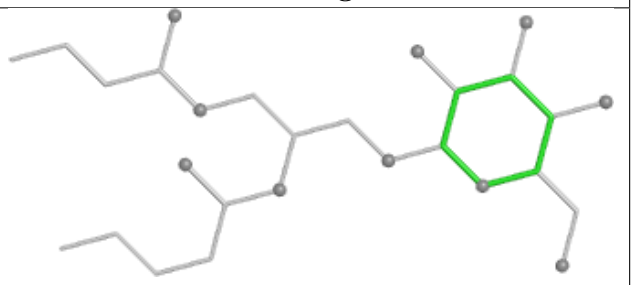
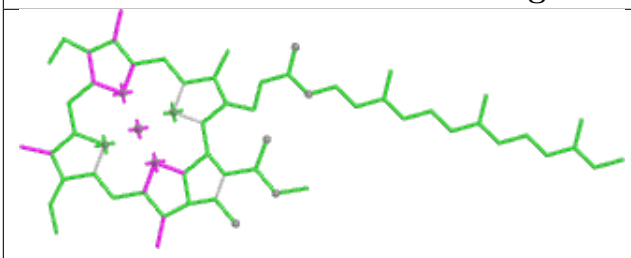


Rings

Ligand CLA 1 321



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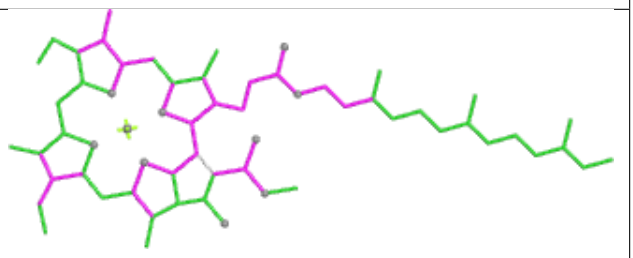

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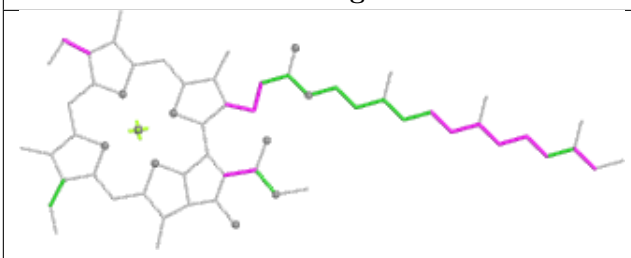

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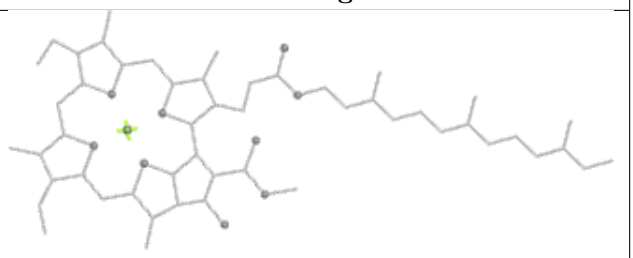

Rings

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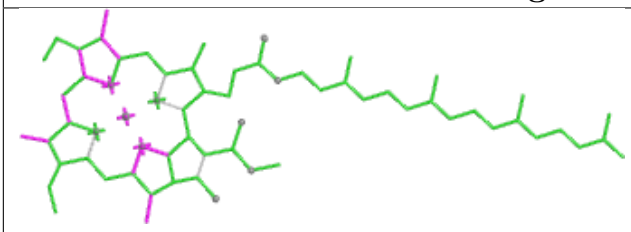

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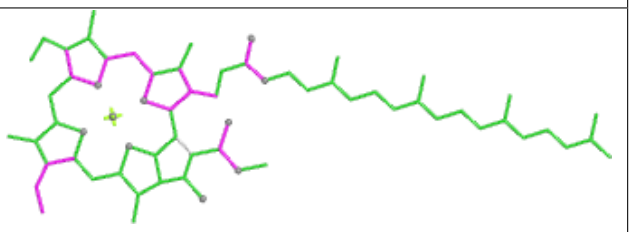

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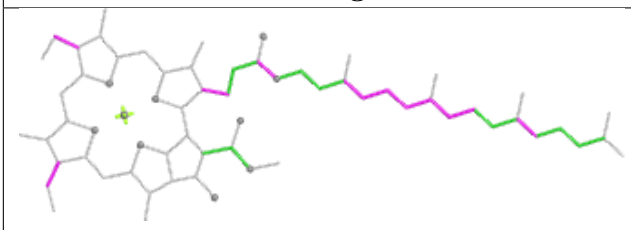

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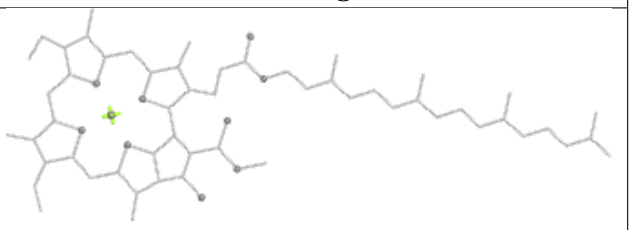
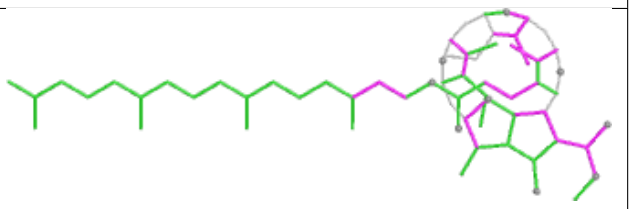


Rings

Ligand PHO a 405



Bond lengths



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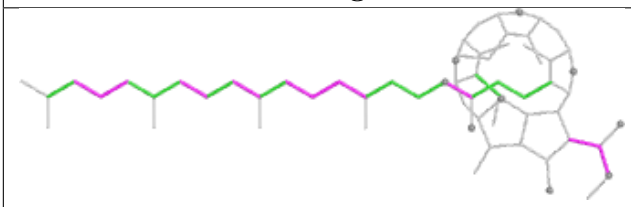

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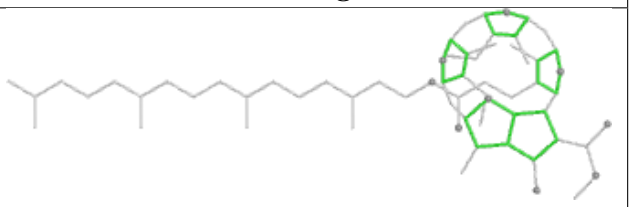
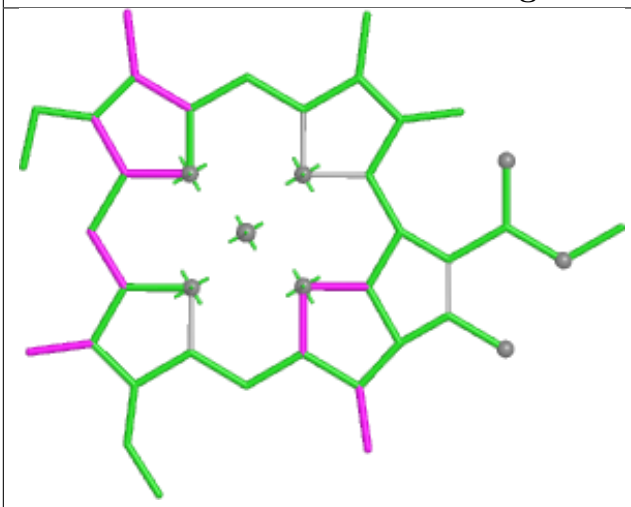


Rings

Ligand CLA 11 316



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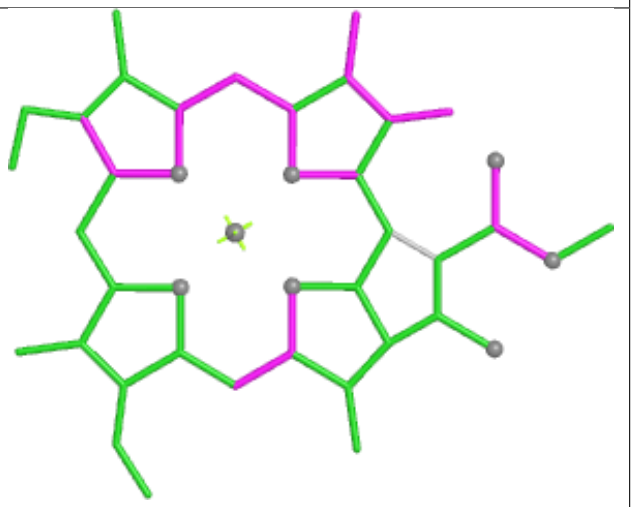

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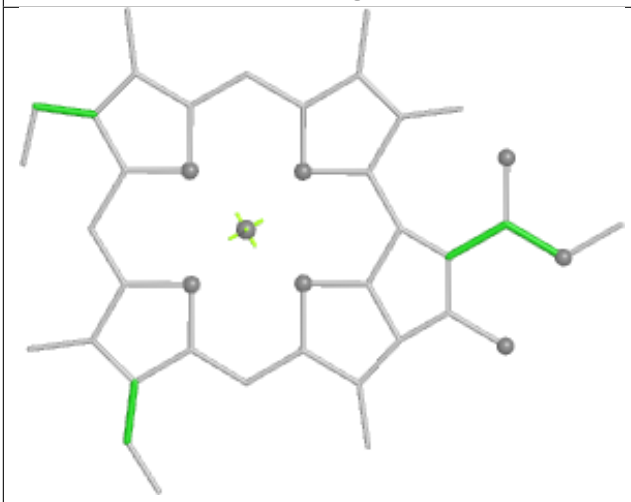

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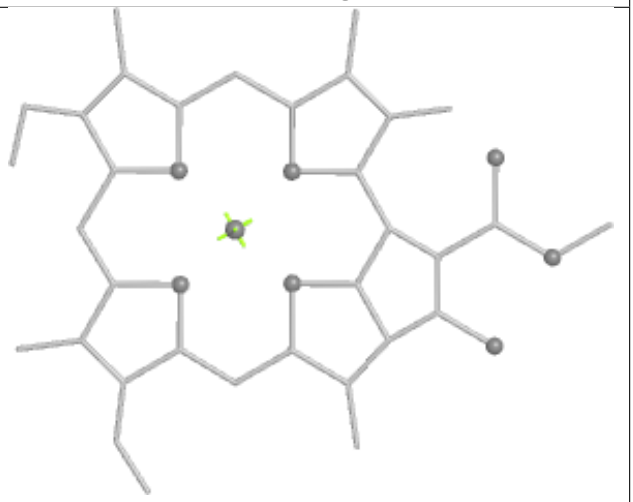

Rings

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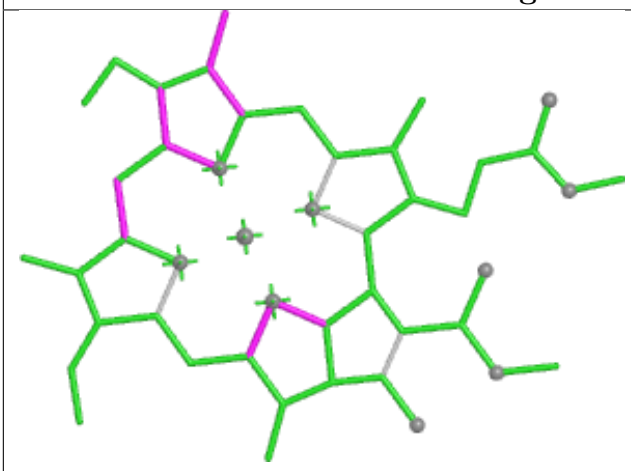

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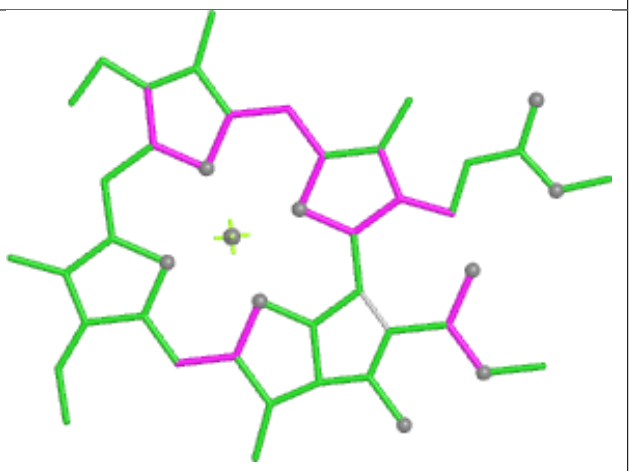

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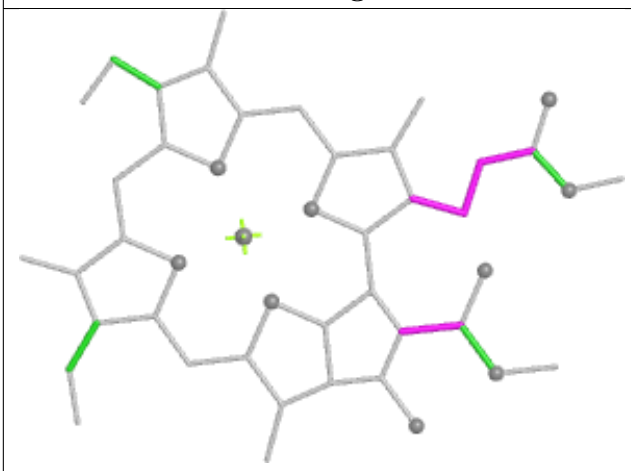

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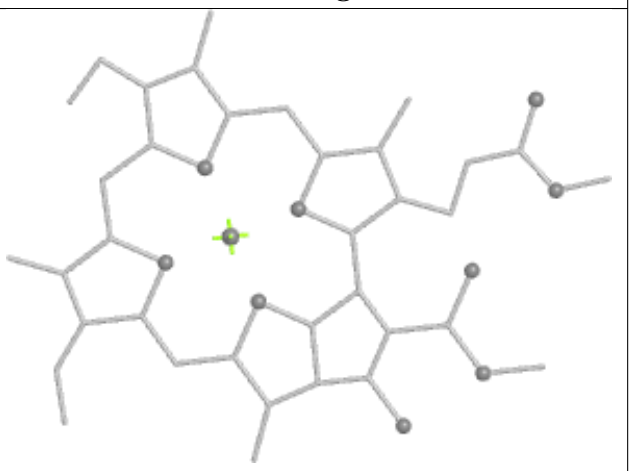
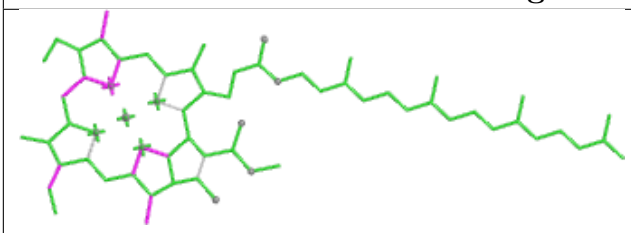


Rings

Ligand CLA b 604



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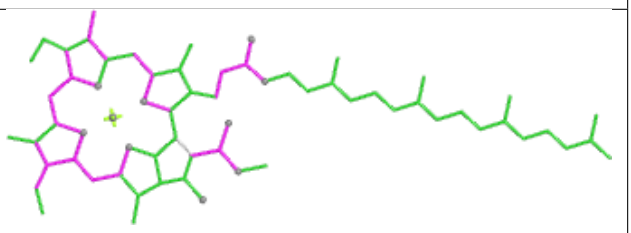
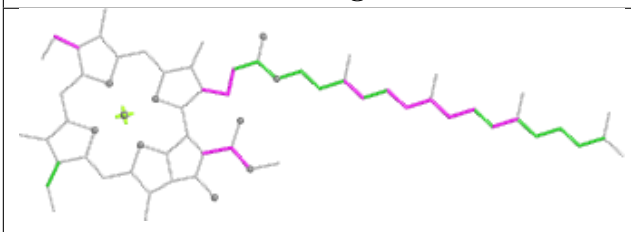


Bond angles



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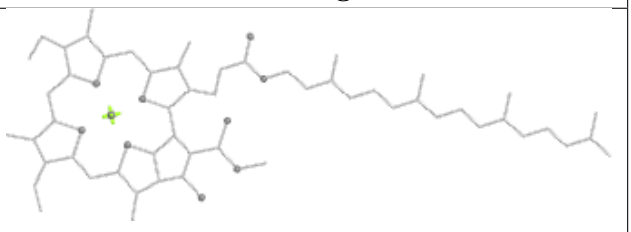
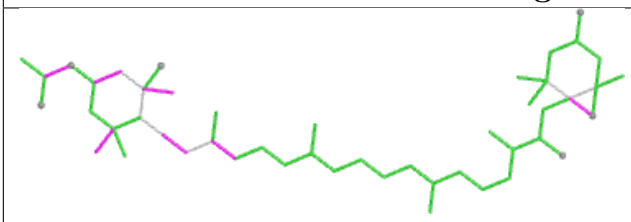


Rings

Ligand A86 2 304



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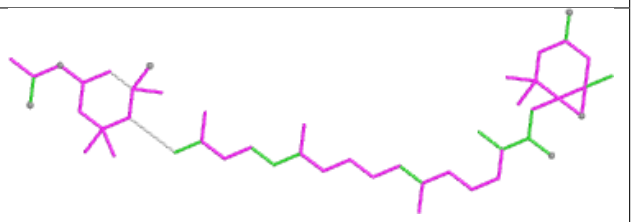
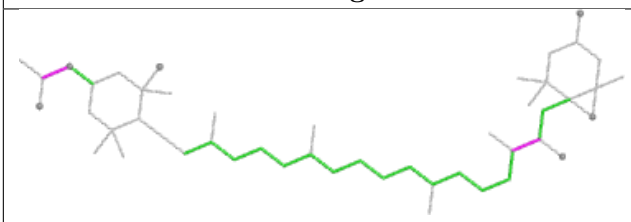


Bond angles



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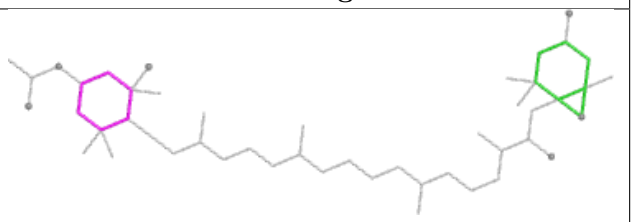
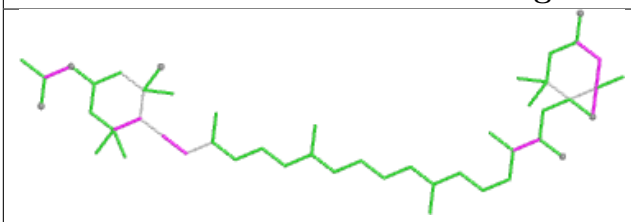


Rings

Ligand A86 4 303



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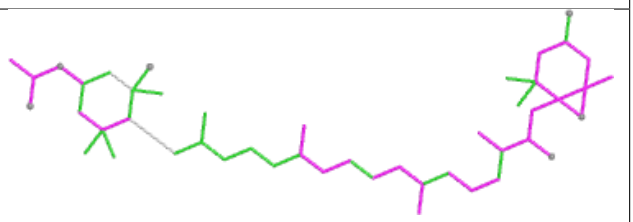
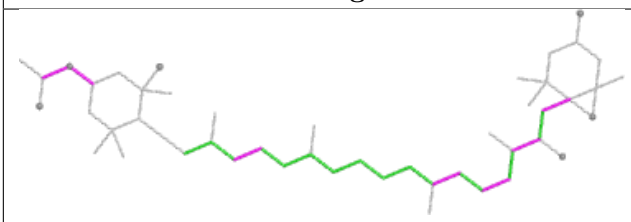


Bond angles



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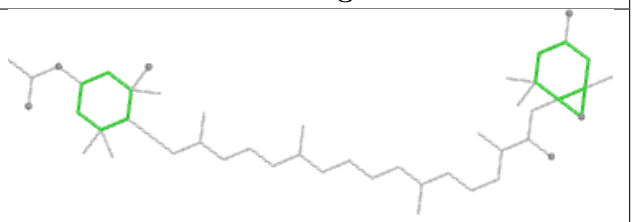
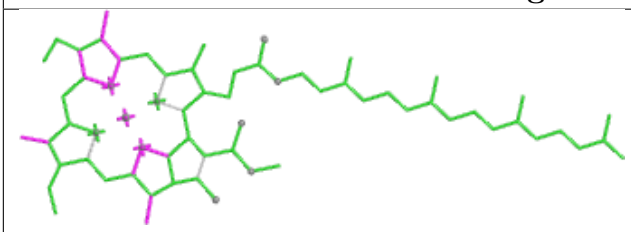


Rings

Ligand CLA p 601



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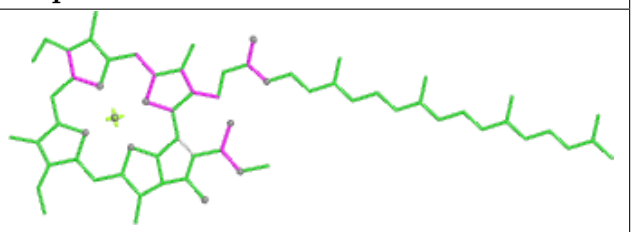
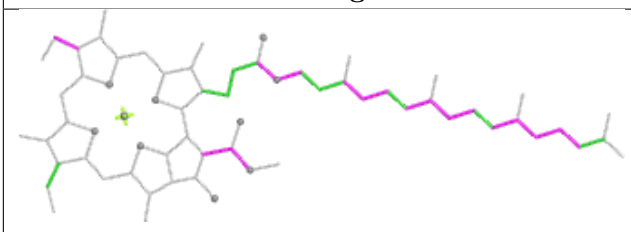


Bond angles



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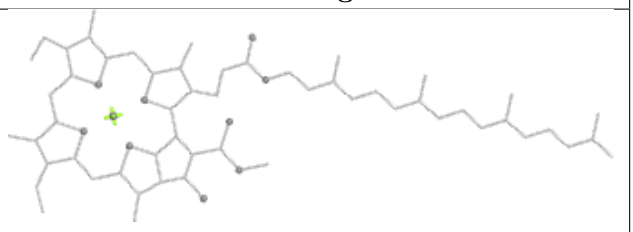
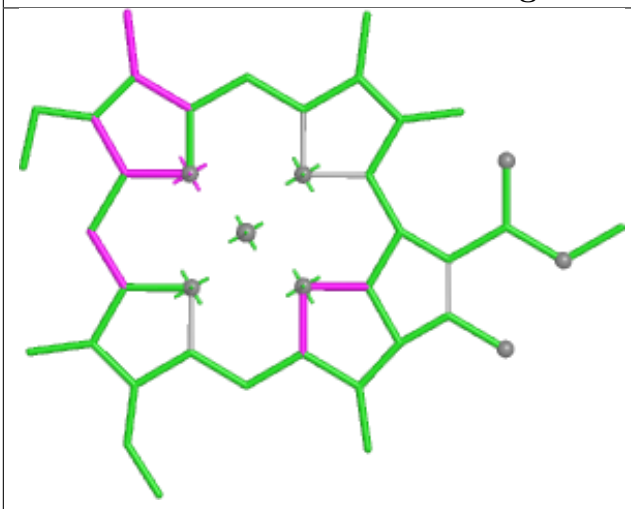
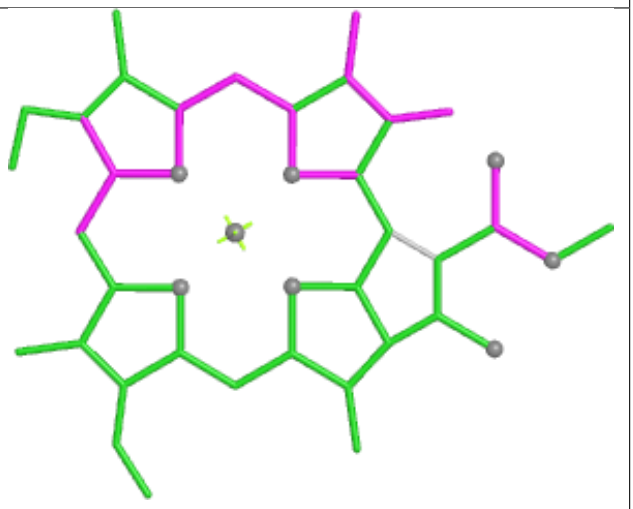


Rings

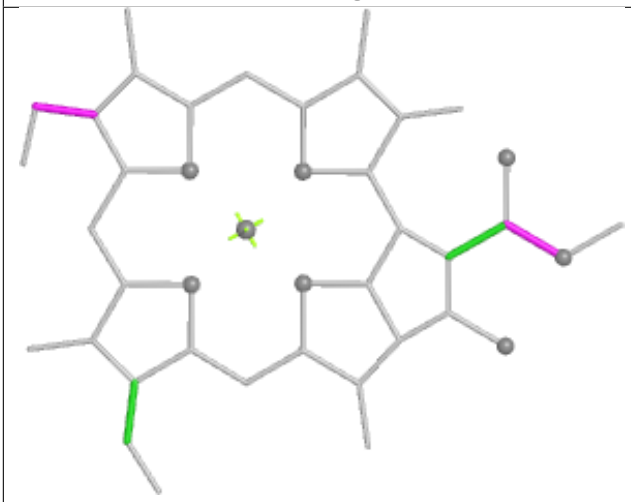
Ligand CLA 13 310



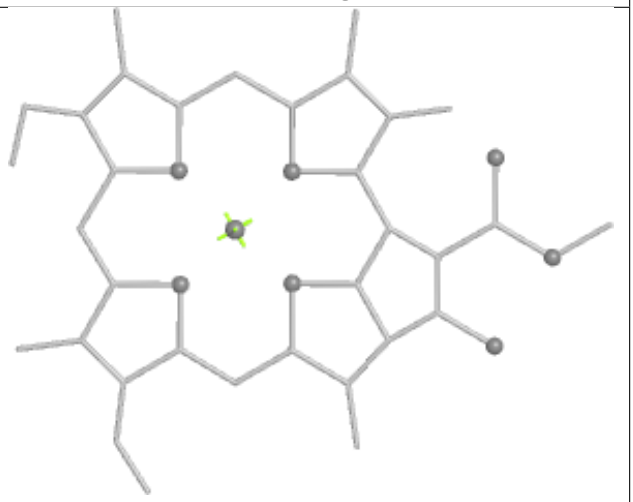
Bond lengths



Bond angles

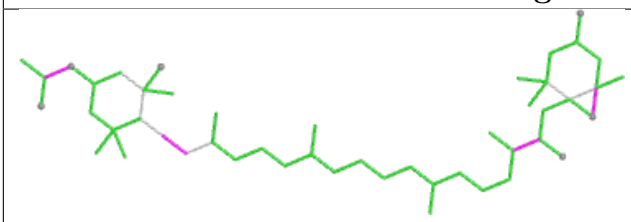


Torsions



Rings

Ligand A86 9 303



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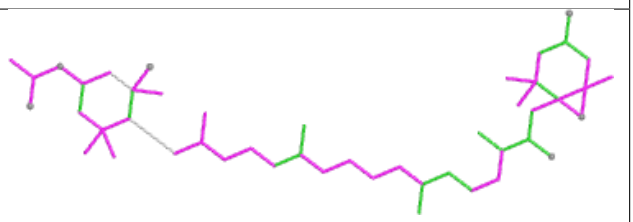

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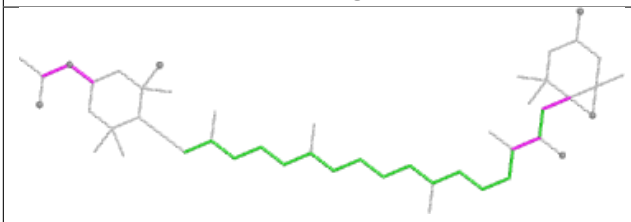

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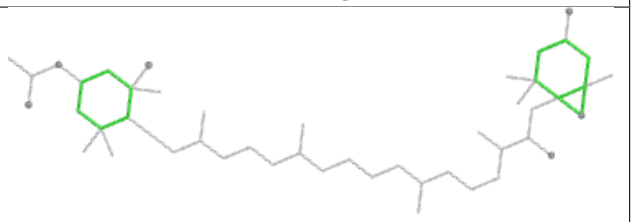

Rings

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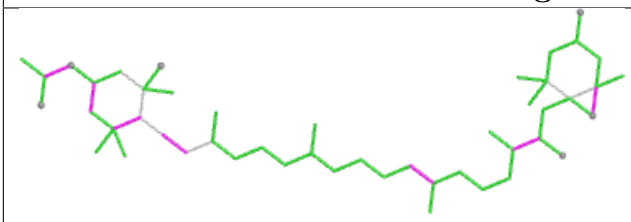

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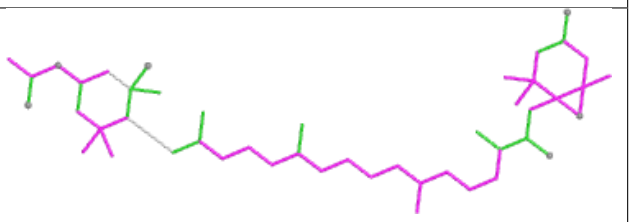

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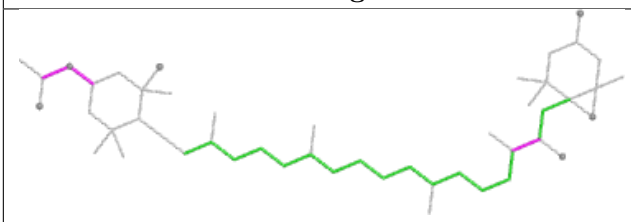

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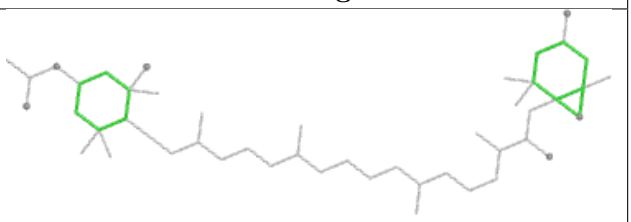
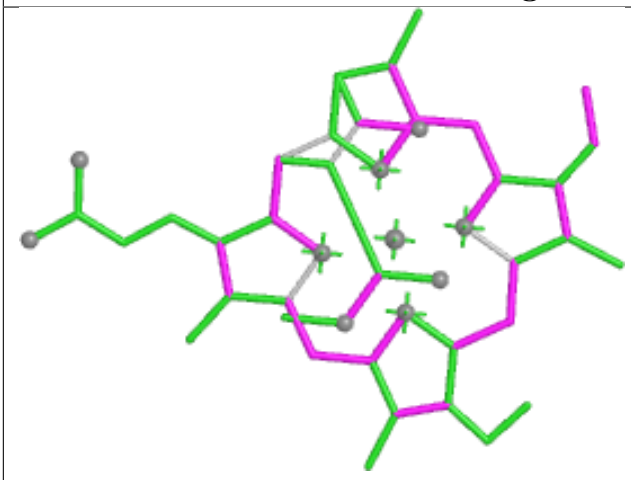


Rings

Ligand KC2 11 309



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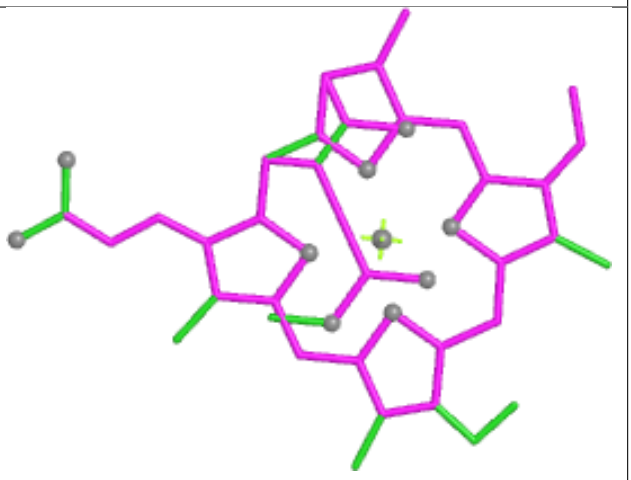

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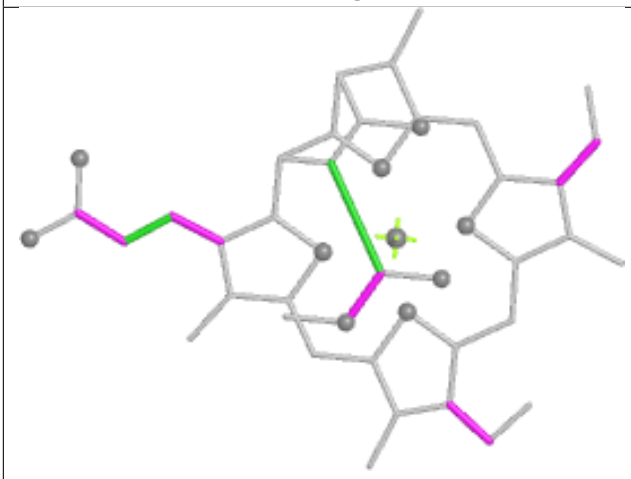

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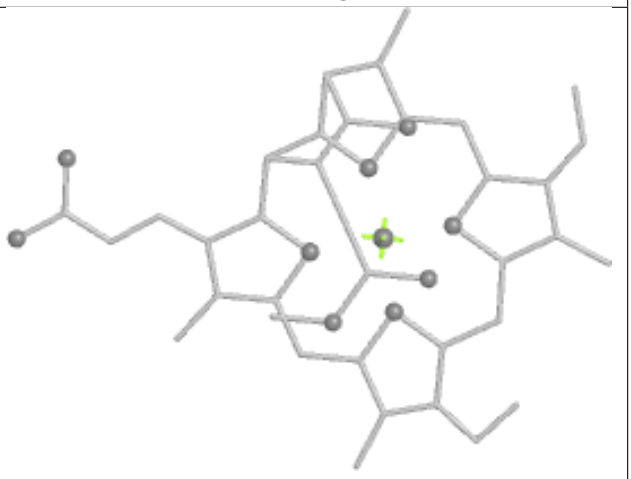

Rings

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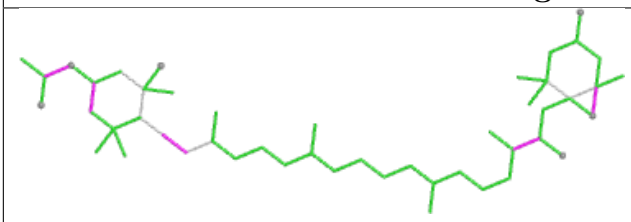
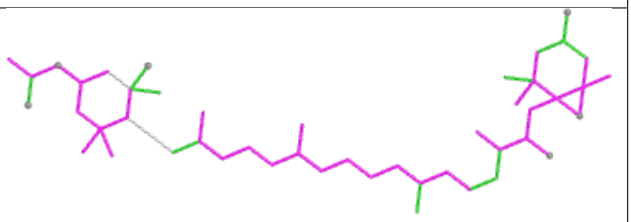
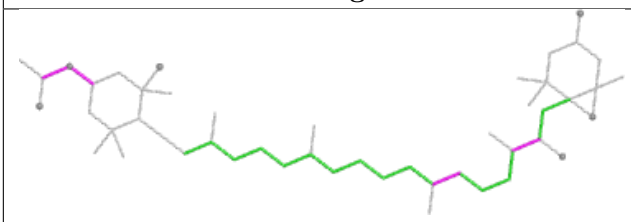
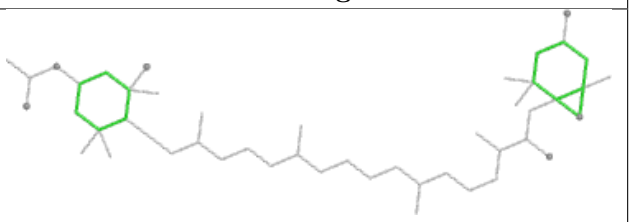
 Bond lengths	 Bond angles
 Torsions	 Rings

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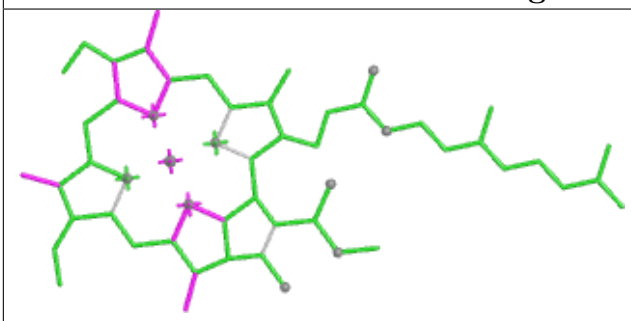
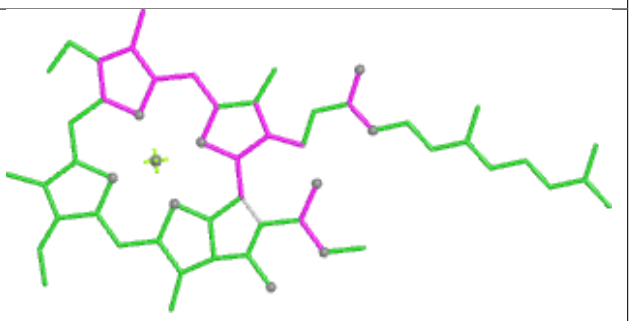
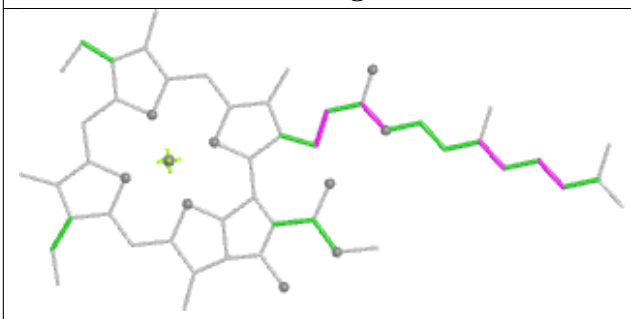
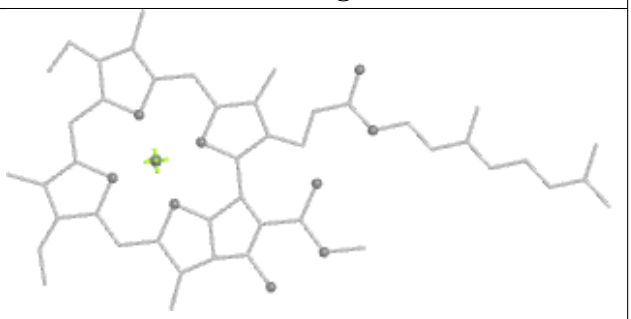
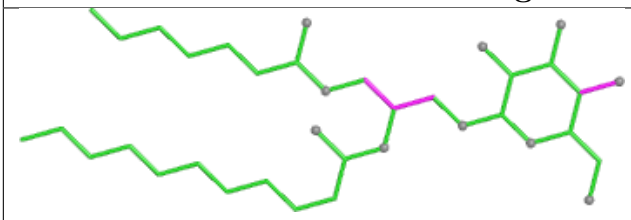
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG 15 314



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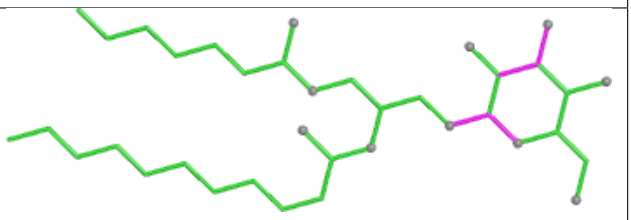
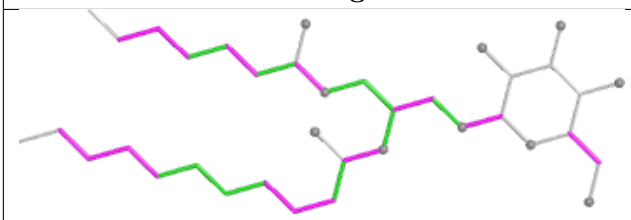


Bond angles



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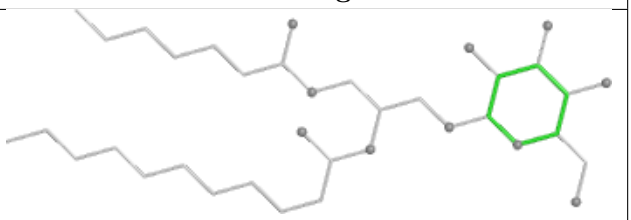
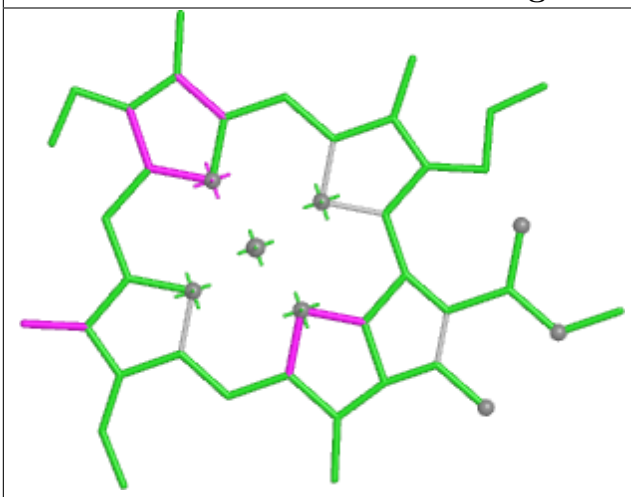


Rings

Ligand CLA 2 309



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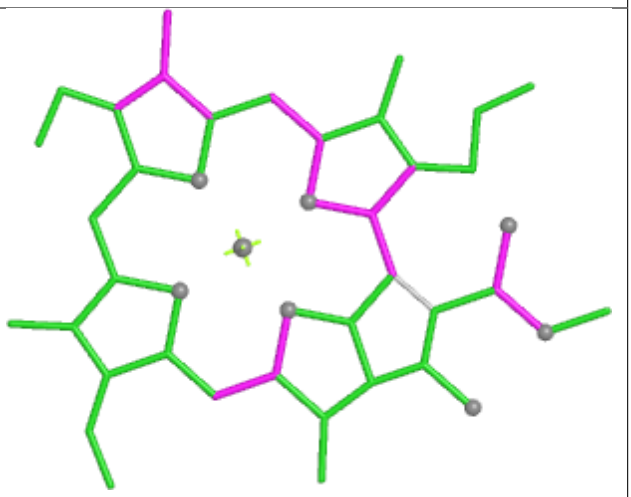

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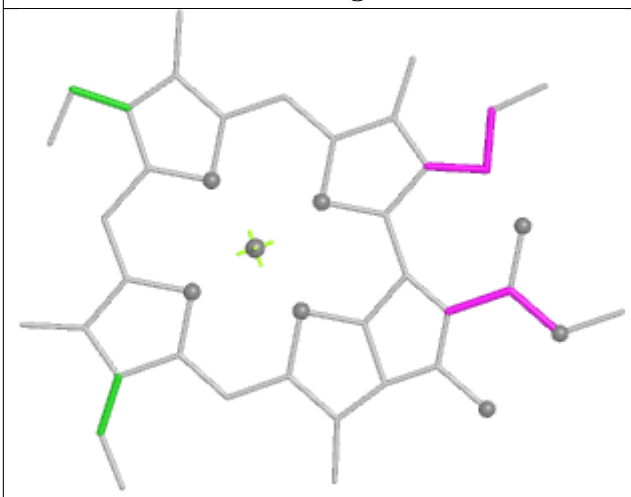

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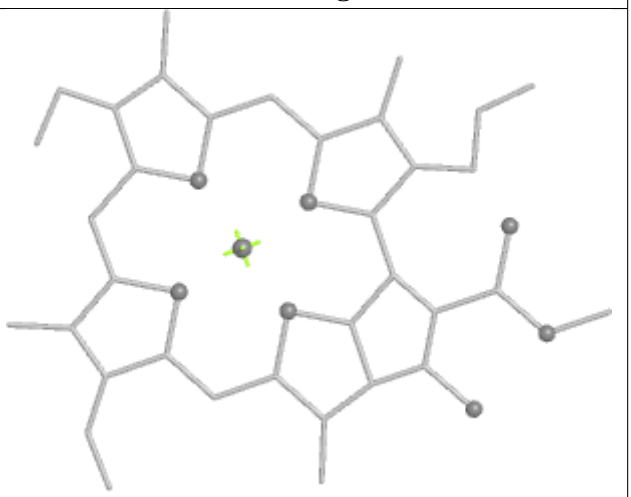

Rings

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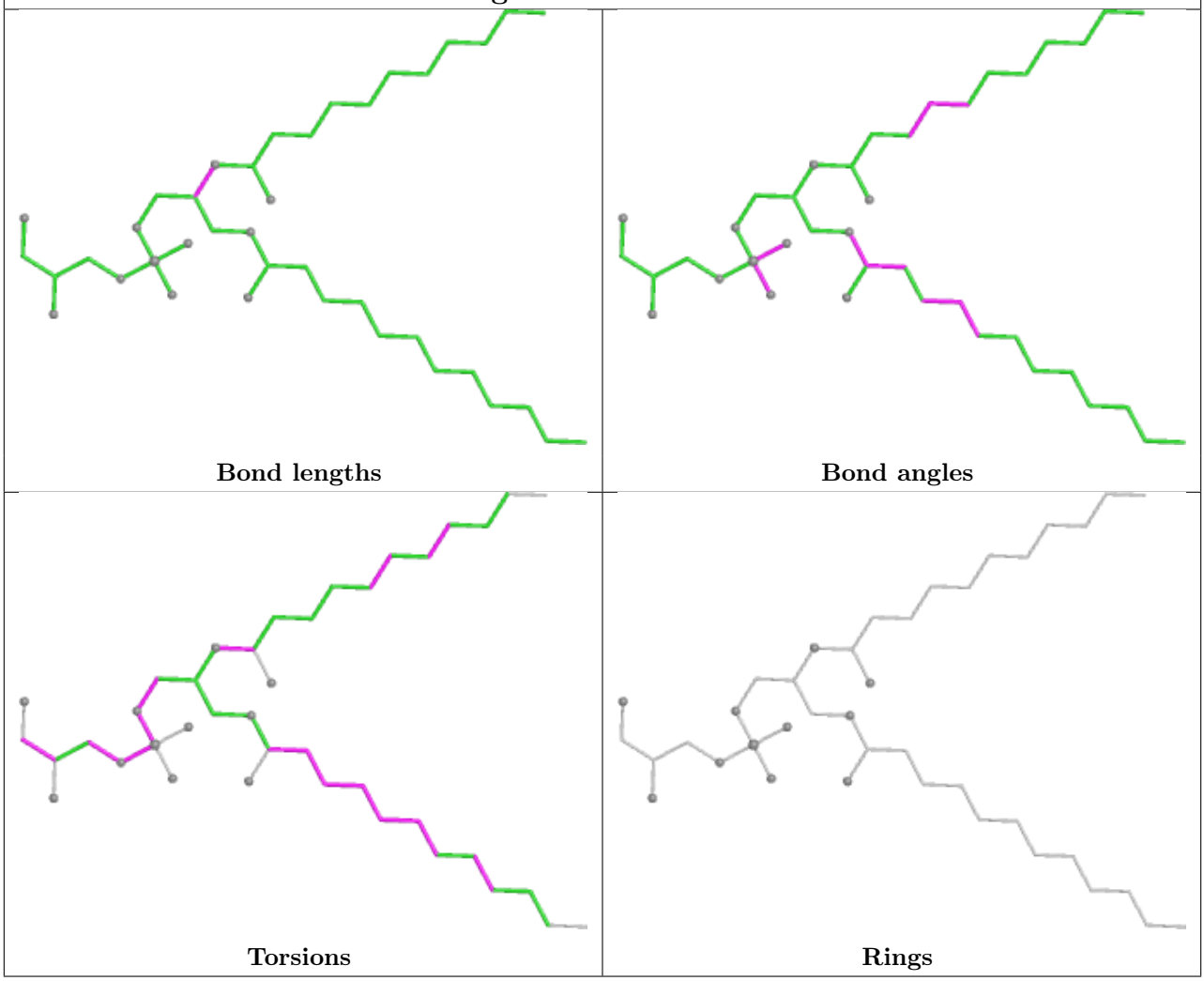
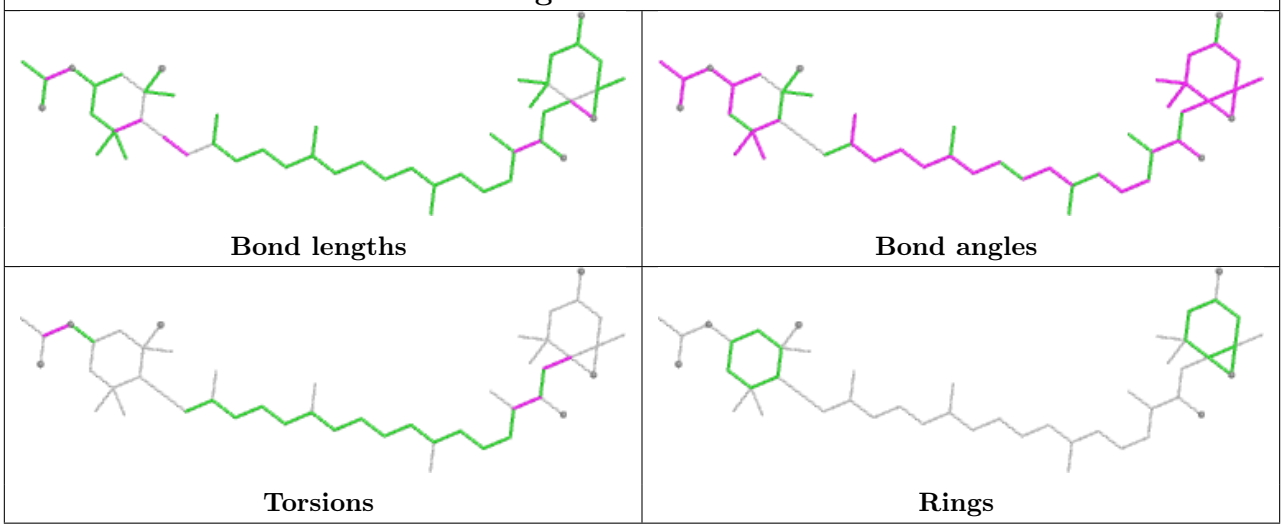


Ligand A86 0 304



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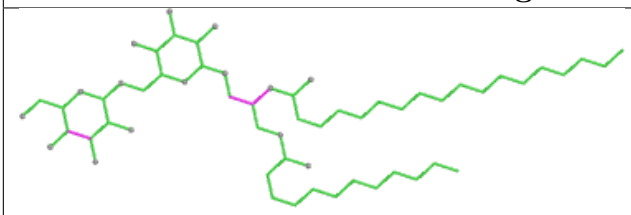

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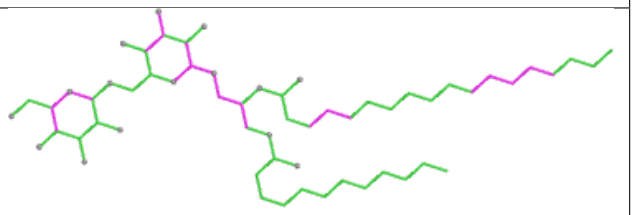
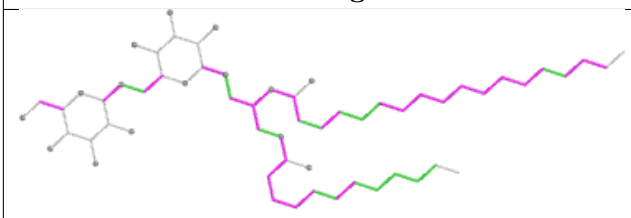


Bond angles



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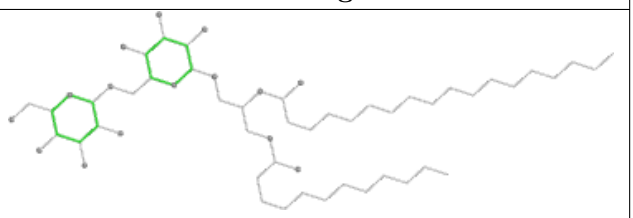

Rings

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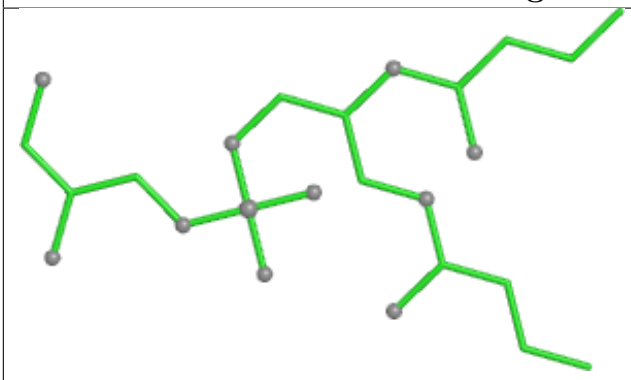

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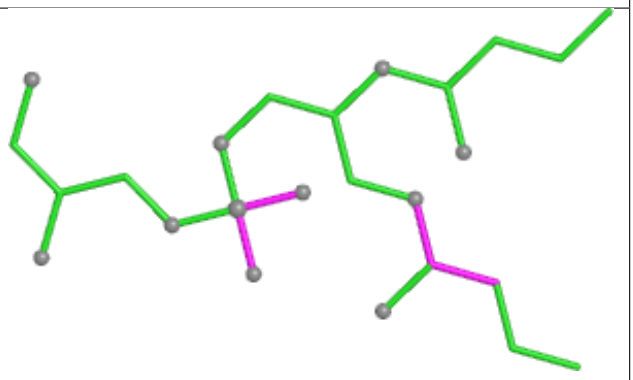

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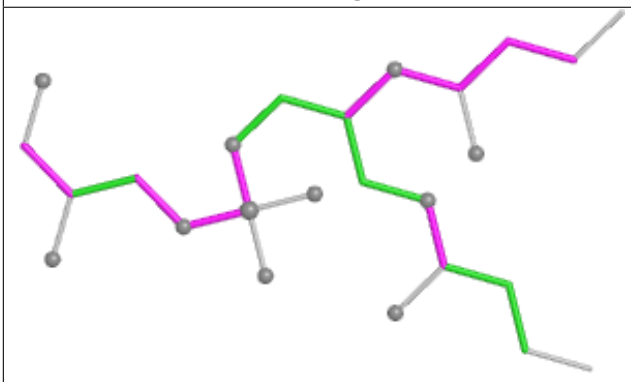

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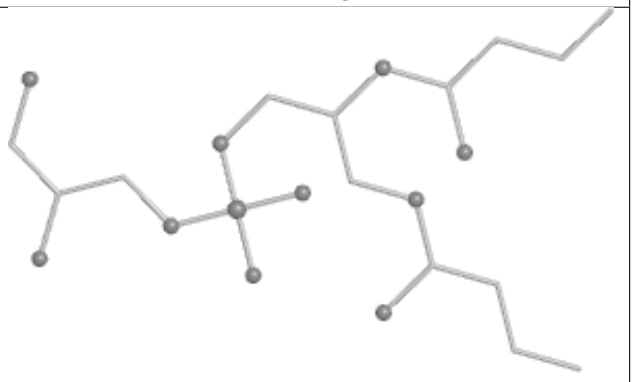

Rings

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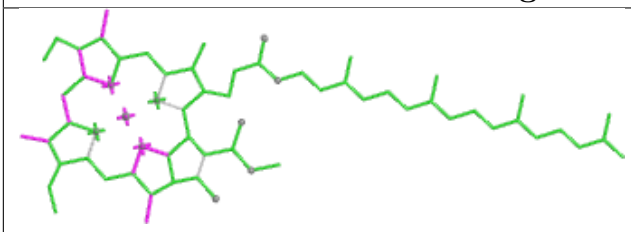

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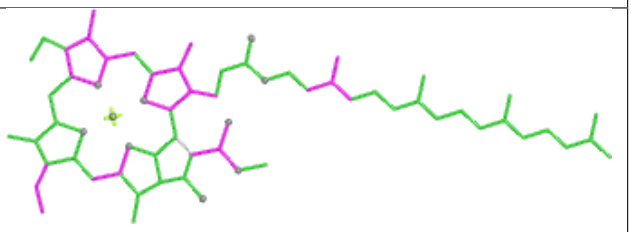
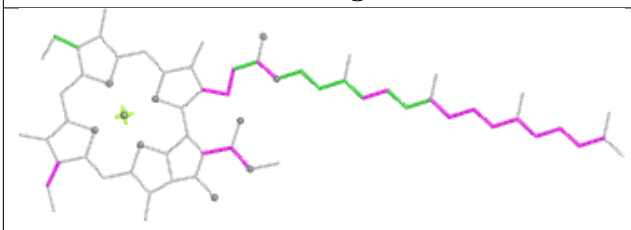


Bond angles



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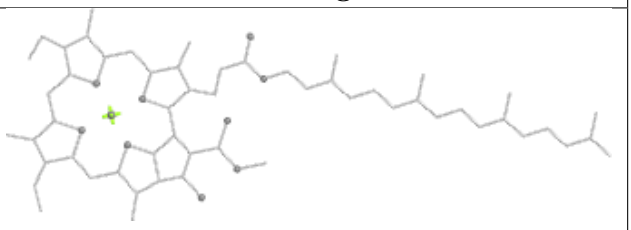
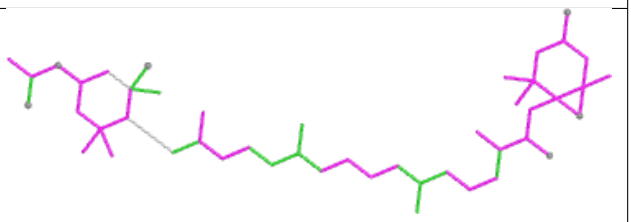


Rings

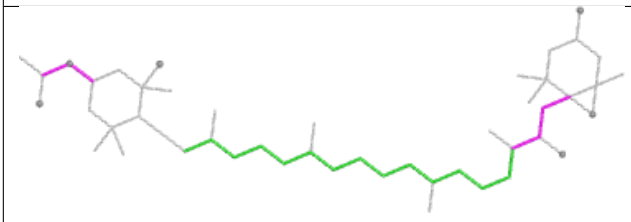
Ligand A86 15 304



Bond lengths



Bond angles



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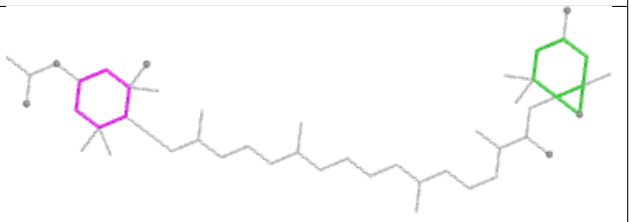
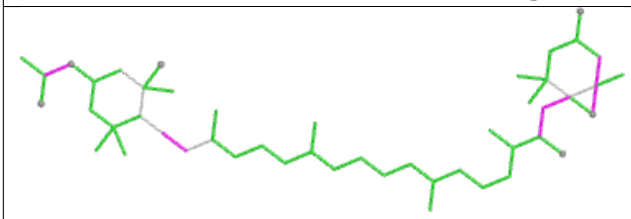


Rings

Ligand A86 19 305



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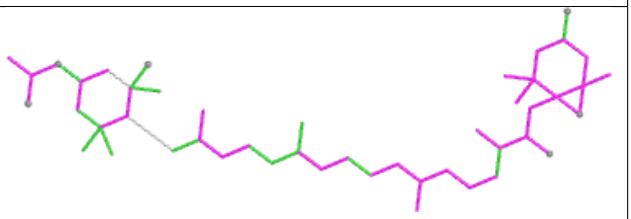

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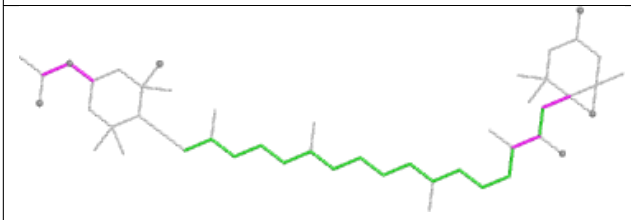

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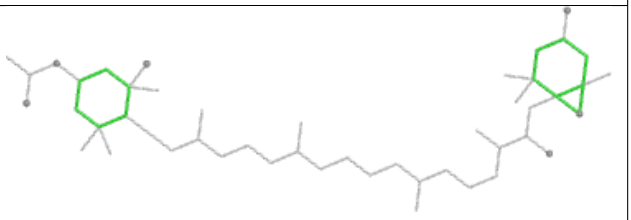
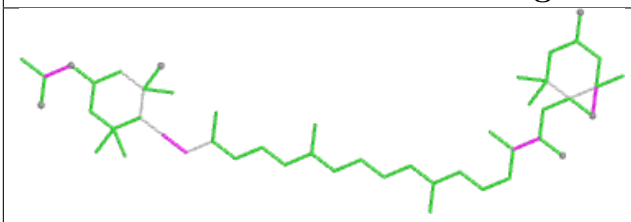


Rings

Ligand A86 5 318



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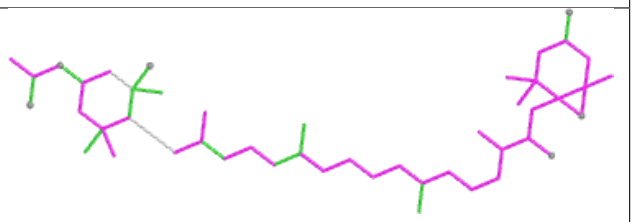
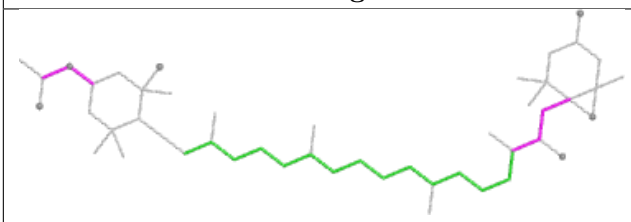


Bond angles



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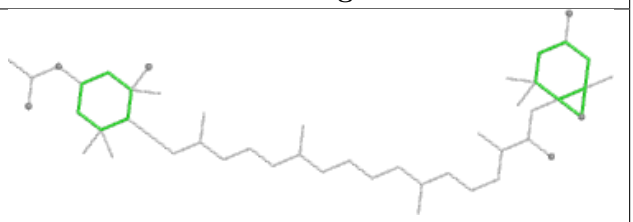
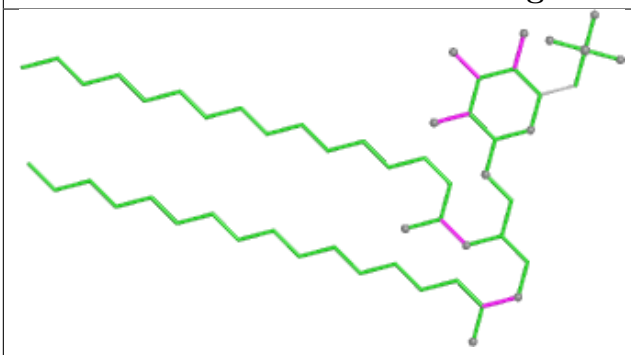


Rings

Ligand SQD L 102



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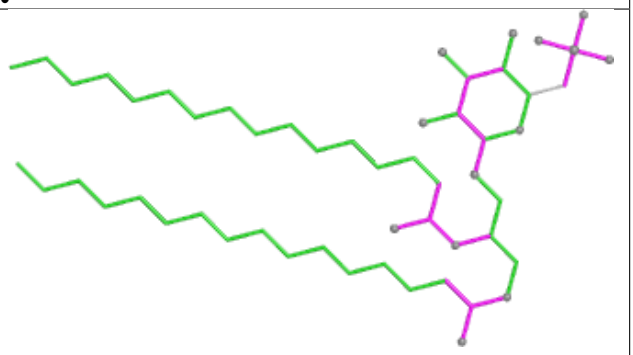
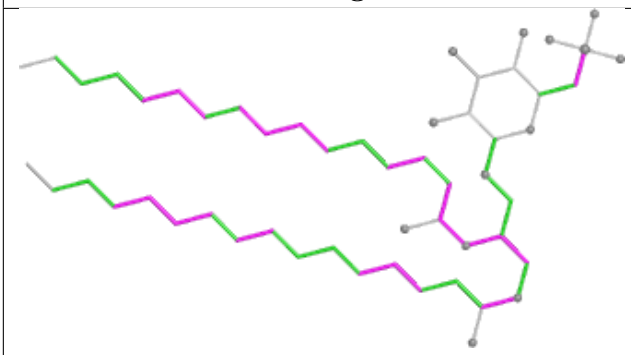
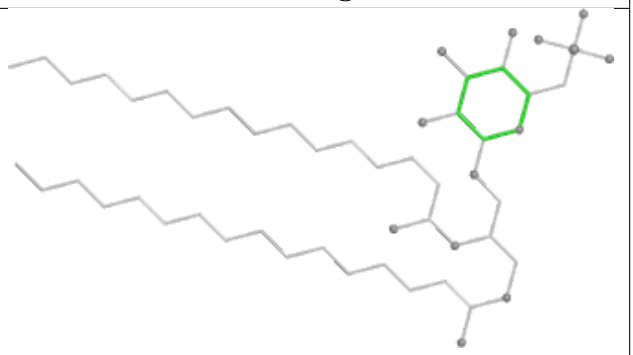


Bond angles



Torsions



Rings

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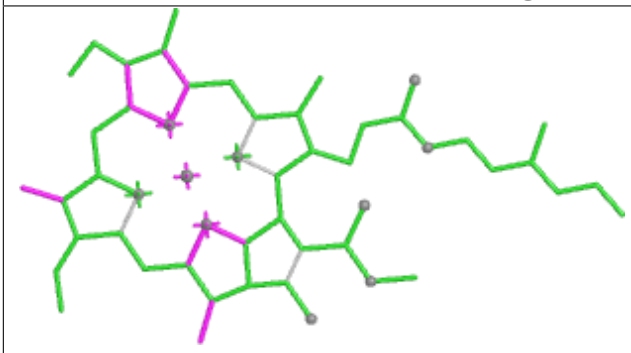
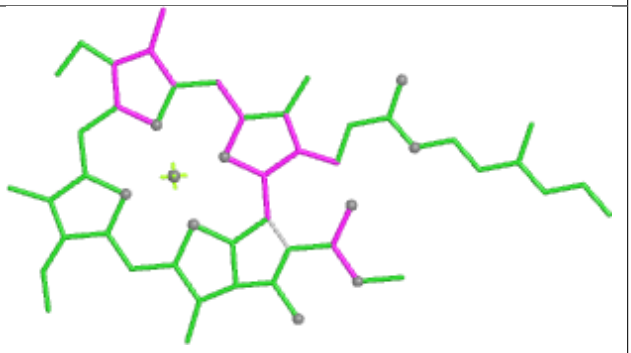
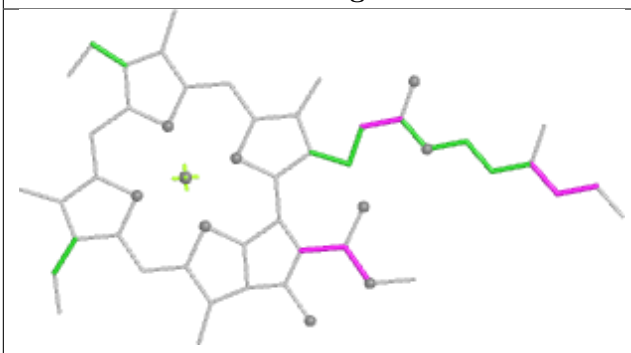
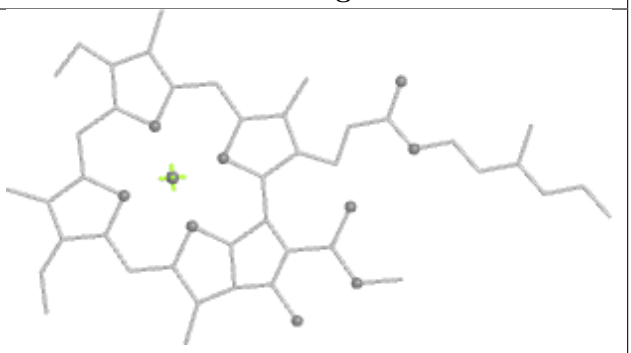
 Bond lengths	 Bond angles
 Torsions	 Rings

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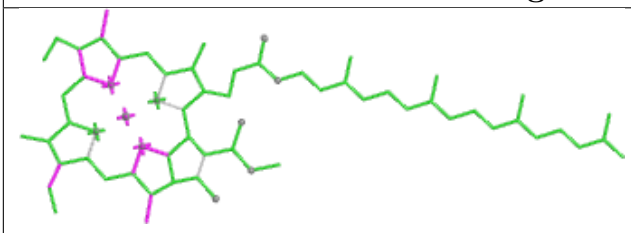
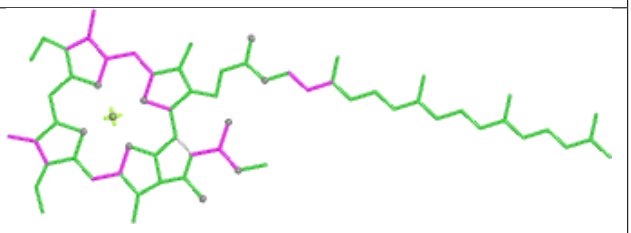
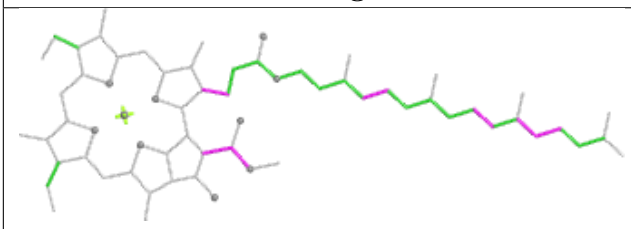
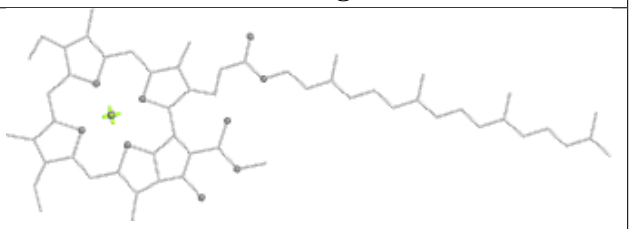
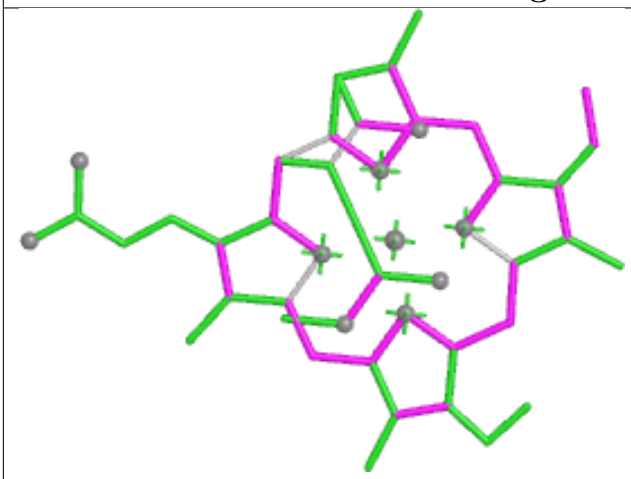
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 4 308



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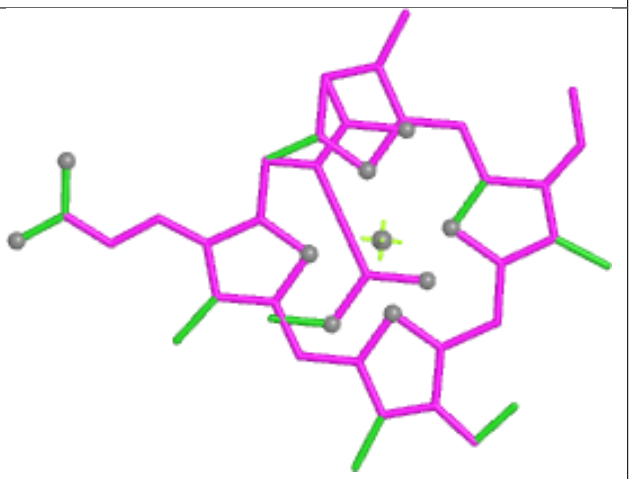

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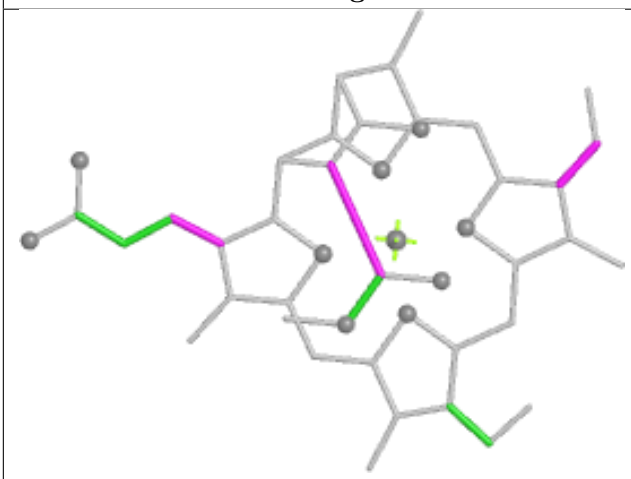

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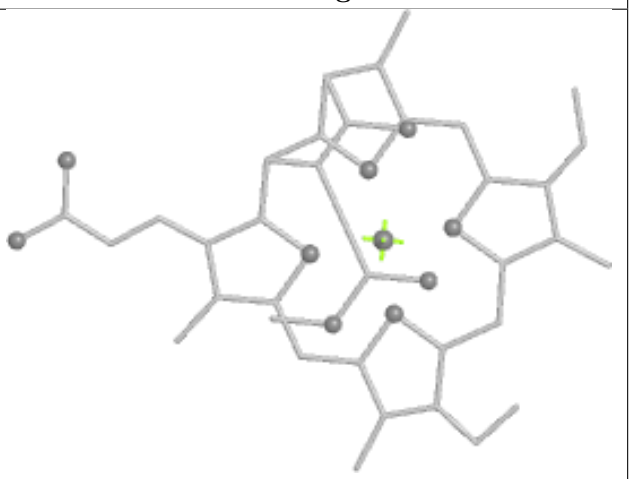

Rings

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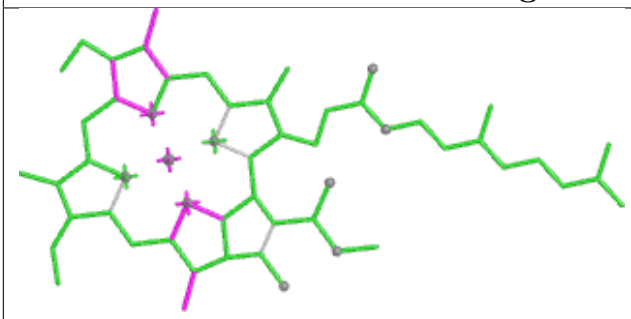

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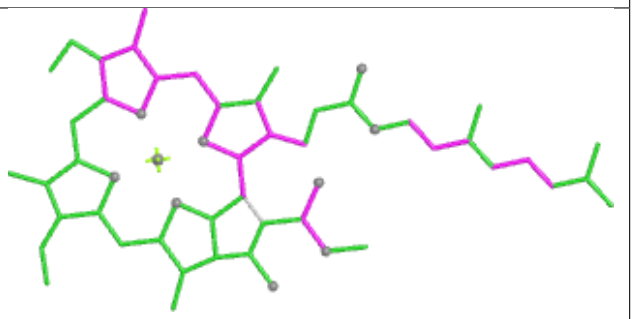

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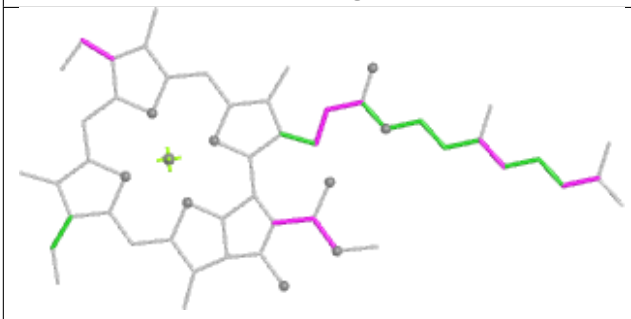

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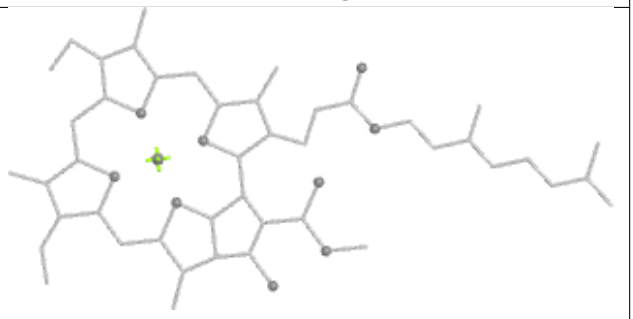

Rings

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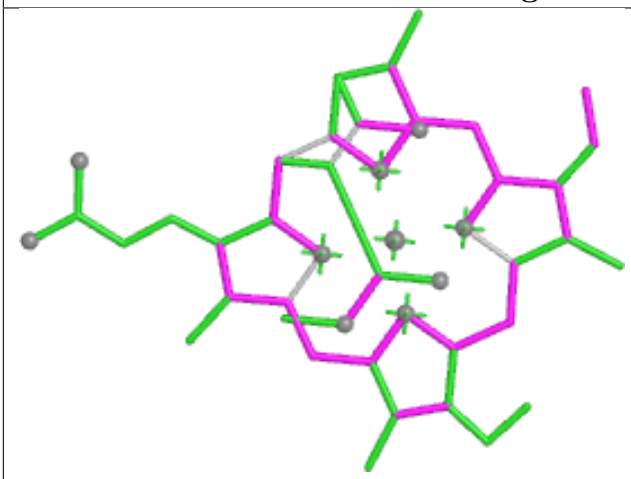

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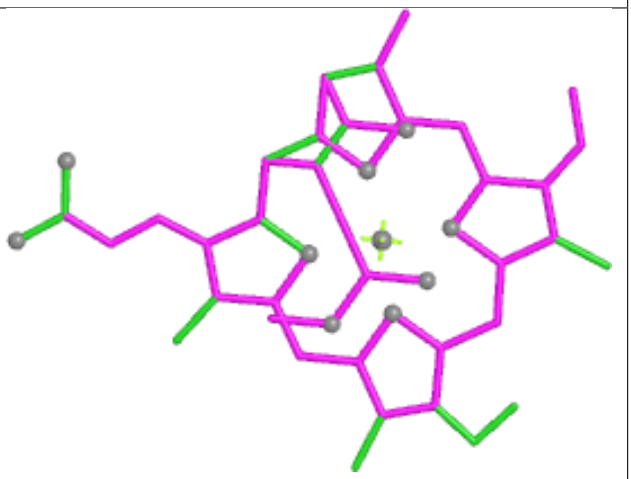

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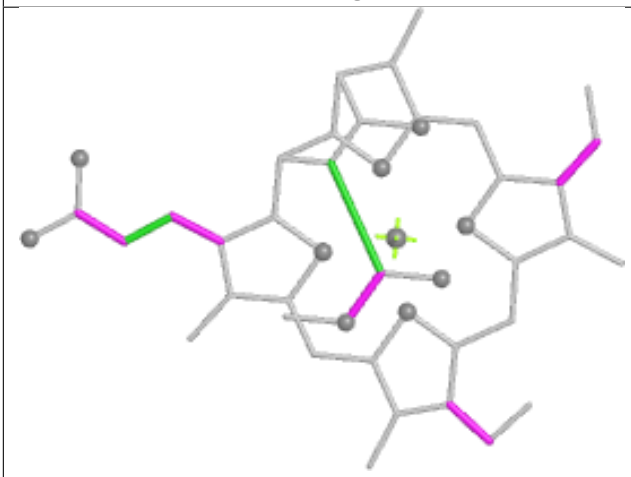

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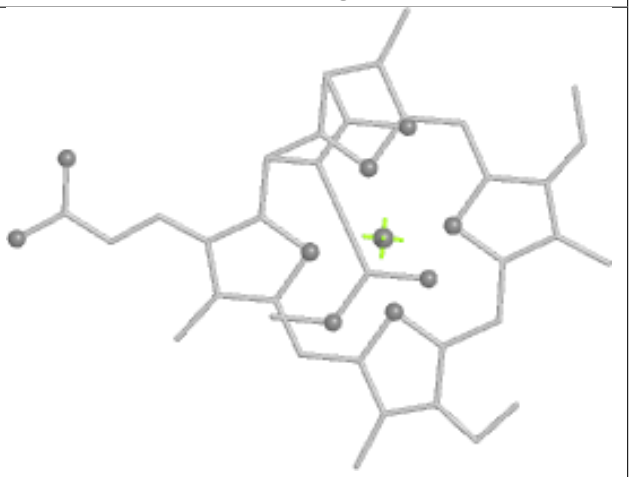

Rings

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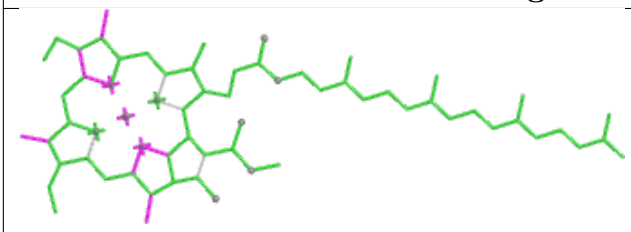

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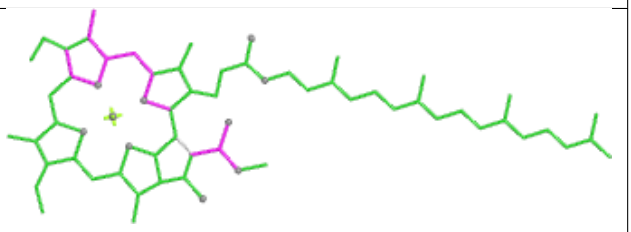

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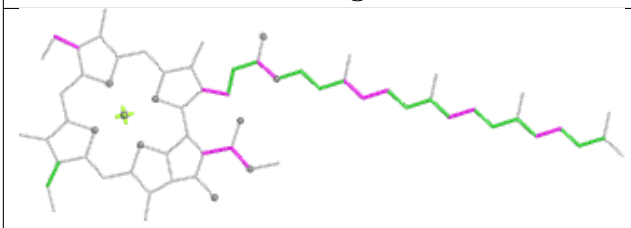

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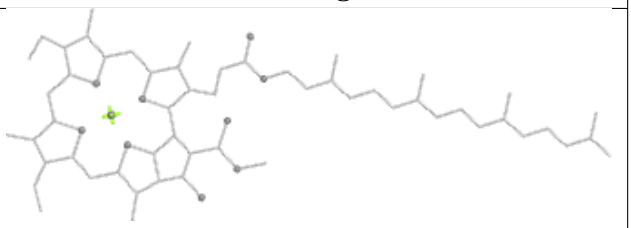

Rings

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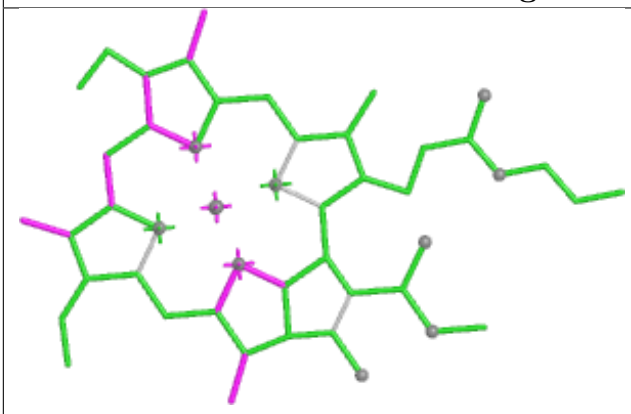

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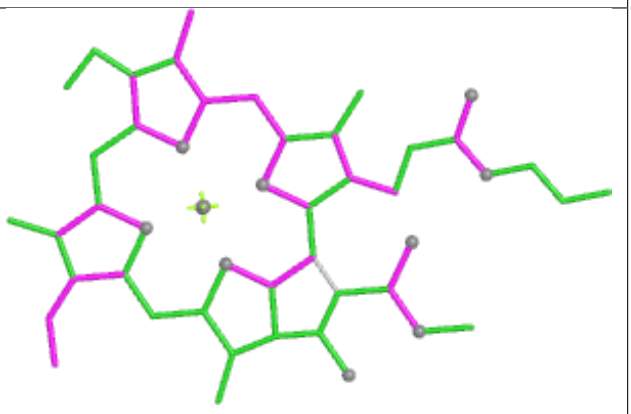

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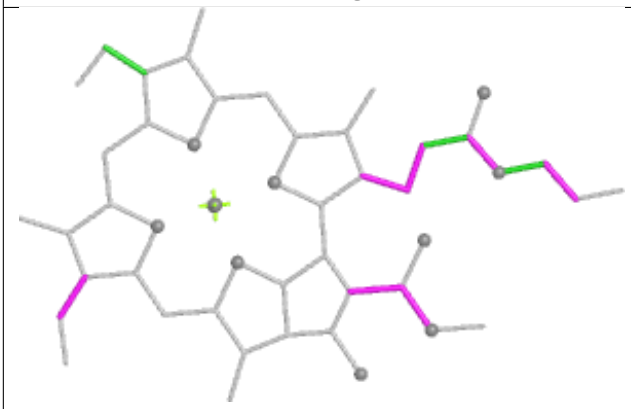

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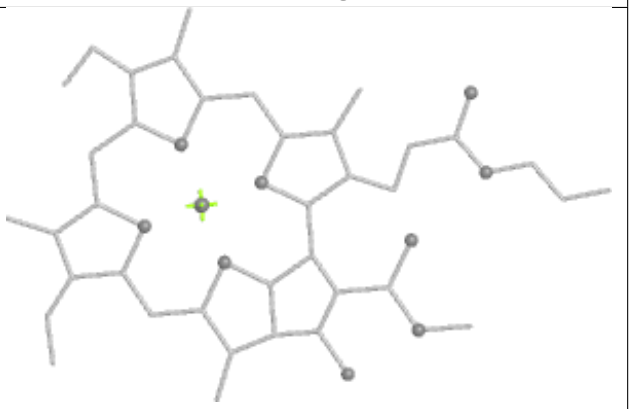

Rings

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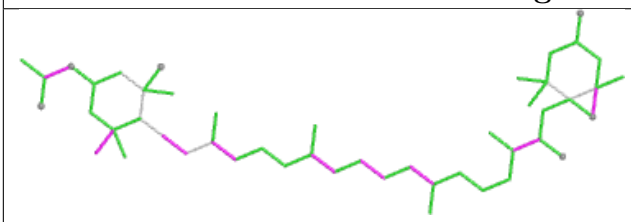

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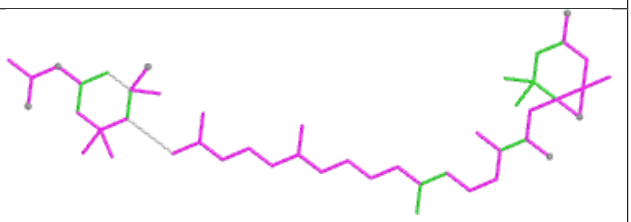

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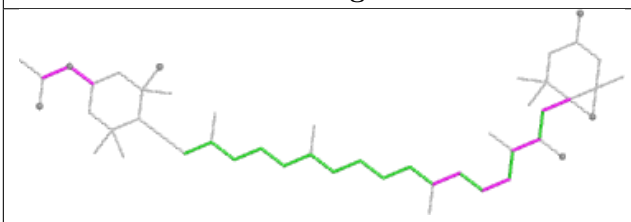

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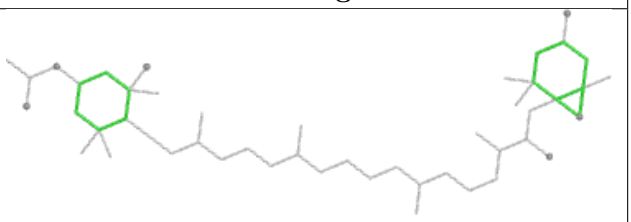

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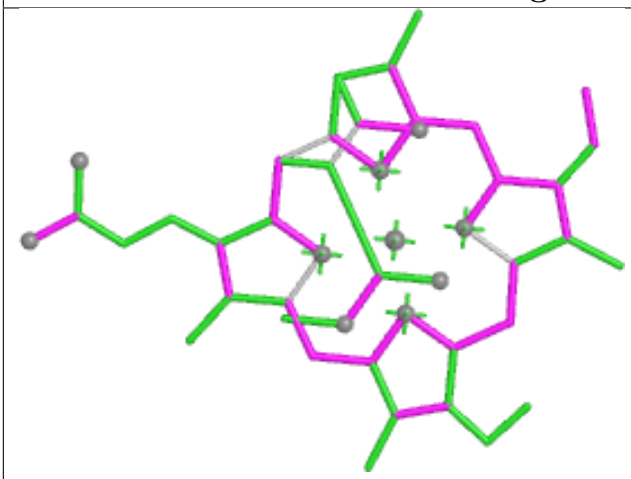

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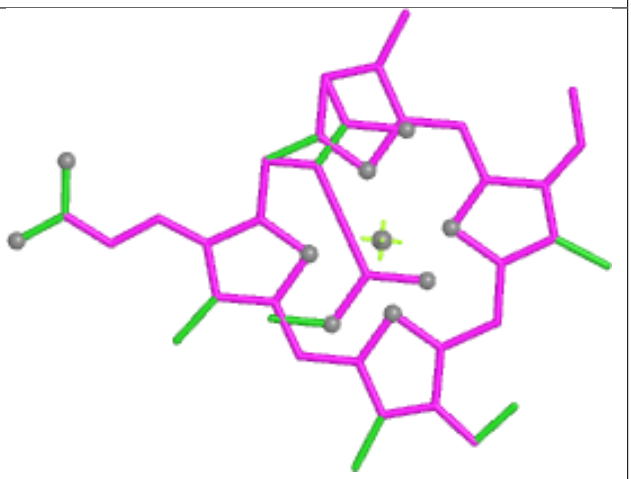

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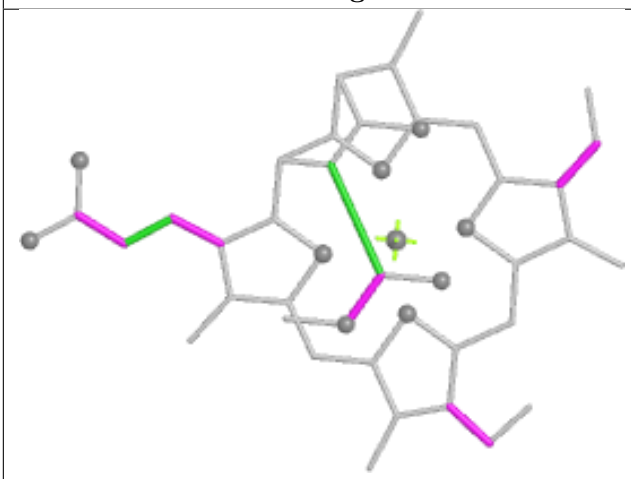

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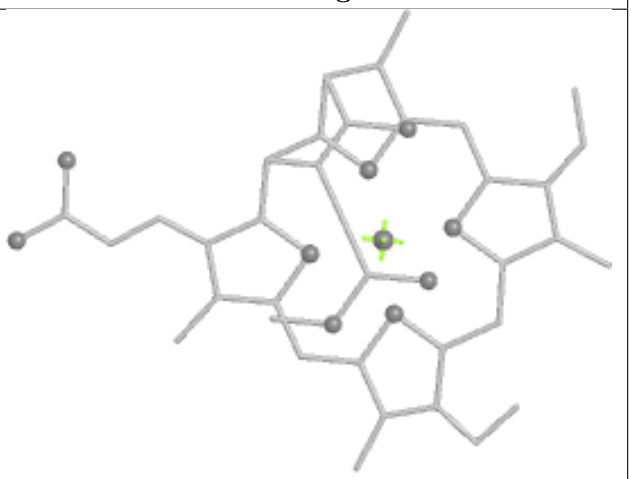

Rings

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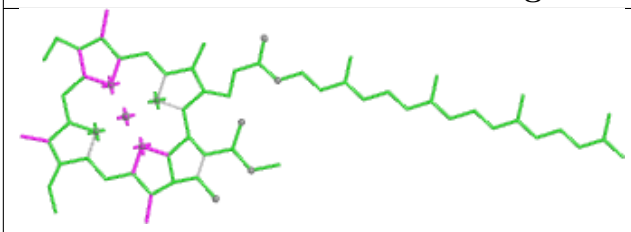

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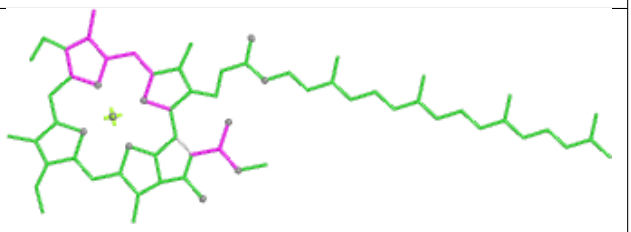

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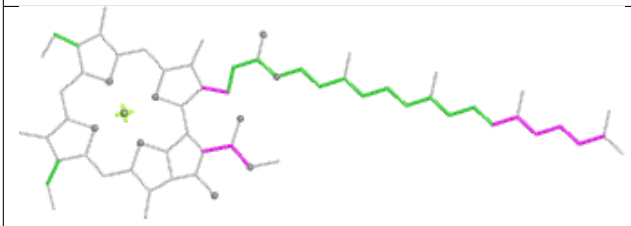

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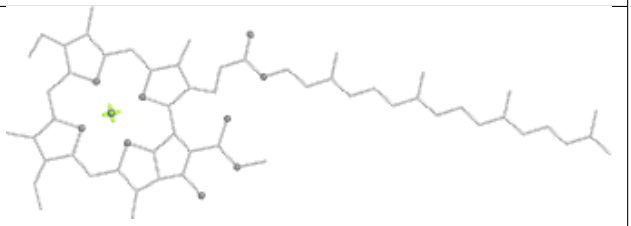

Rings

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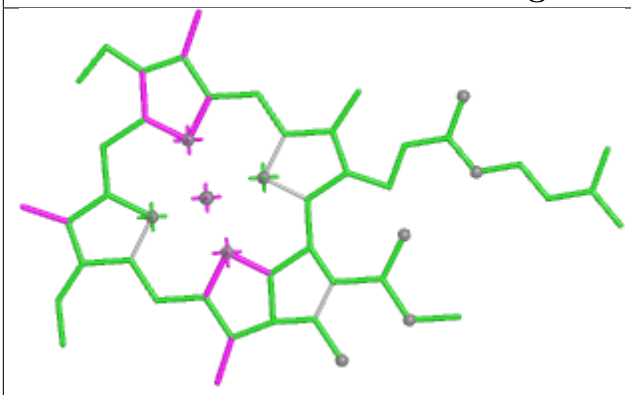

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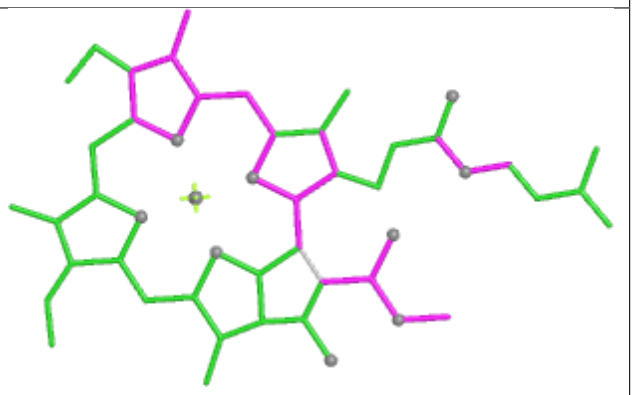

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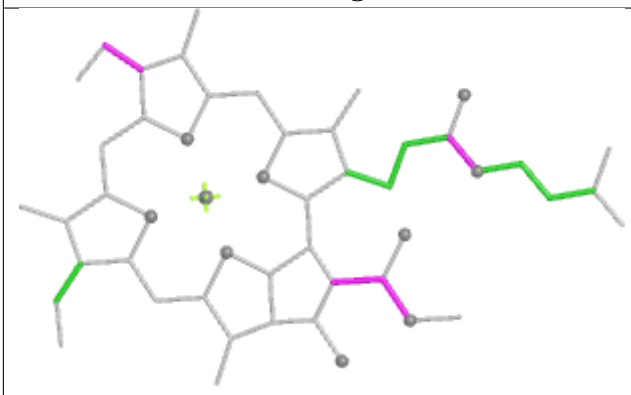

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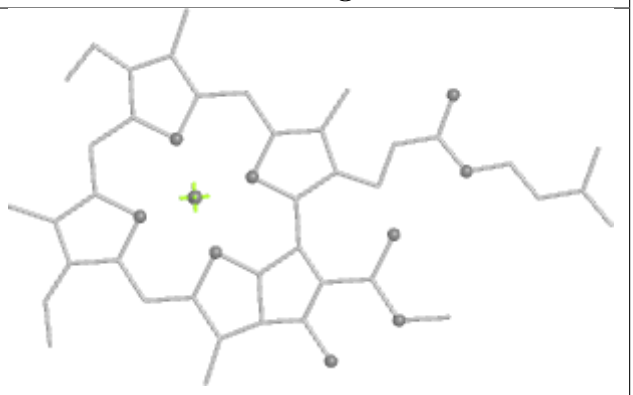

Rings

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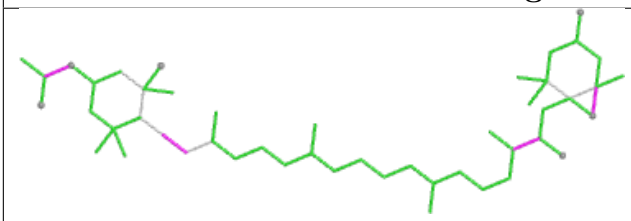

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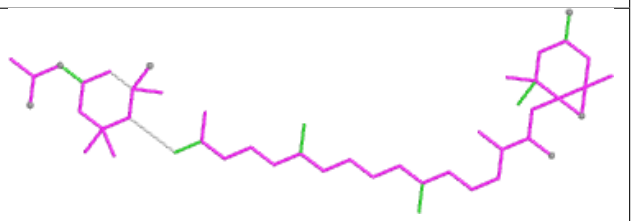

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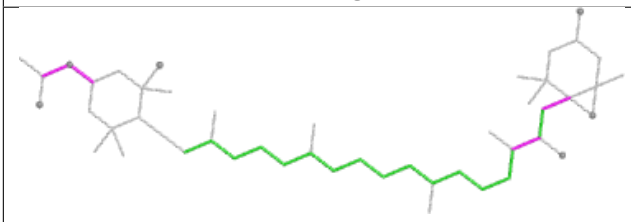

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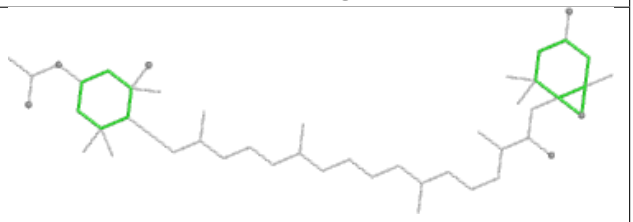
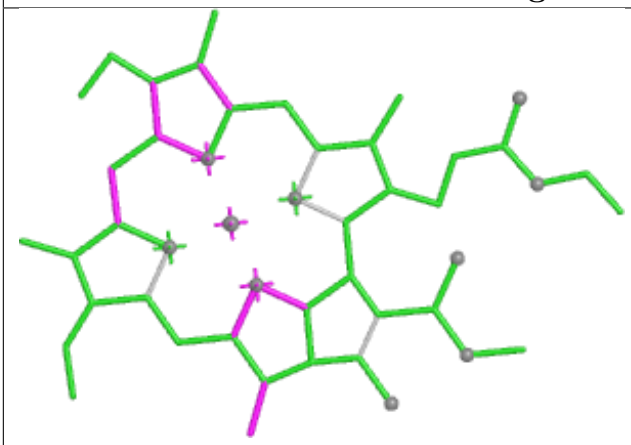


Rings

Ligand CLA 6 313



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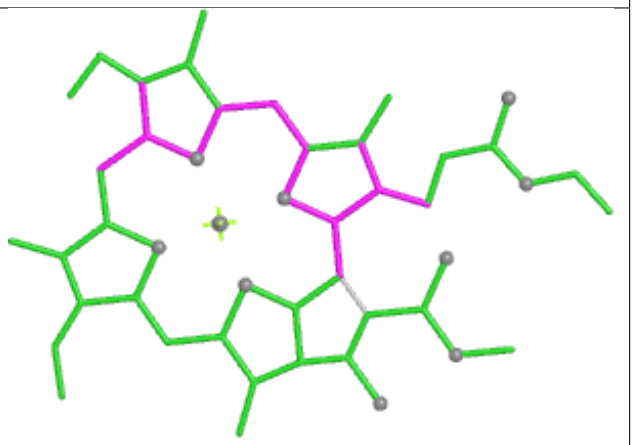

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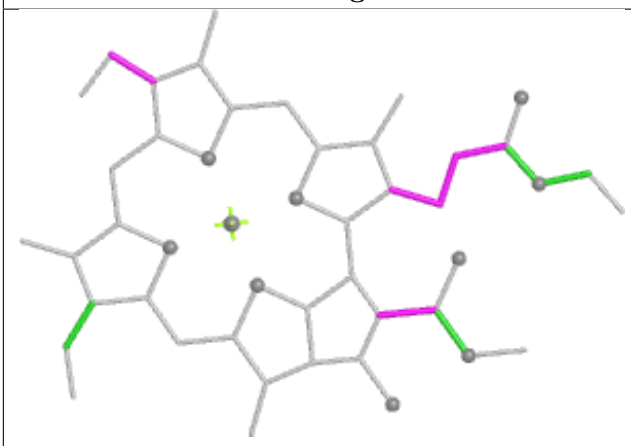

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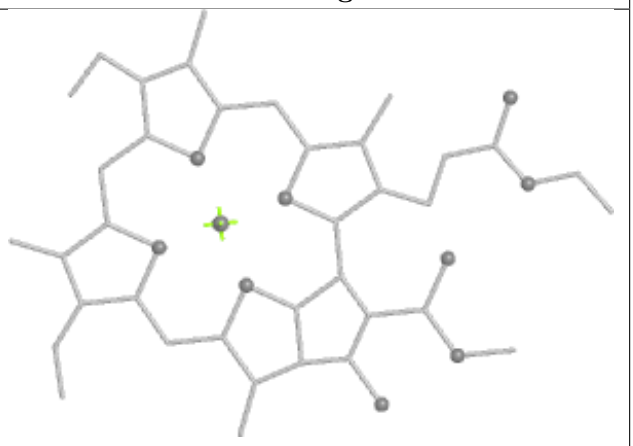

Rings

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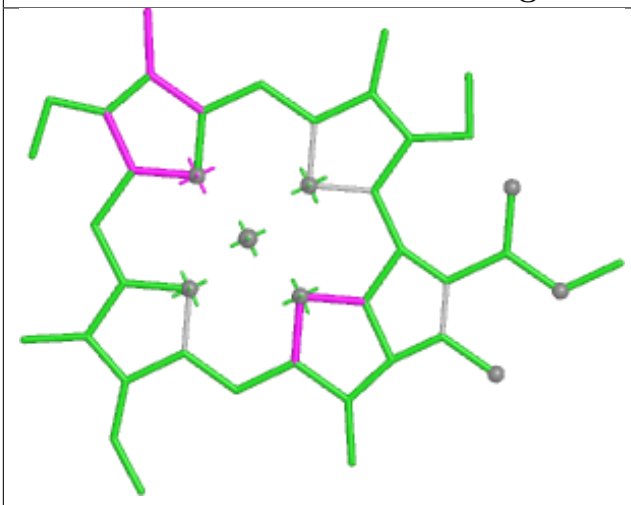

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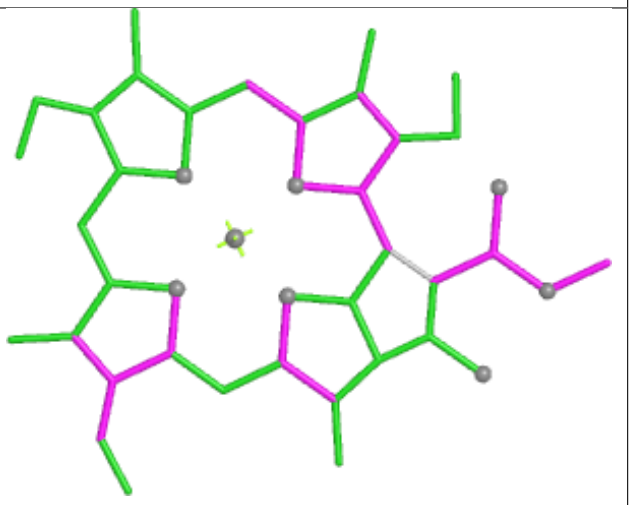
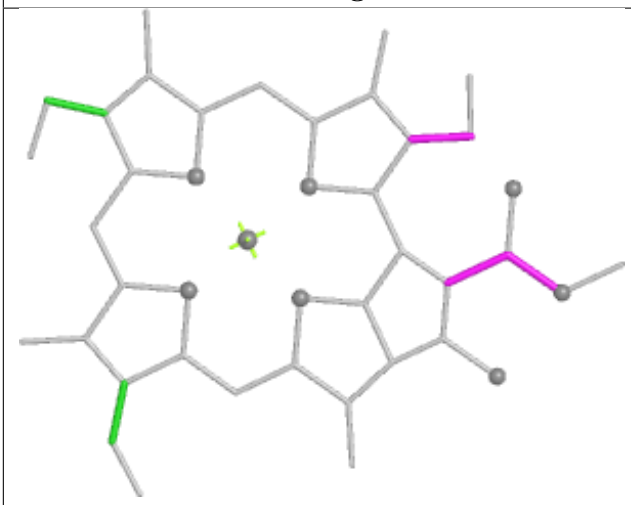


Bond angles

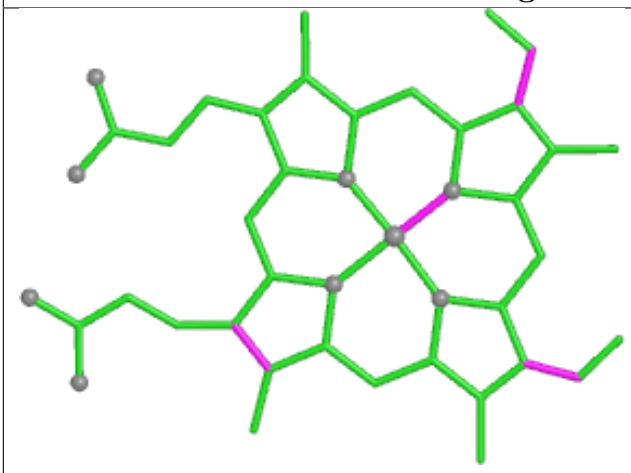


Torsions

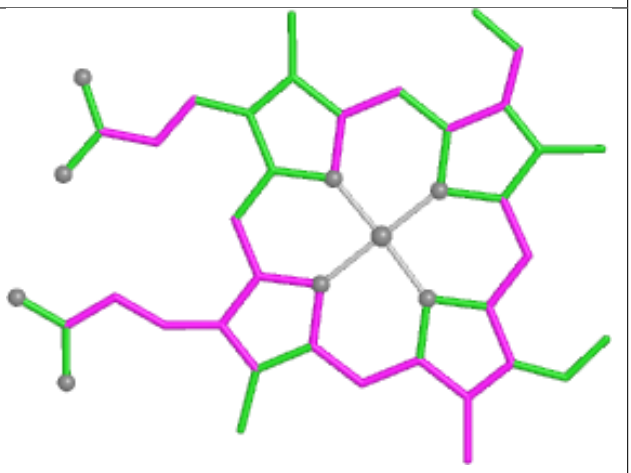


Rings

Ligand HEM V 201



Bond lengths



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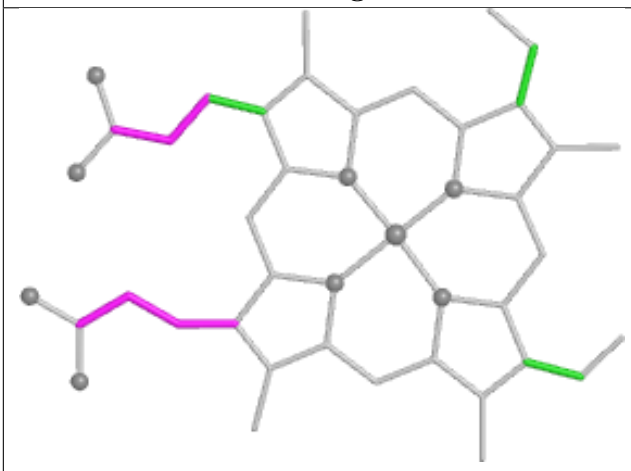

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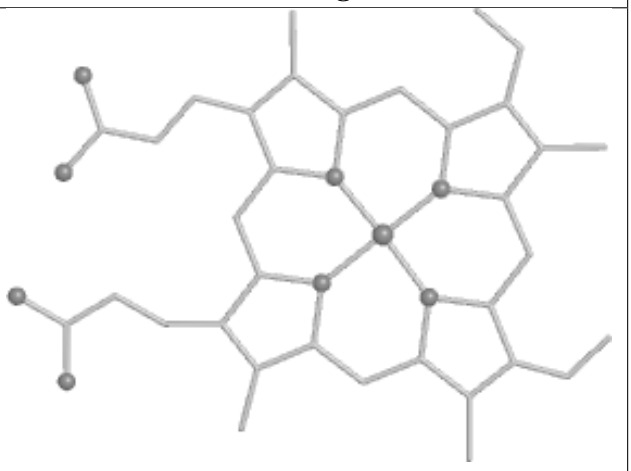

Rings

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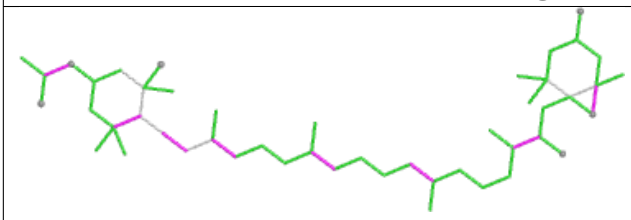

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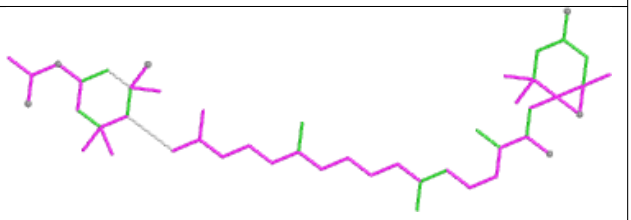

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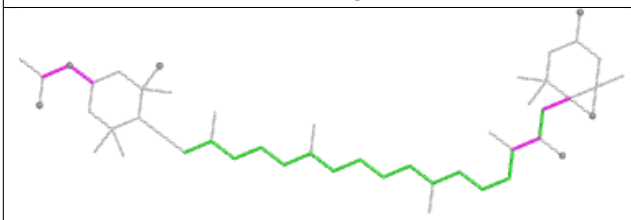

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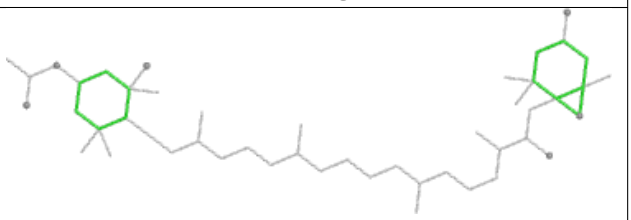

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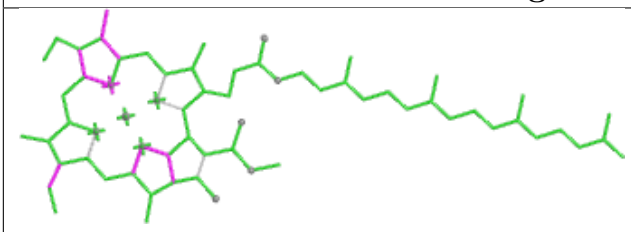

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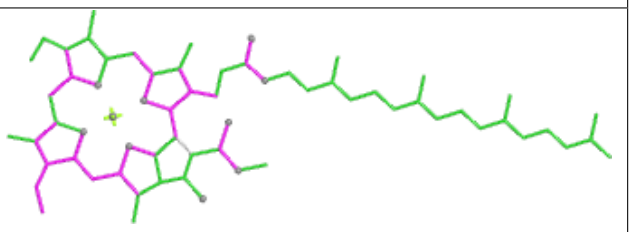

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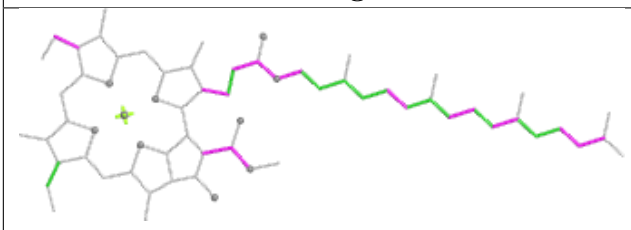

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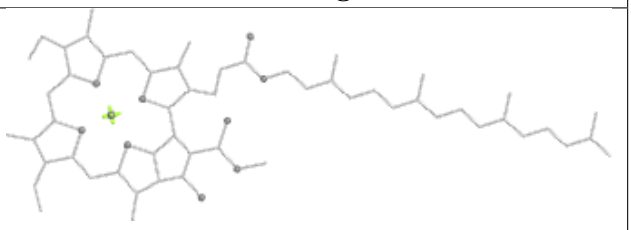

Rings

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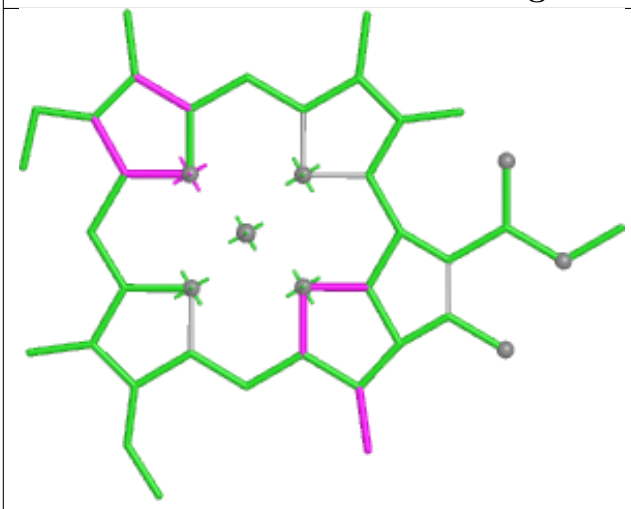

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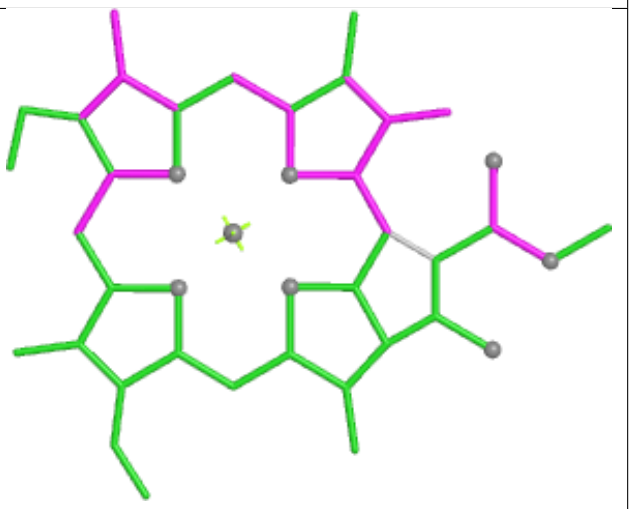

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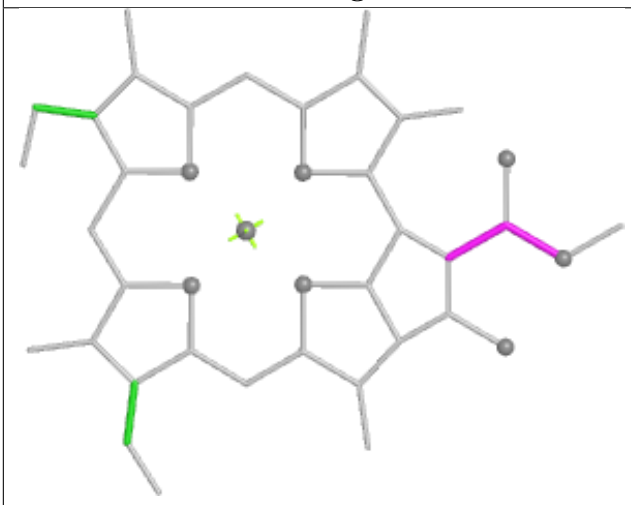

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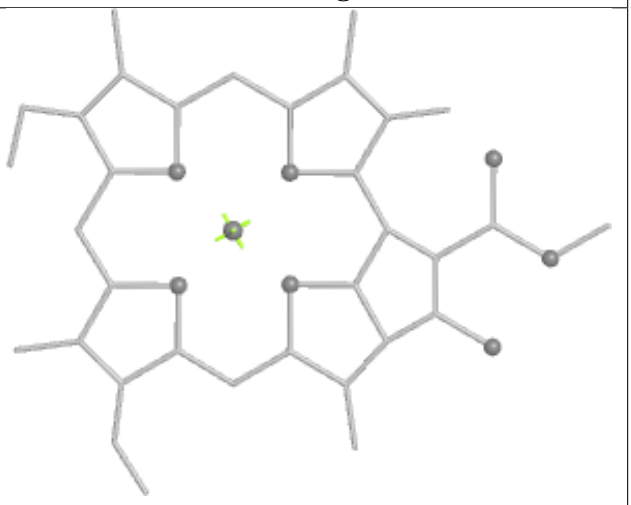

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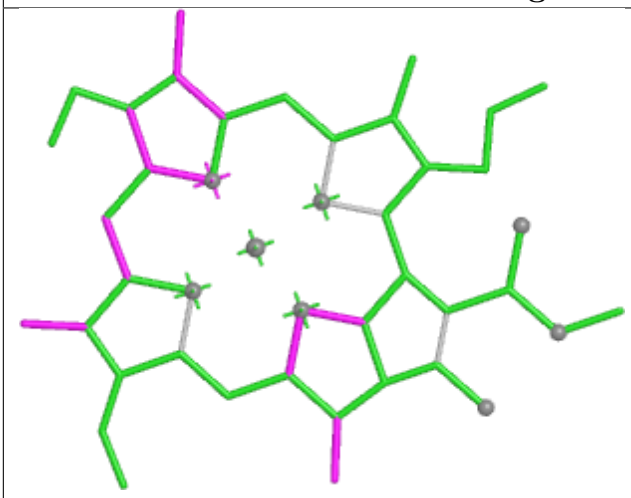

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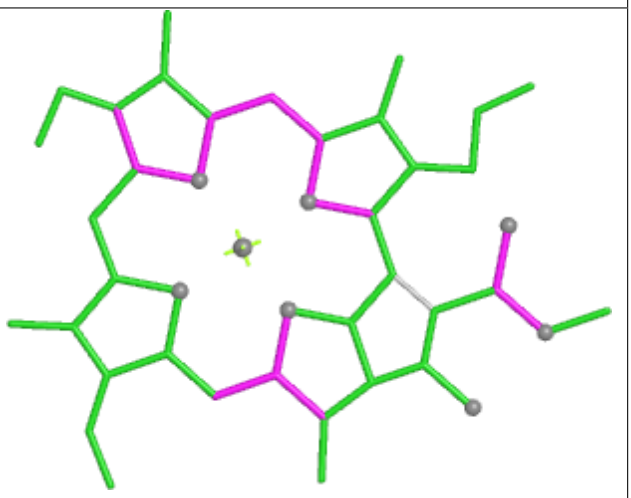

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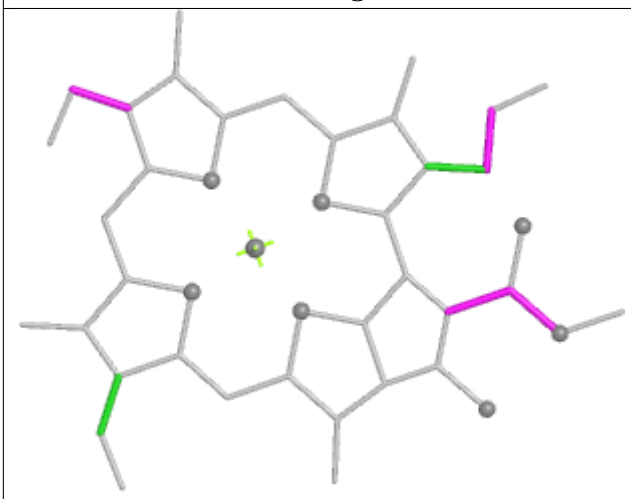

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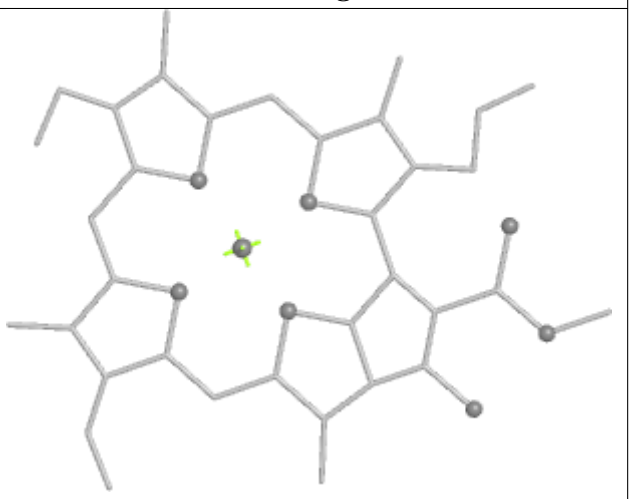

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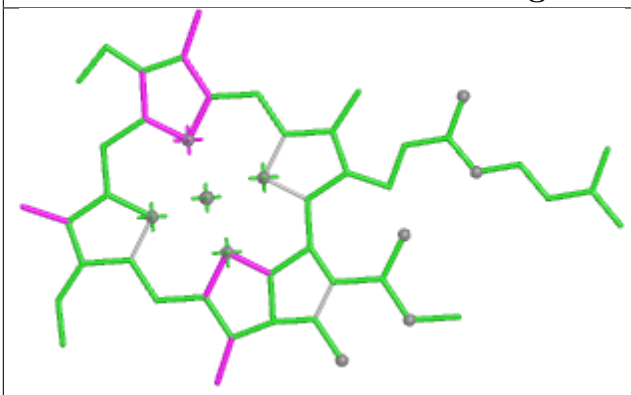

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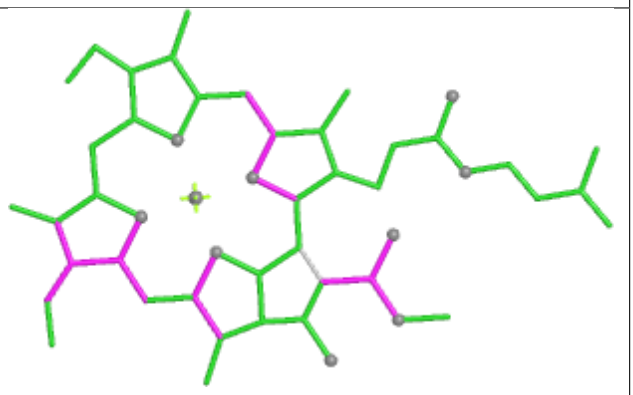

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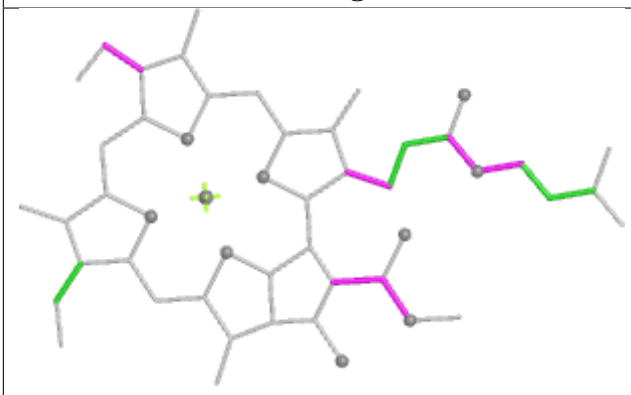

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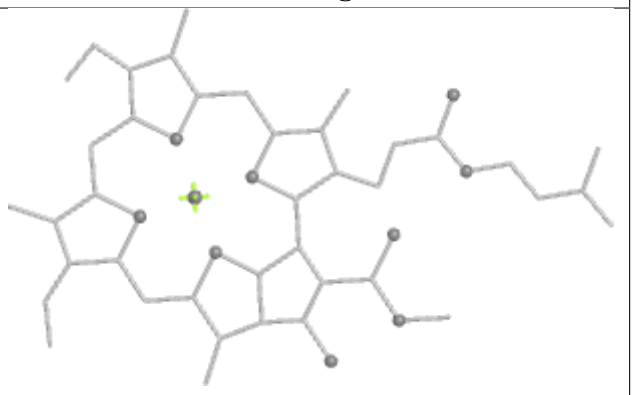

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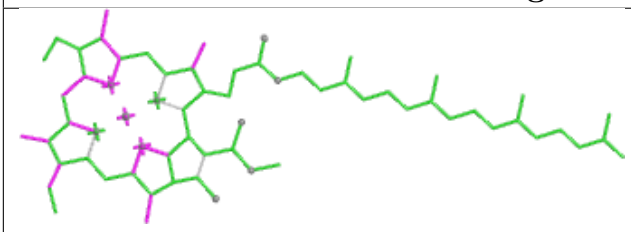

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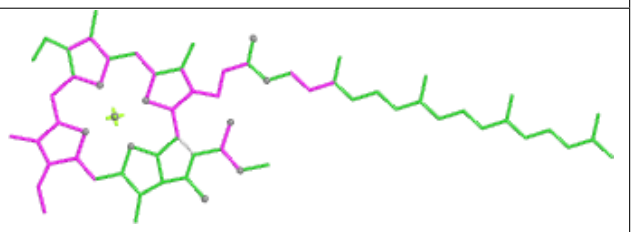

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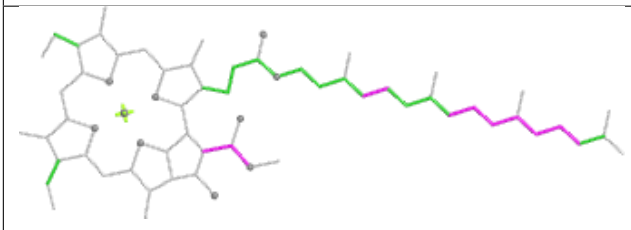

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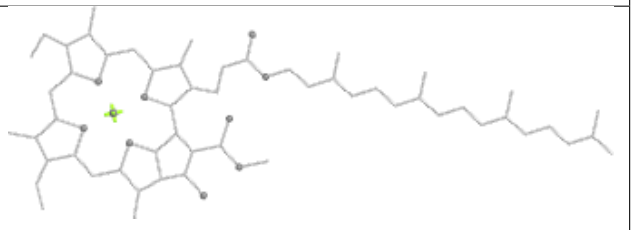

Rings

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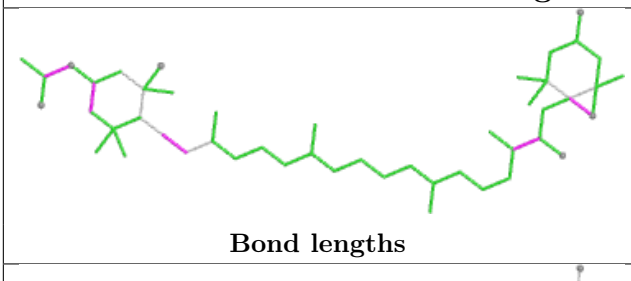
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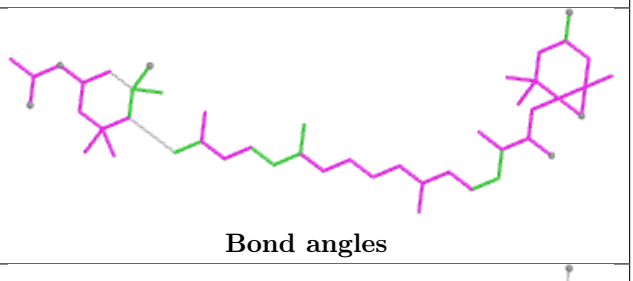
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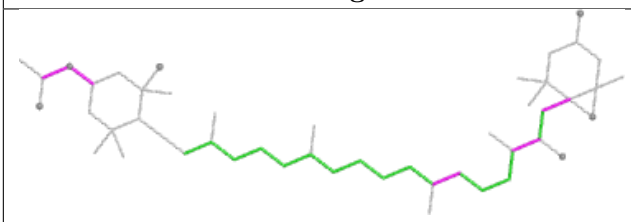
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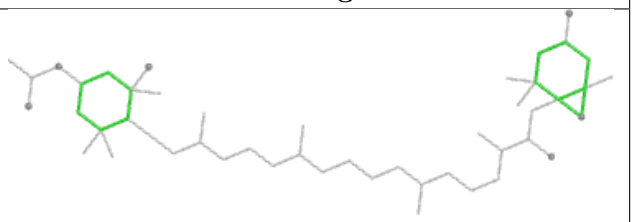
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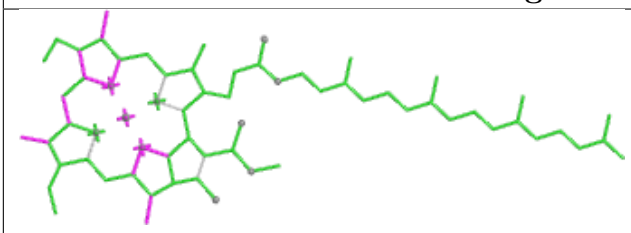
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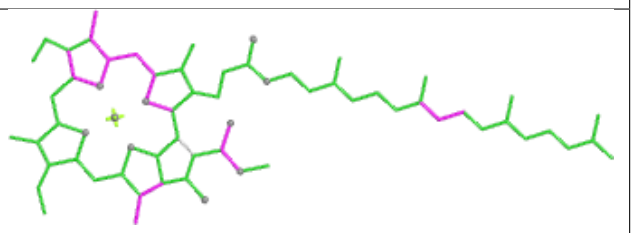
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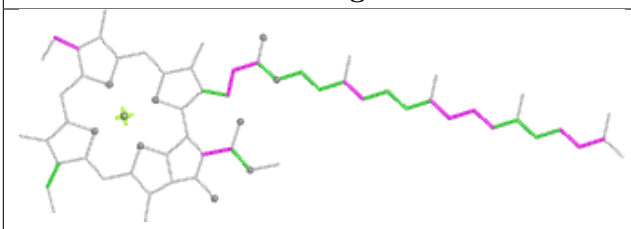
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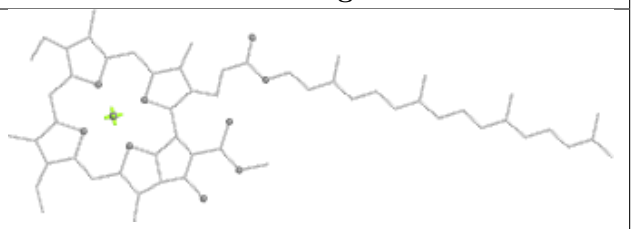
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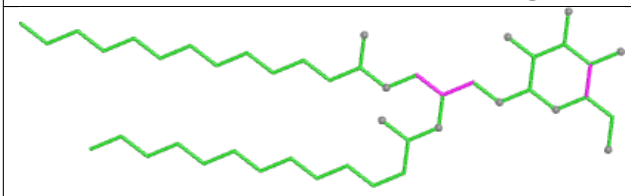
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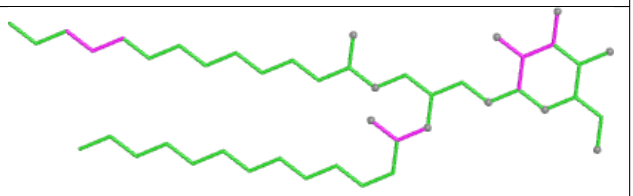
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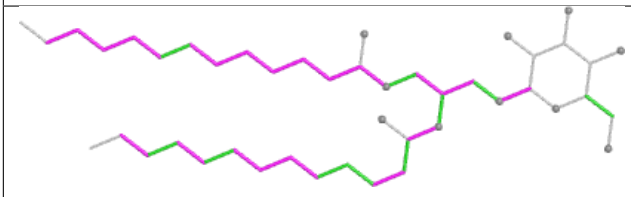
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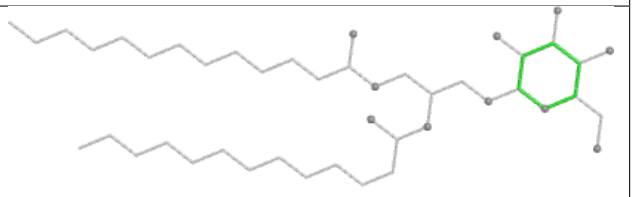
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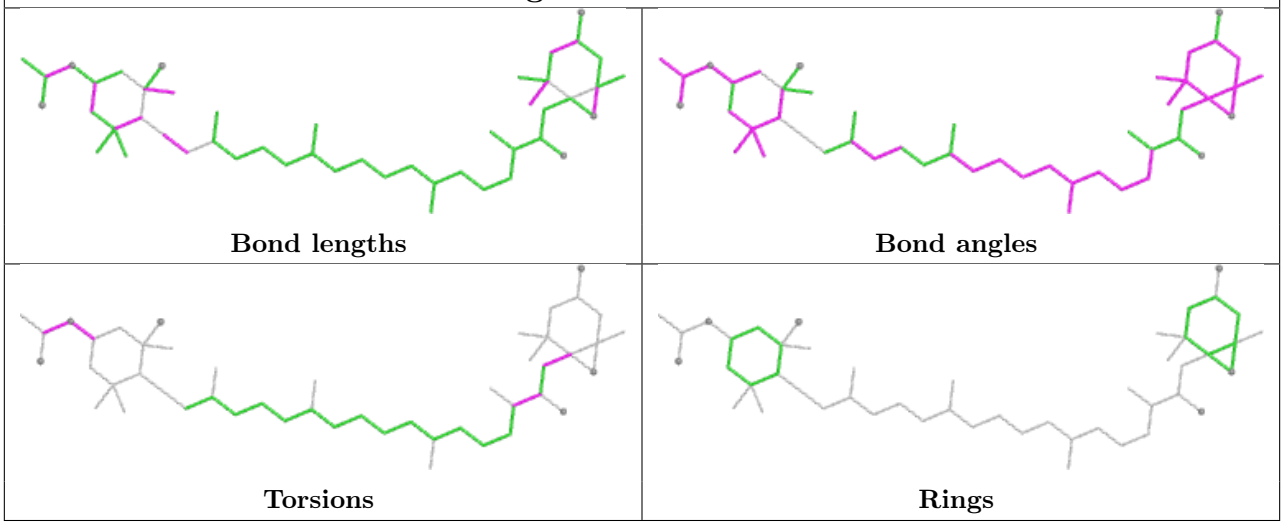

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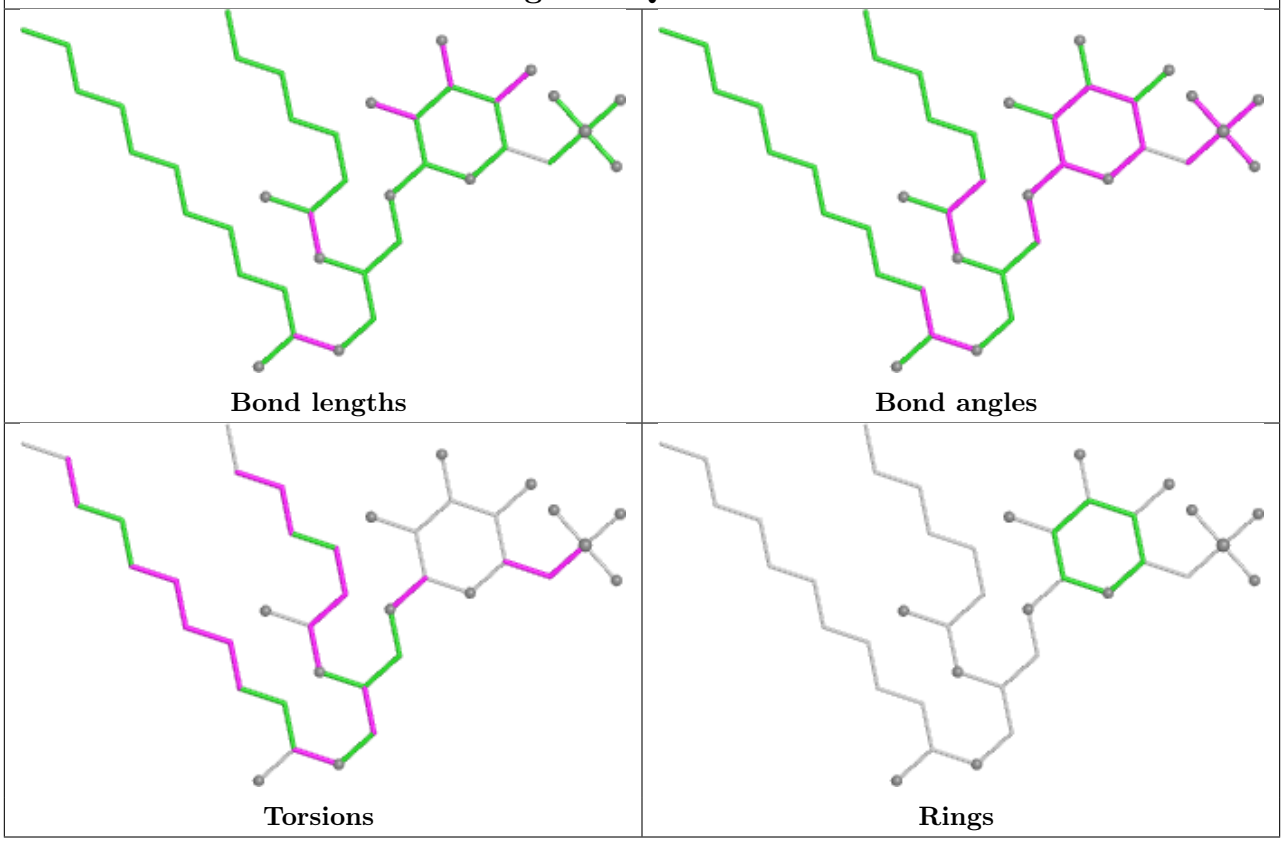

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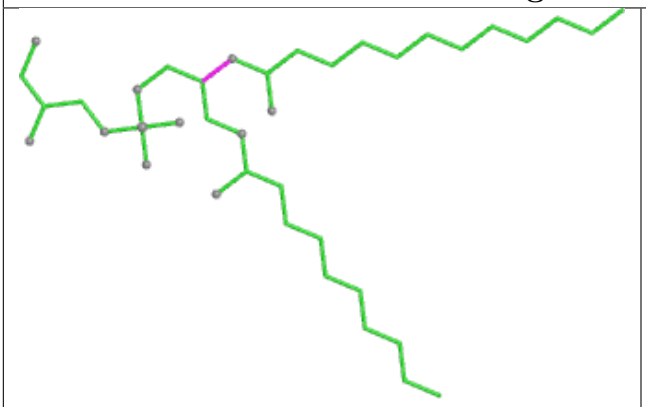

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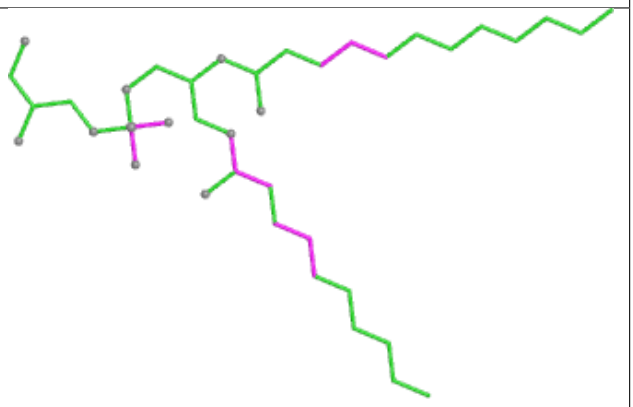

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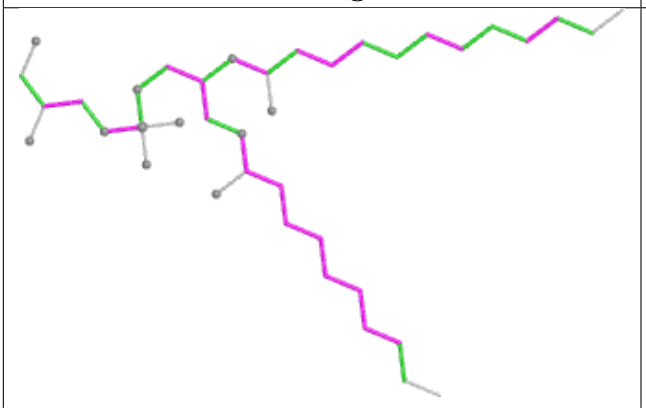

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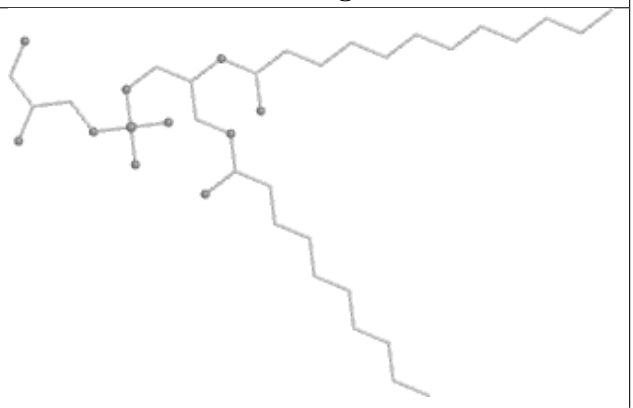

Rings

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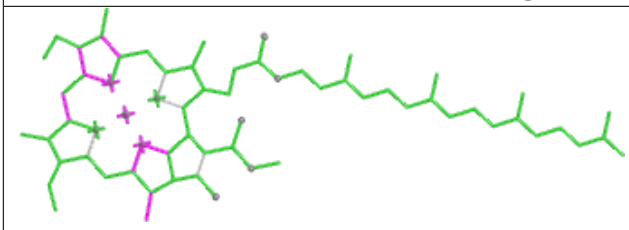

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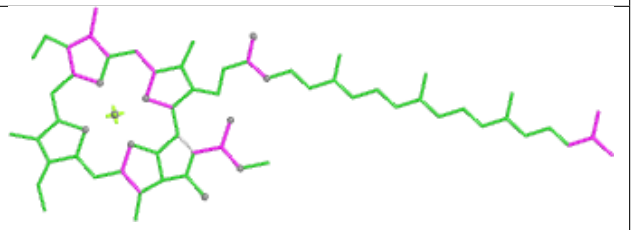

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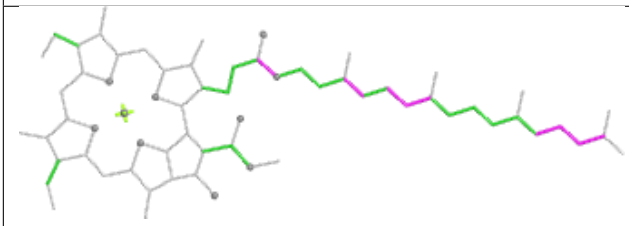

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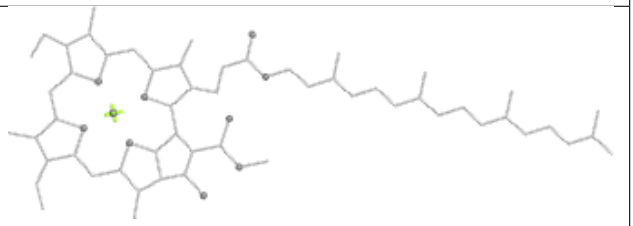

Rings

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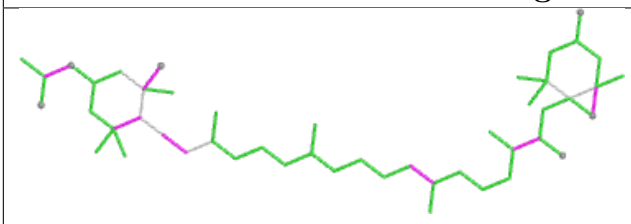

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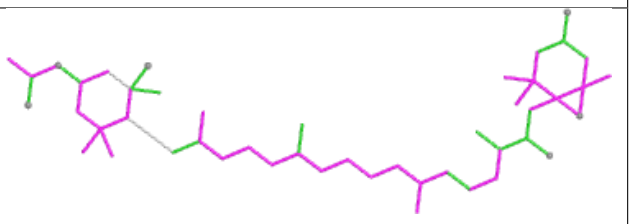
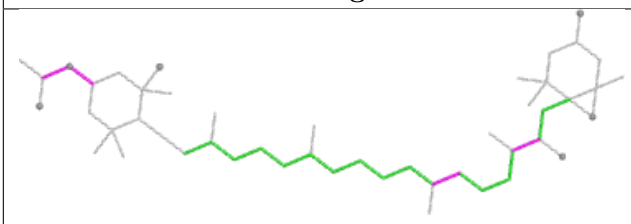


Bond angles



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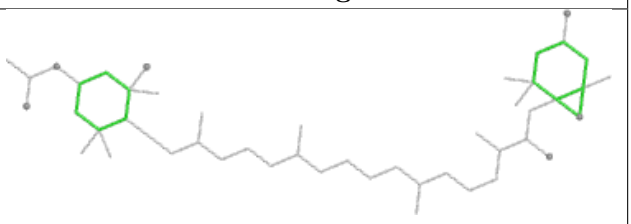
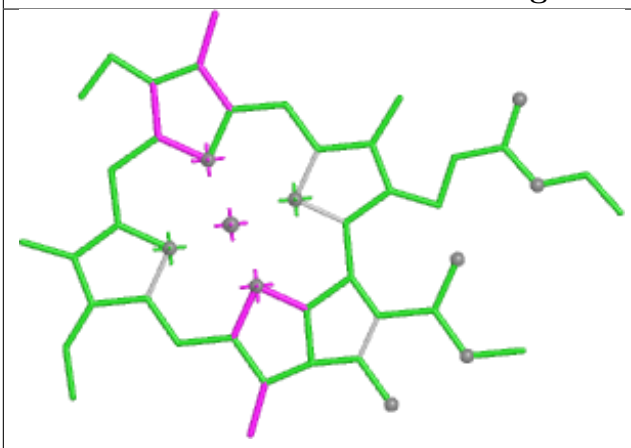


Rings

Ligand CLA r 101



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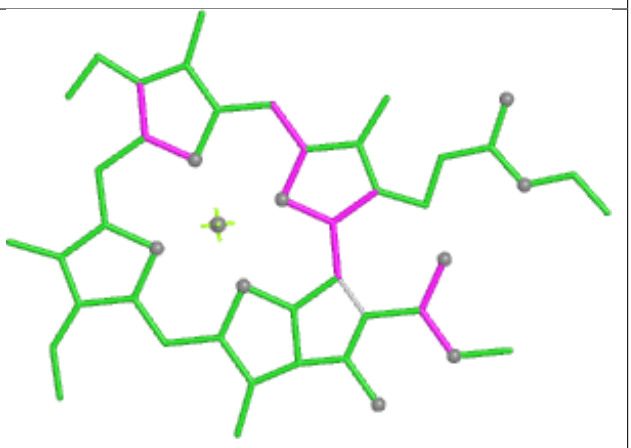
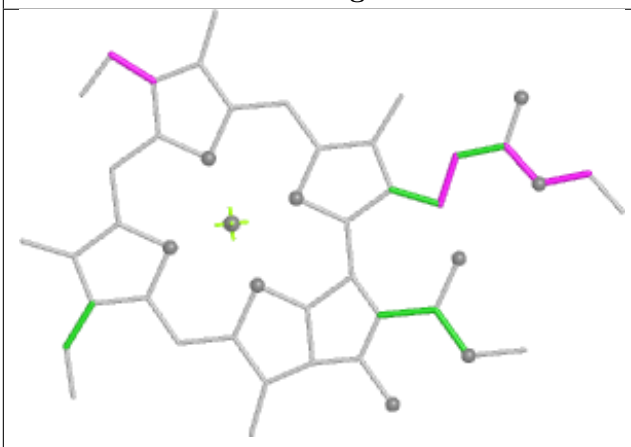


Bond angles



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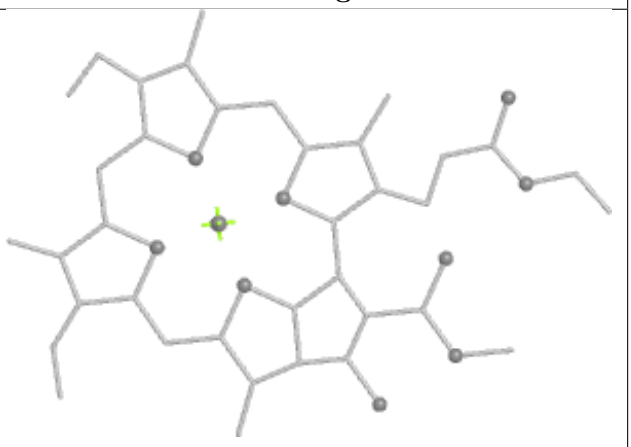

Rings

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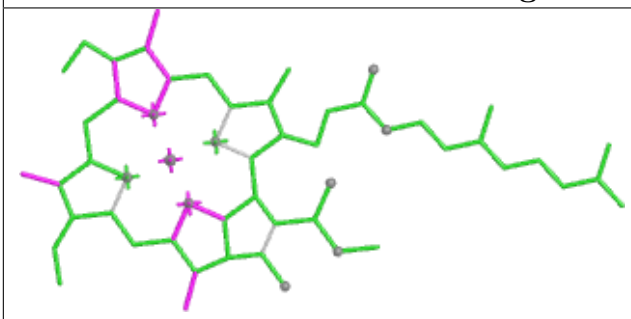
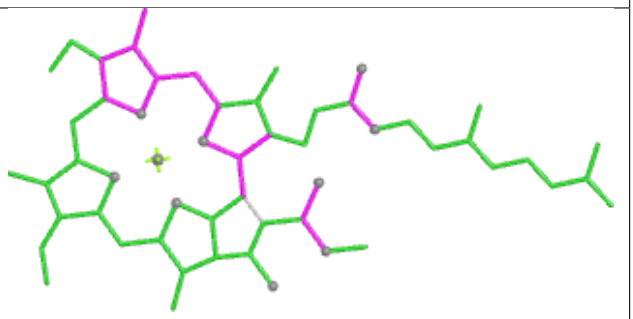
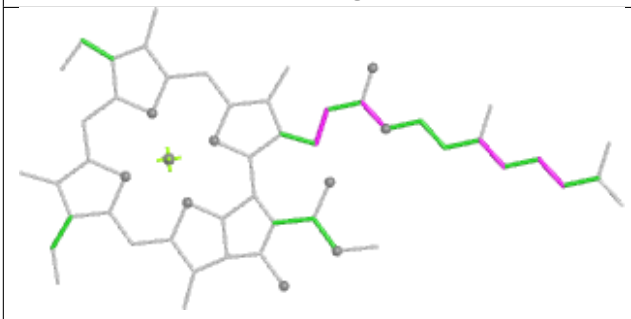


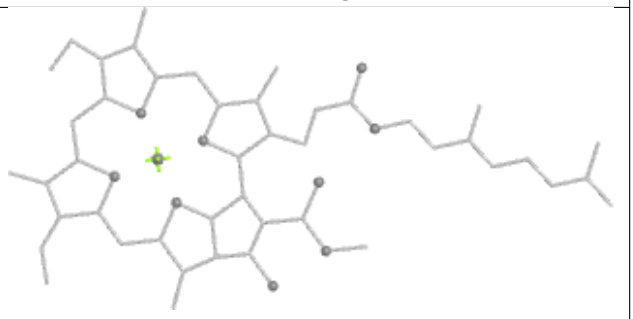
Bond lengths



Bond angles

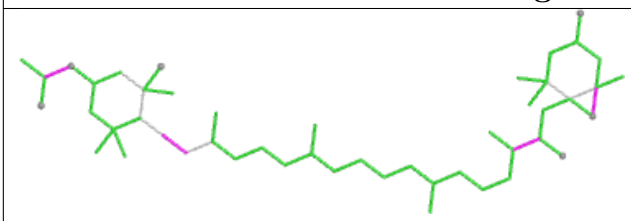


Torsions



Rings

Ligand A86 1 319



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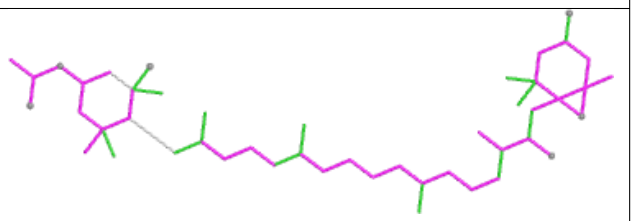

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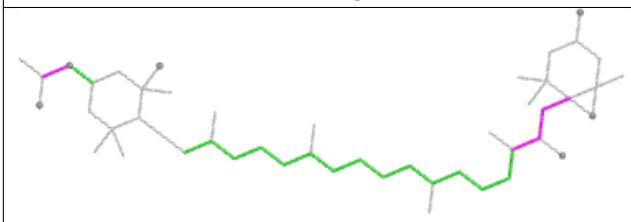

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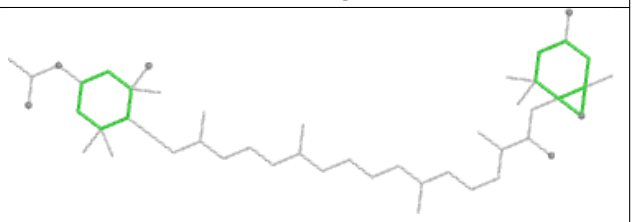
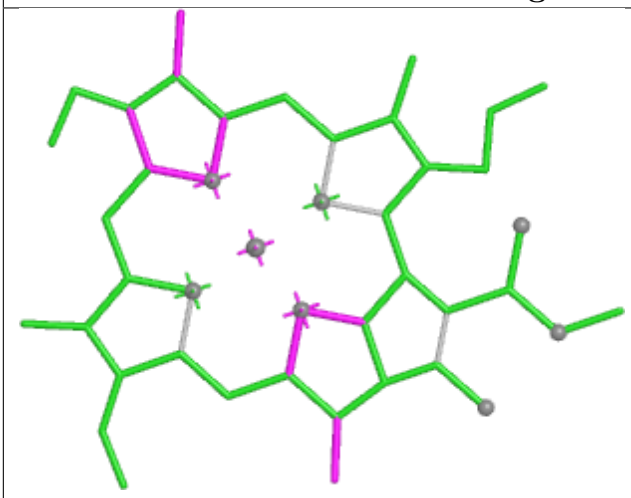


Rings

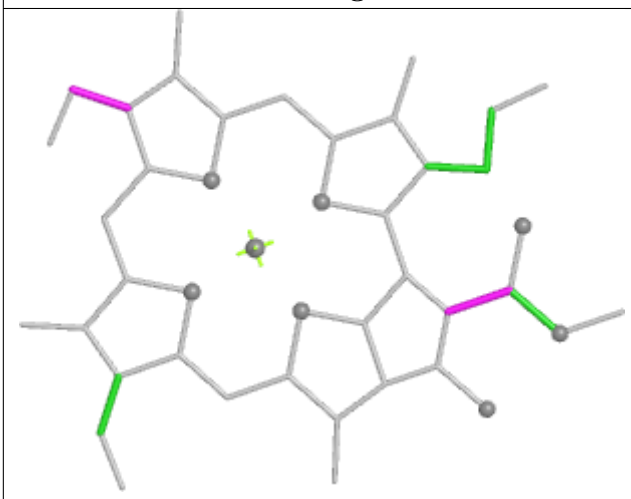
Ligand CLA 1 307



Bond lengths



Bond angles



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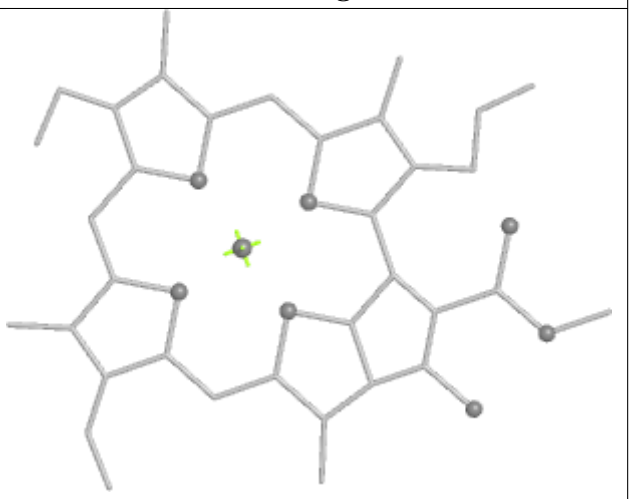

Rings

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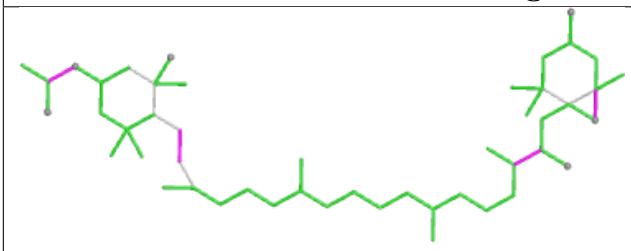

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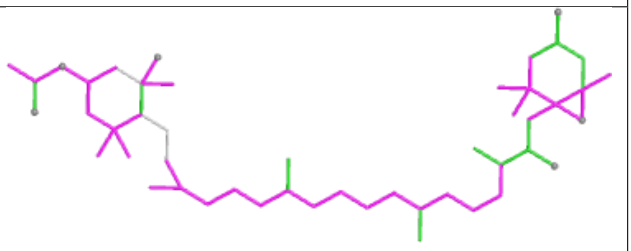

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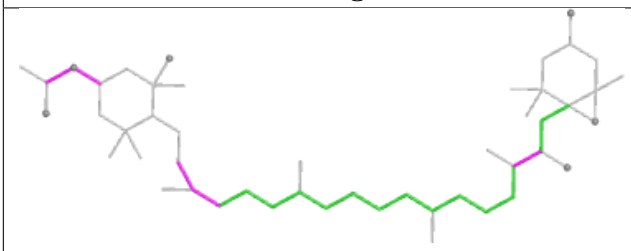

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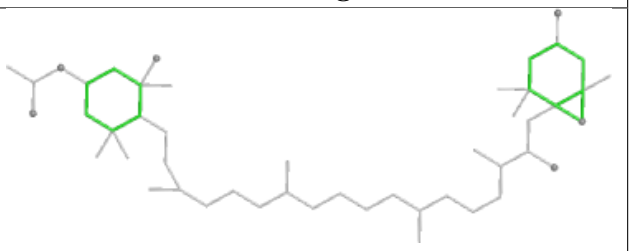

Rings

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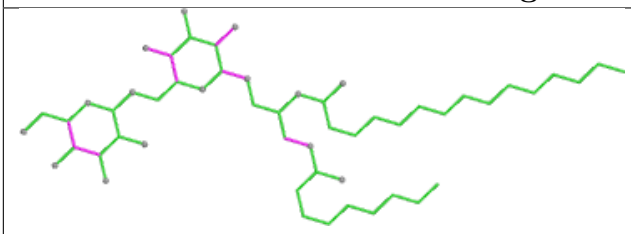

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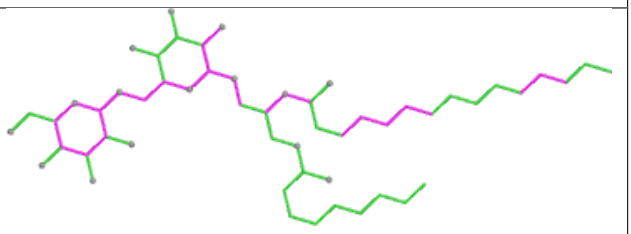
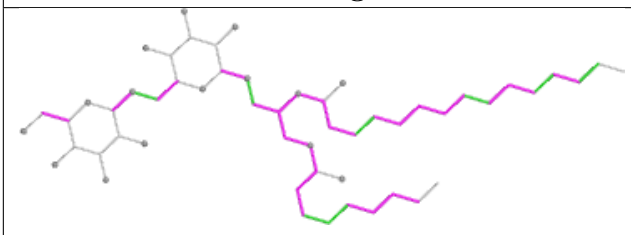


Bond angles



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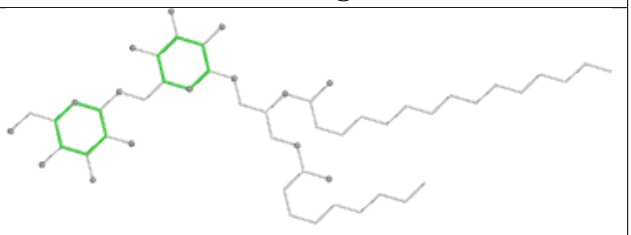

Rings

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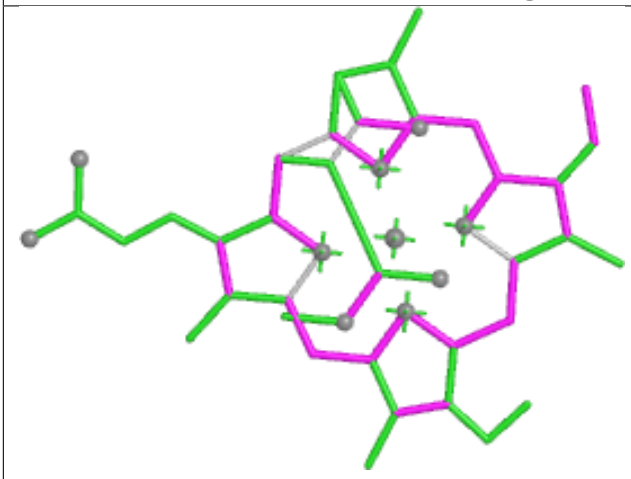

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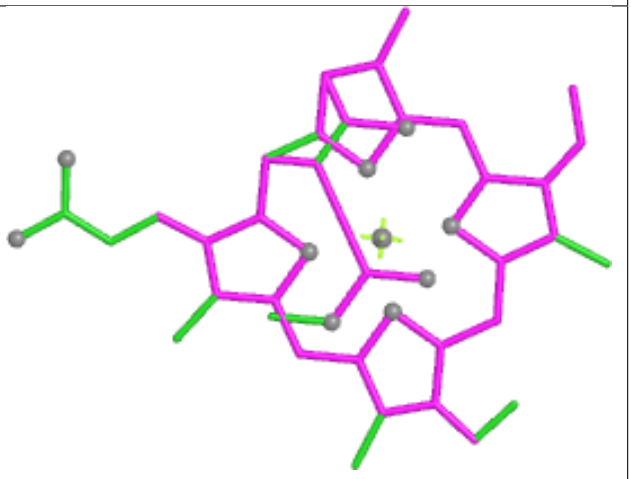

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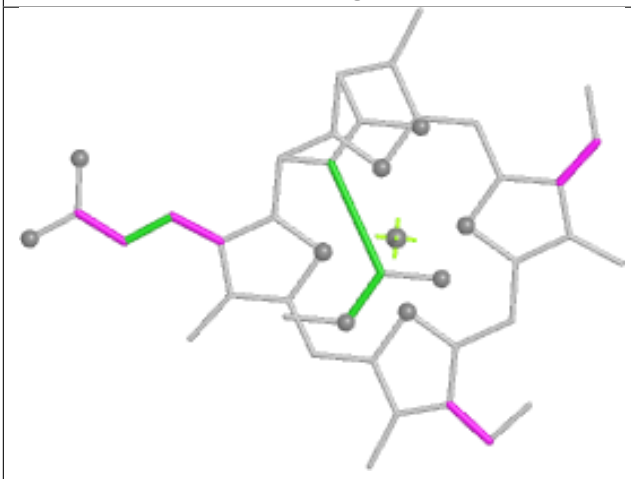

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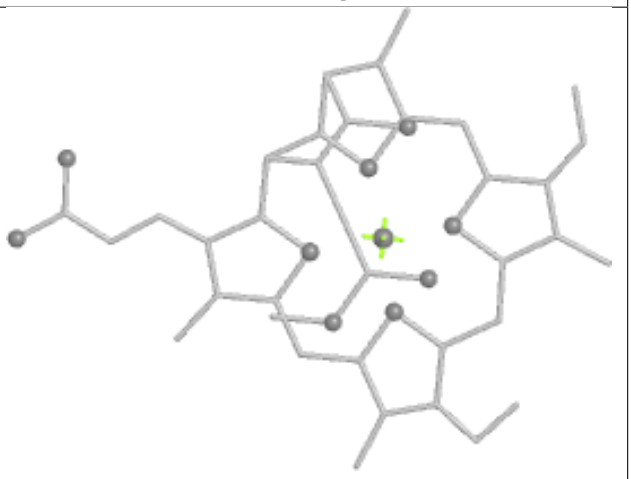

Rings

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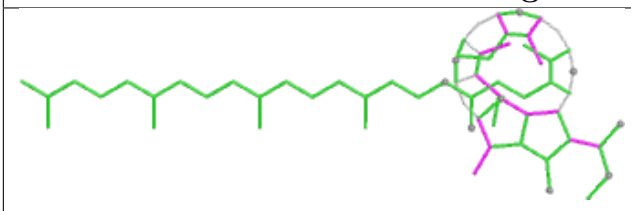

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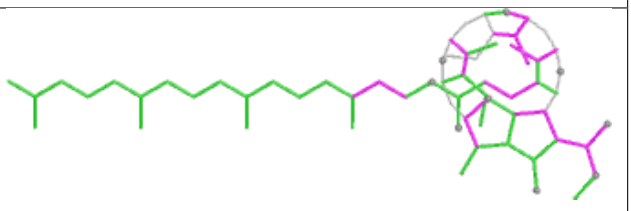
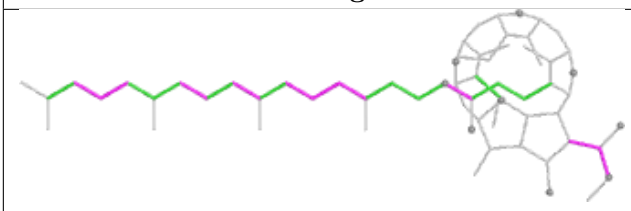


Bond angles



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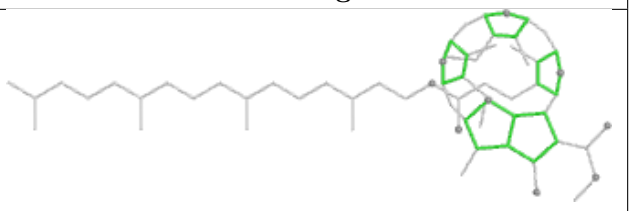
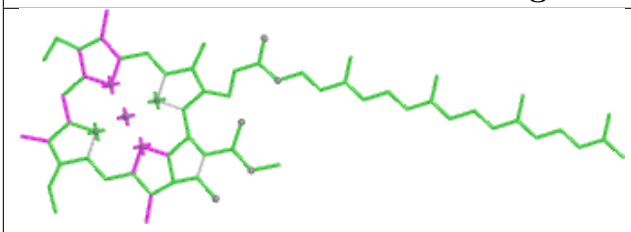


Rings

Ligand CLA c 506



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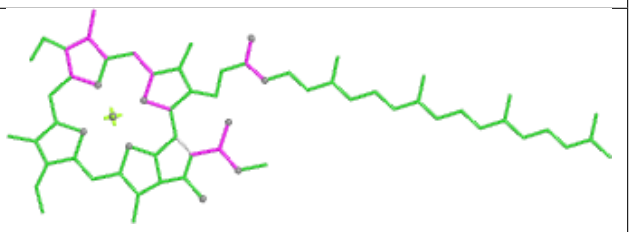

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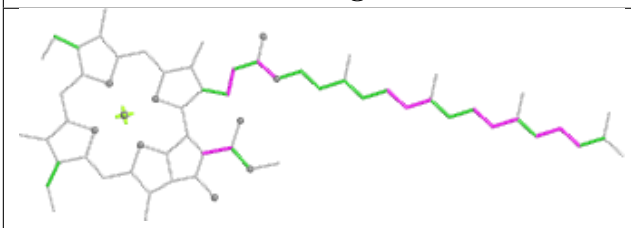

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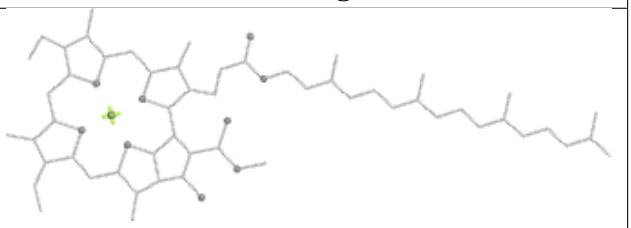

Rings

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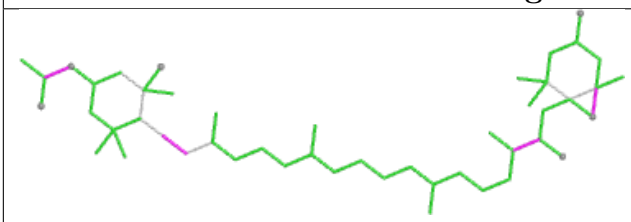

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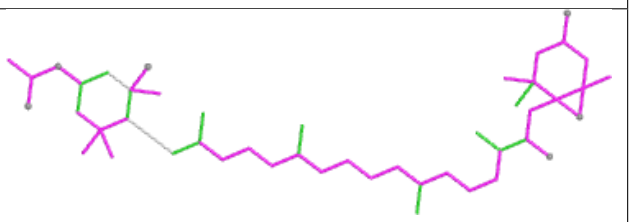

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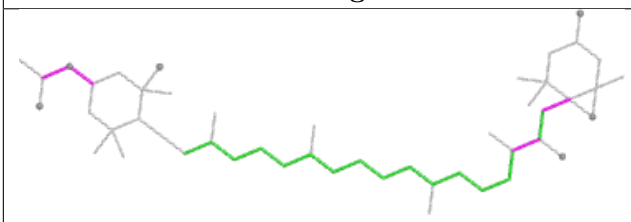

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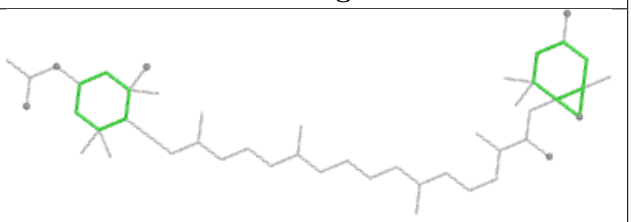

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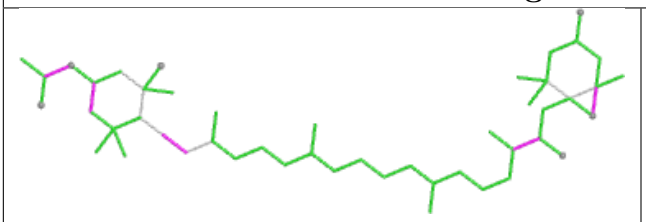

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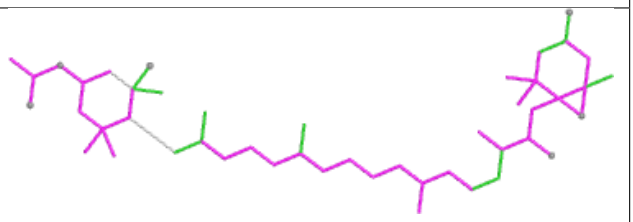

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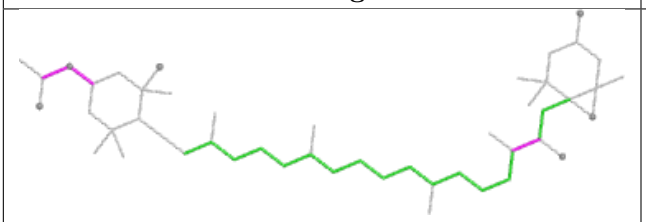

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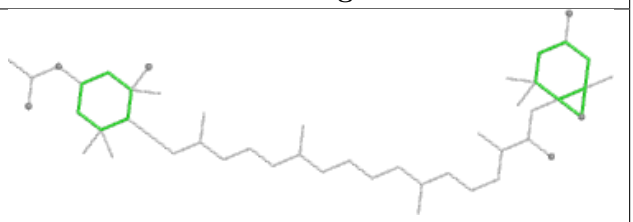
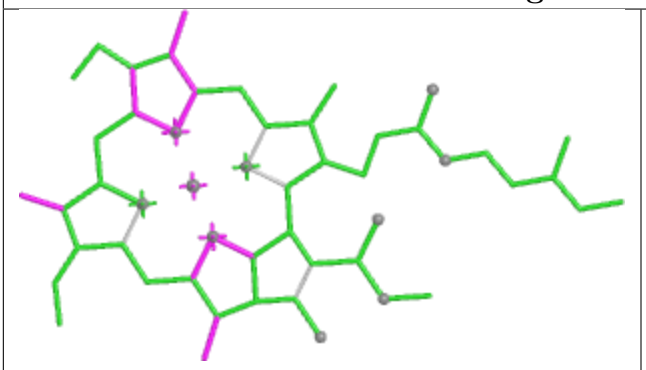


Rings

Ligand CLA Z 101



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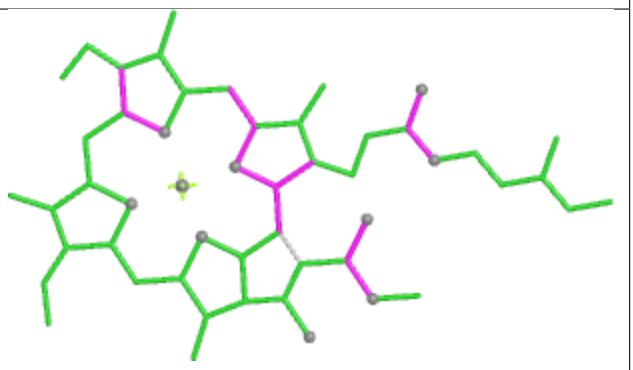

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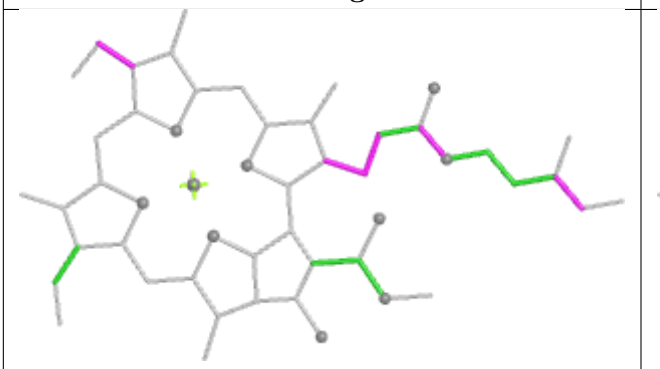

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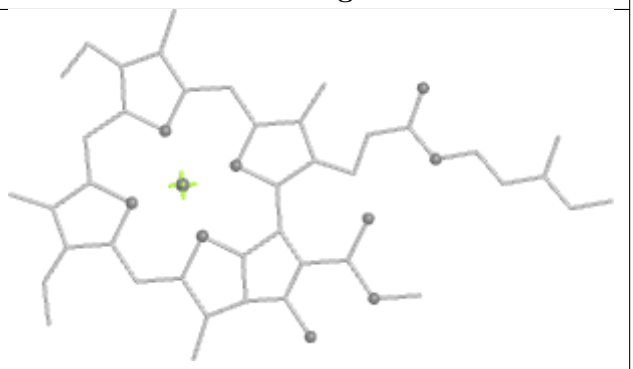
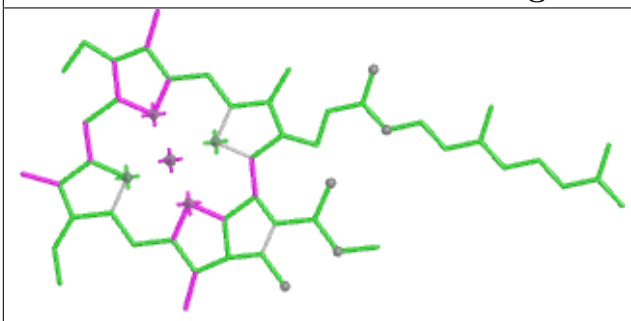


Rings

Ligand CLA 8 313



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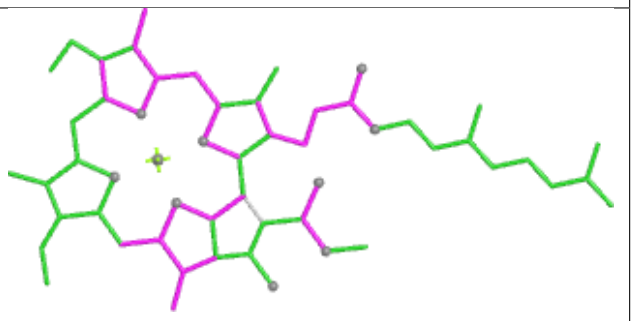

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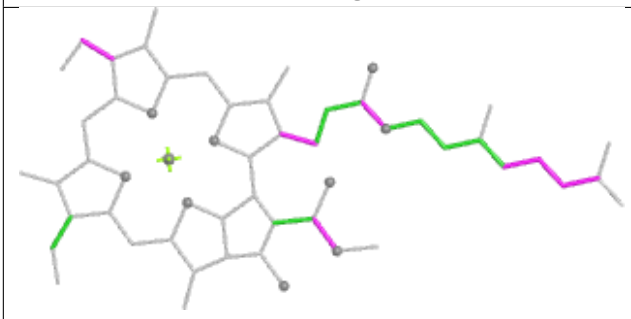

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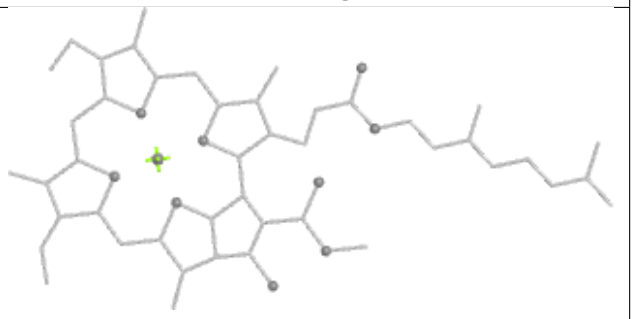
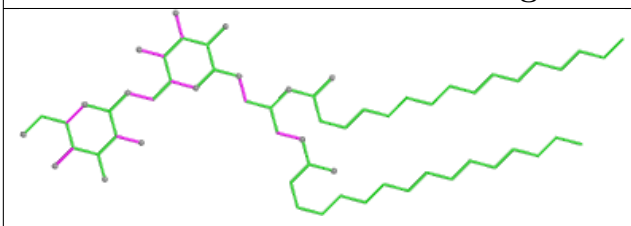


Rings

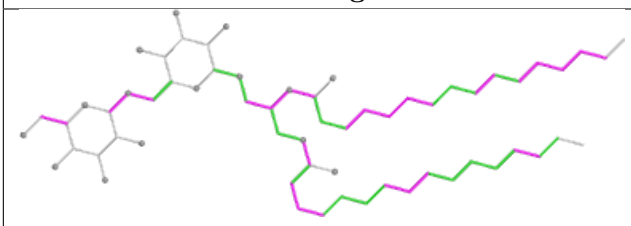
Ligand DGD C 519



Bond lengths



Bond angles



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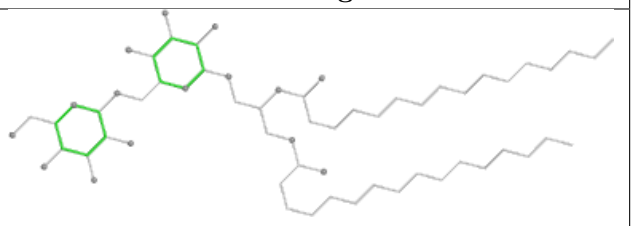
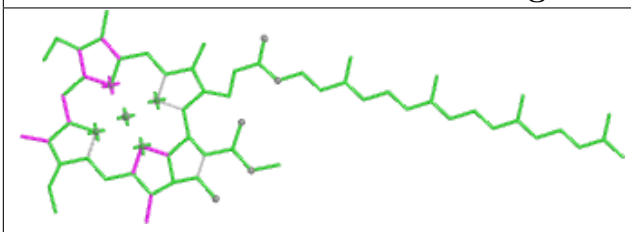


Rings

Ligand CLA 9 308



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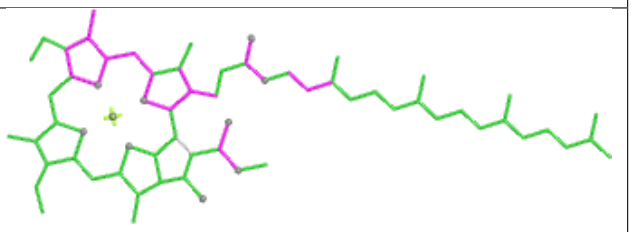
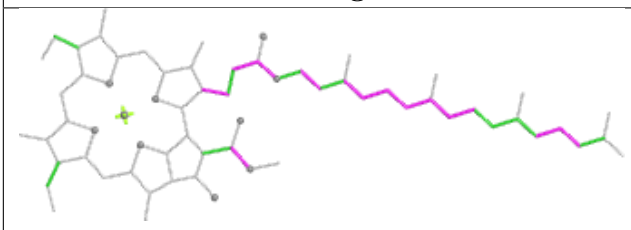


Bond angles



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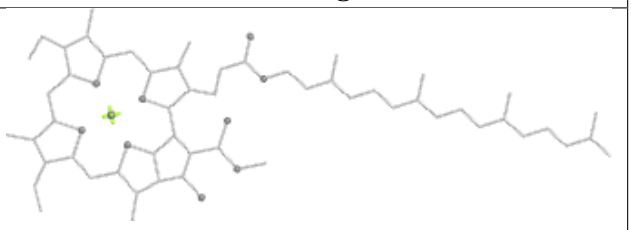
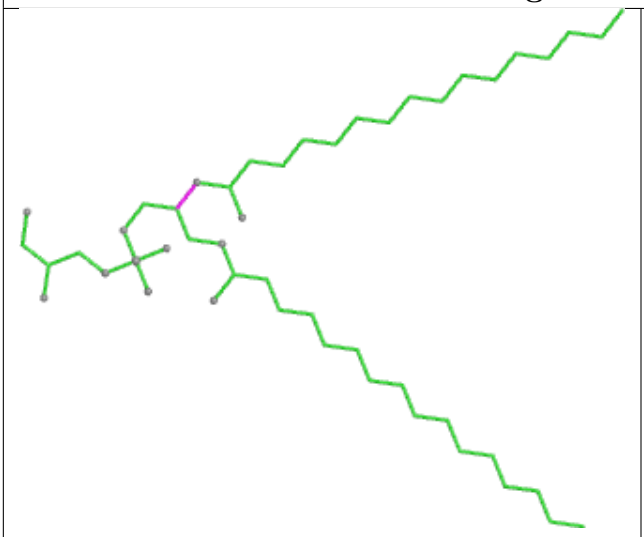


Rings

Ligand LHG d 408



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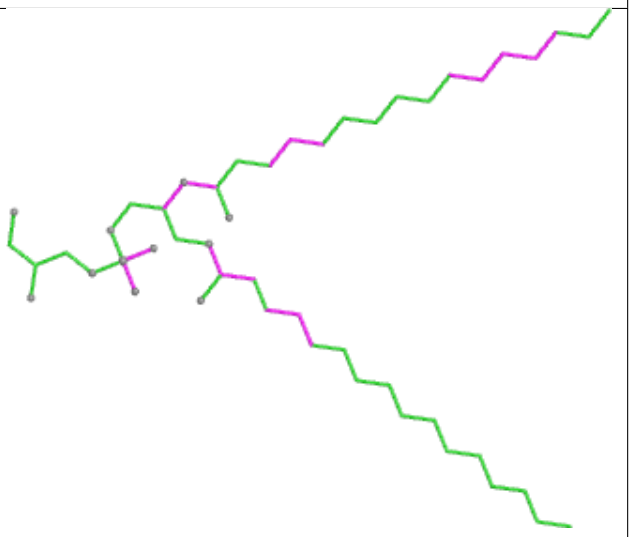
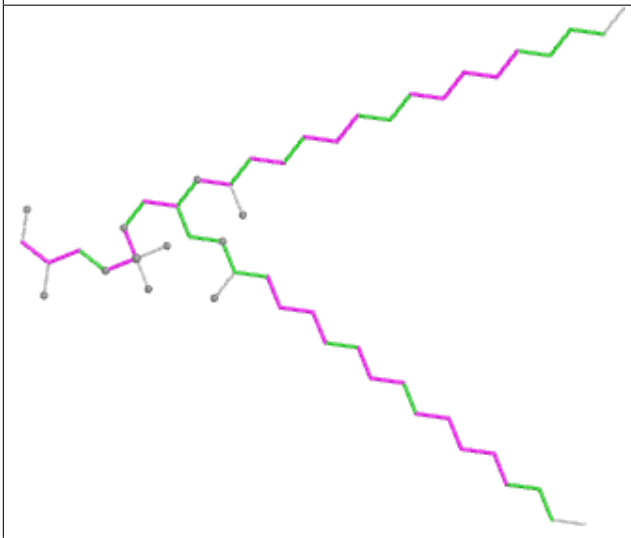


Bond angles



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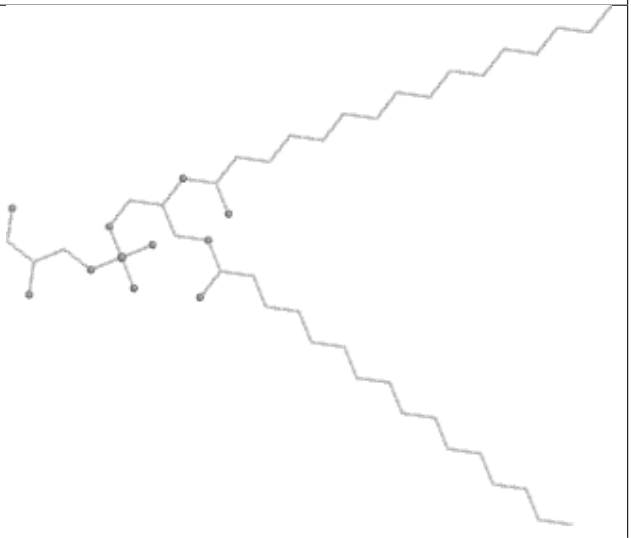
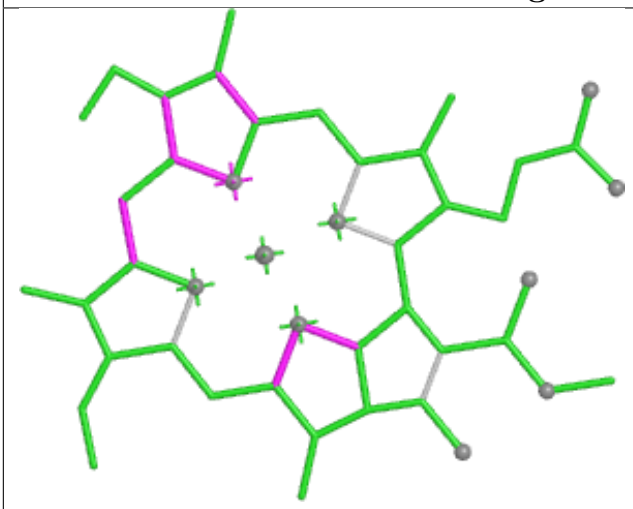
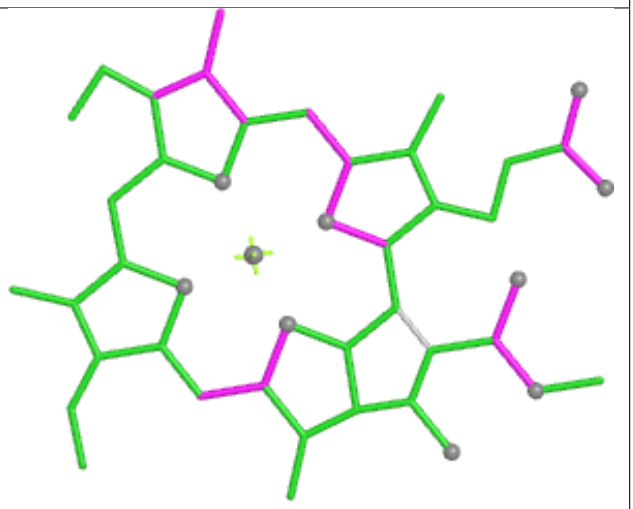


Rings

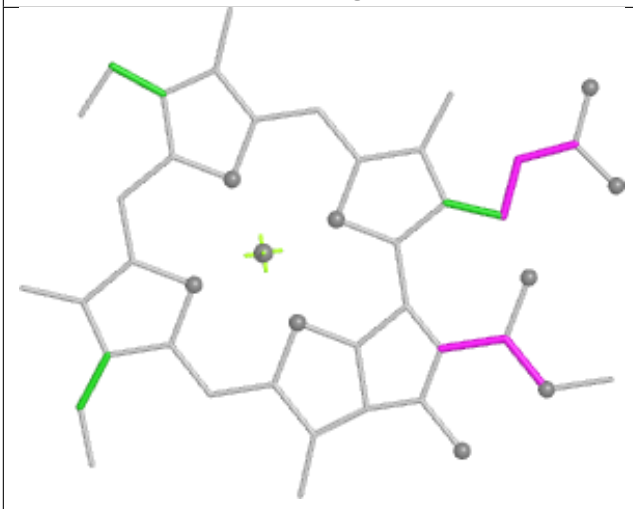
Ligand CLA 7 310



Bond lengths



Bond angles

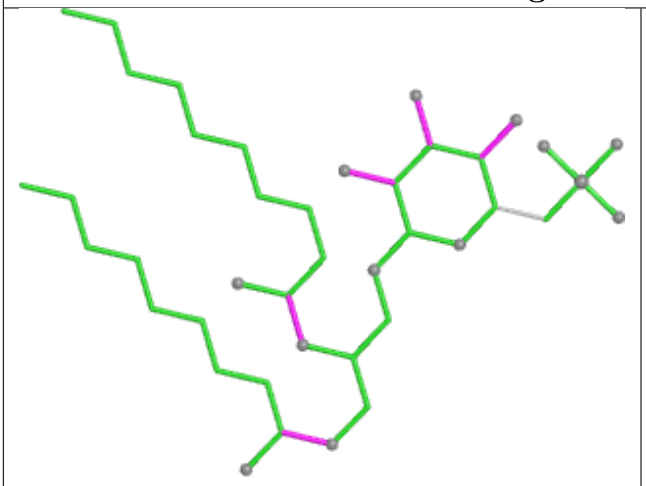


Torsions

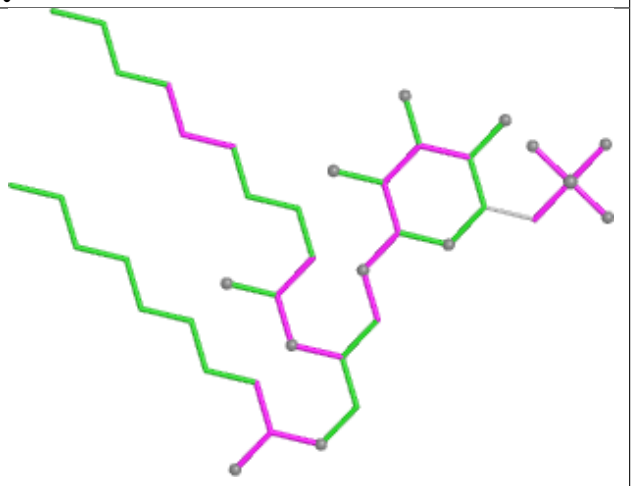


Rings

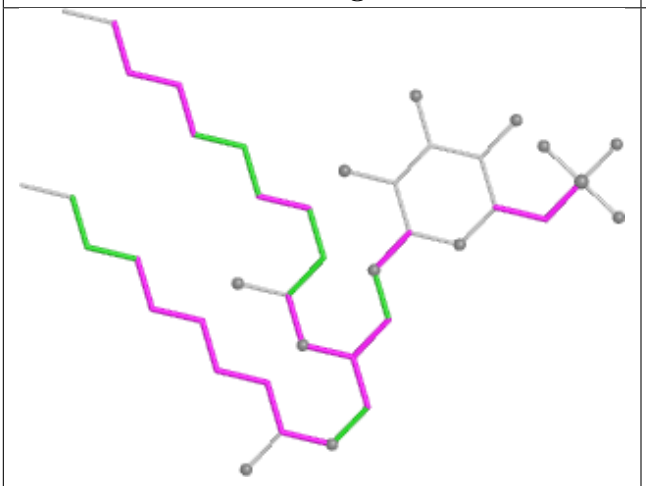
Ligand SQD 8 301



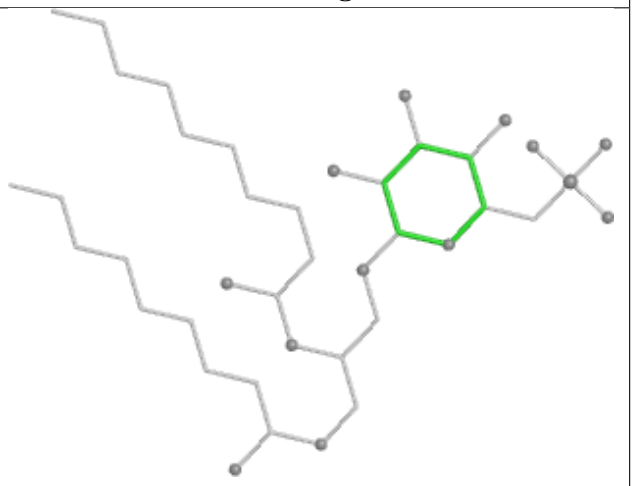
Bond lengths



Bond angles

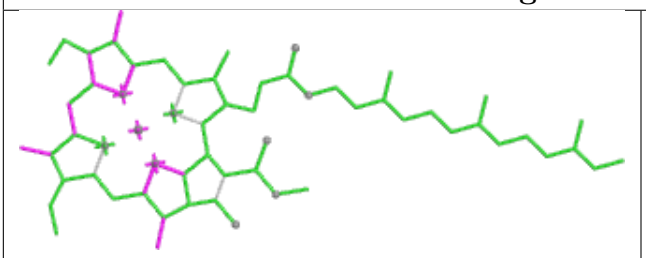


Torsions

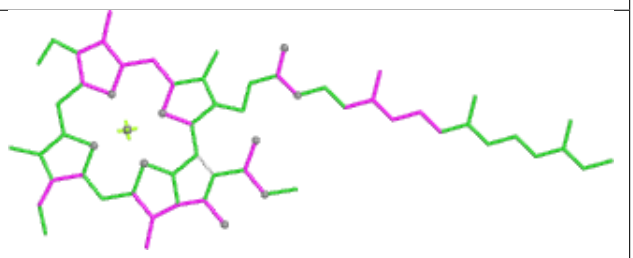


Rings

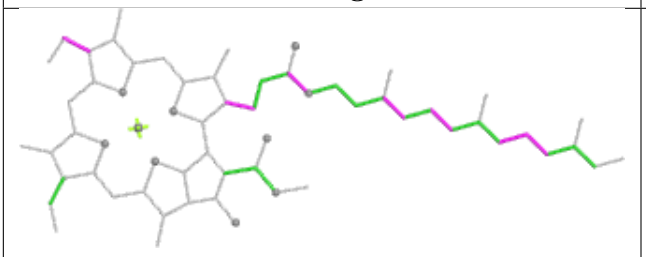
Ligand CLA 18 307



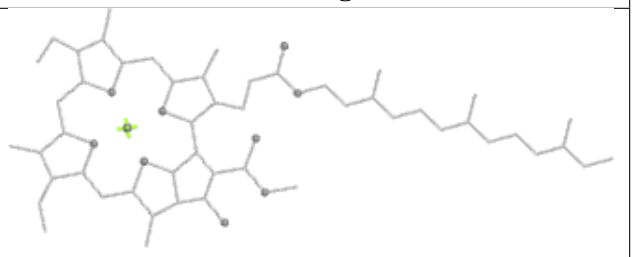
Bond lengths



Bond angles

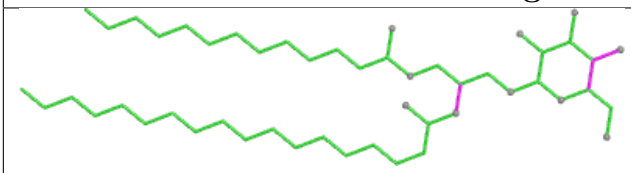


Torsions

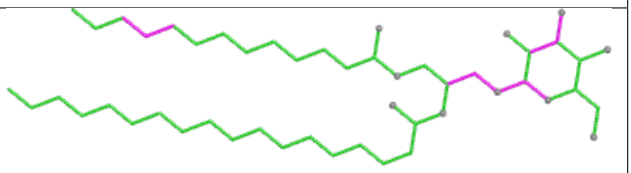


Rings

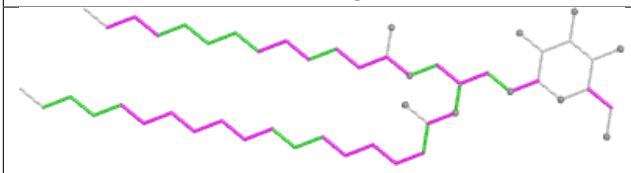
Ligand LMG J 101



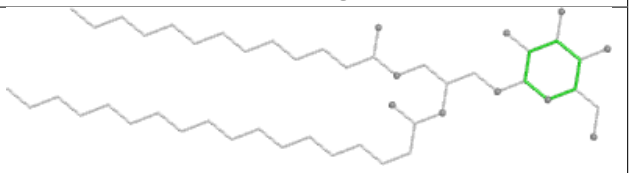
Bond lengths



Bond angles

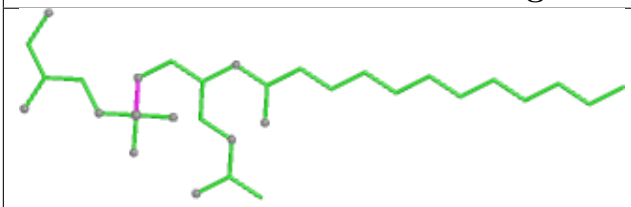


Torsions

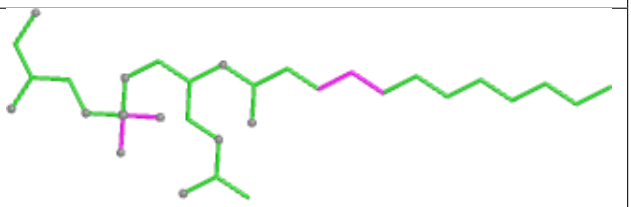


Rings

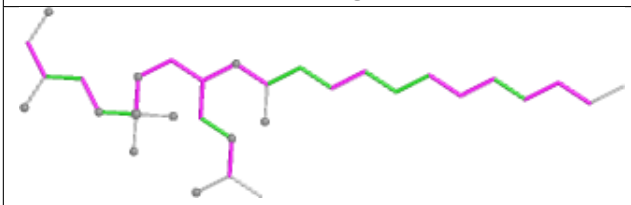
Ligand LHG 8 317



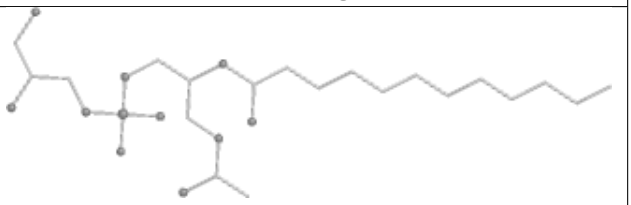
Bond lengths



Bond angles

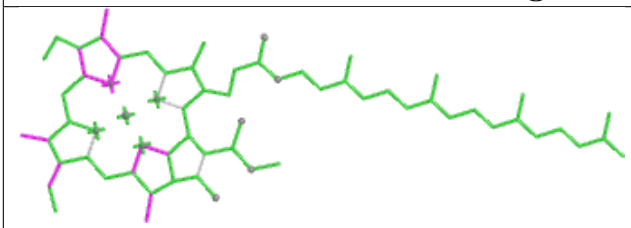


Torsions

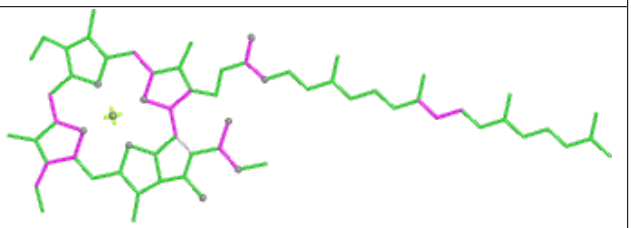


Rings

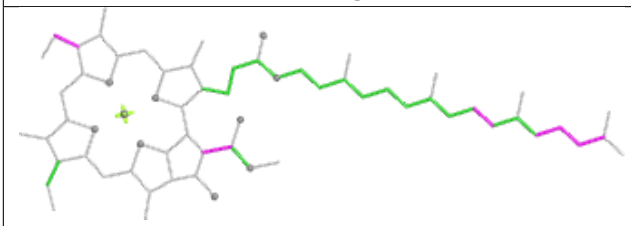
Ligand CLA b 616



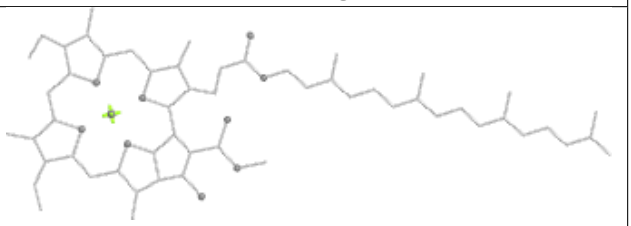
Bond lengths



Bond angles

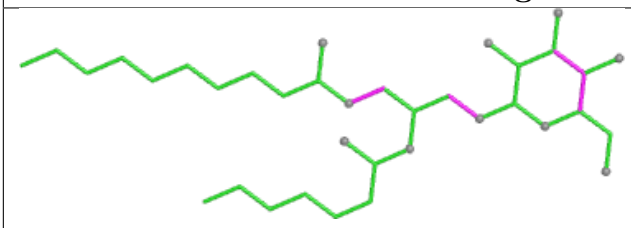


Torsions

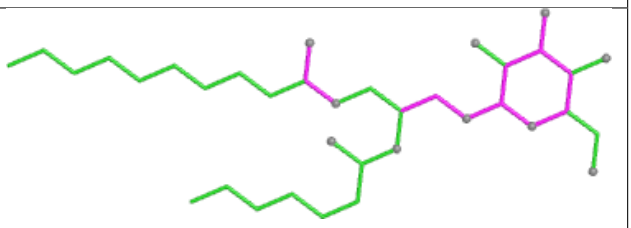


Rings

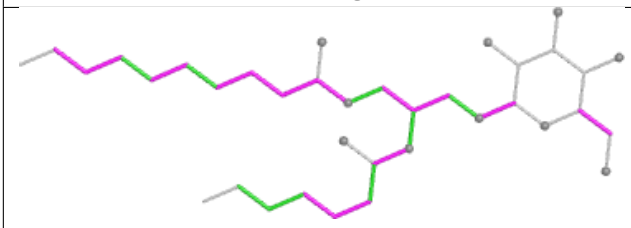
Ligand LMG 15 315



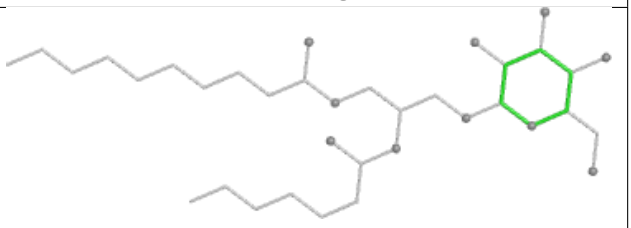
Bond lengths



Bond angles

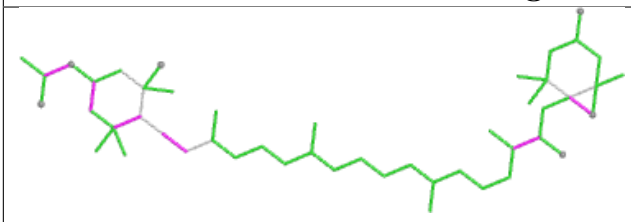


Torsions

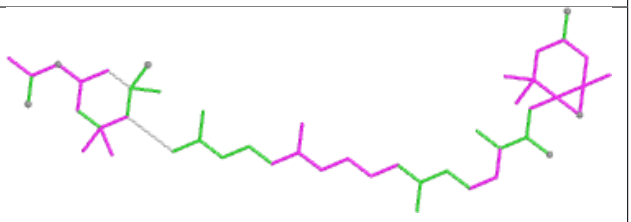


Rings

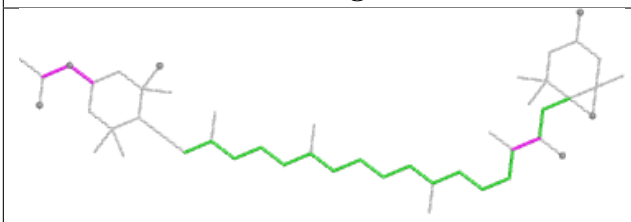
Ligand A86 18 304



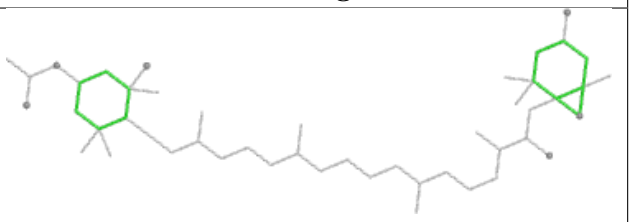
Bond lengths



Bond angles

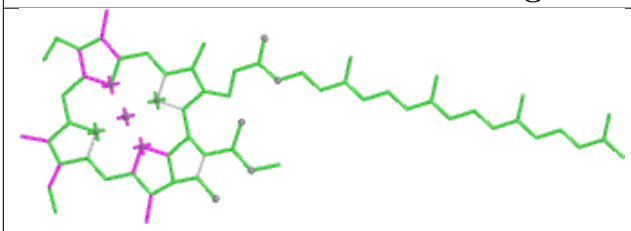


Torsions

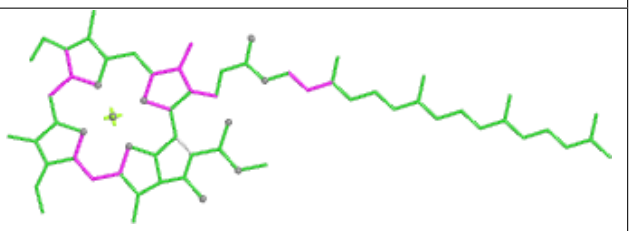


Rings

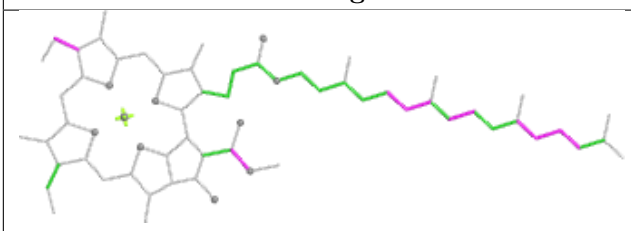
Ligand CLA B 605



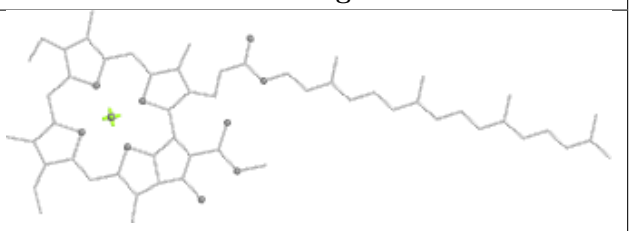
Bond lengths



Bond angles

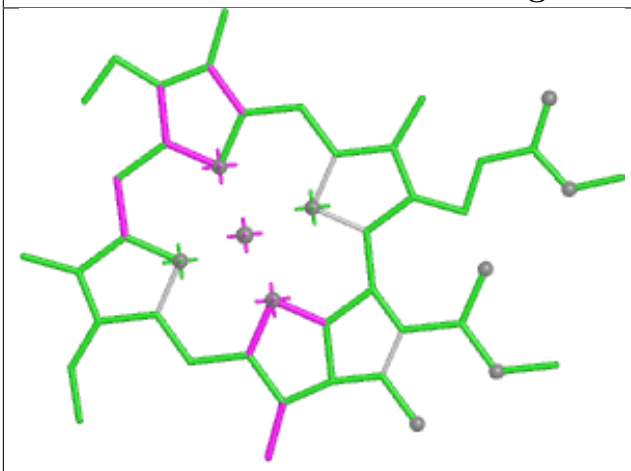


Torsions

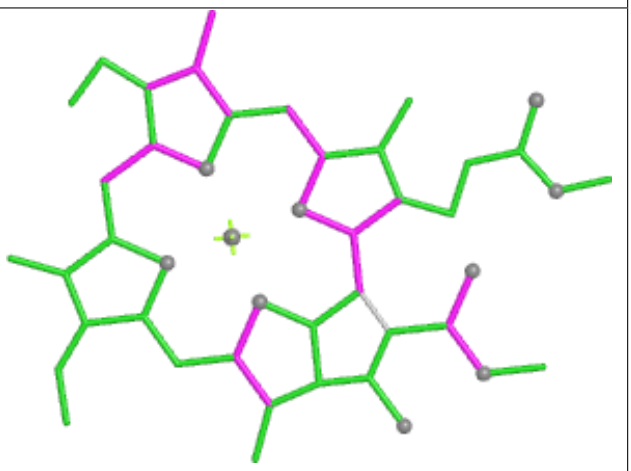


Rings

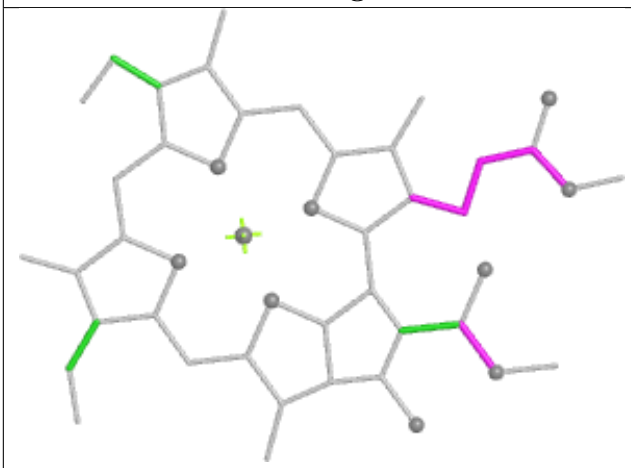
Ligand CLA 4 311



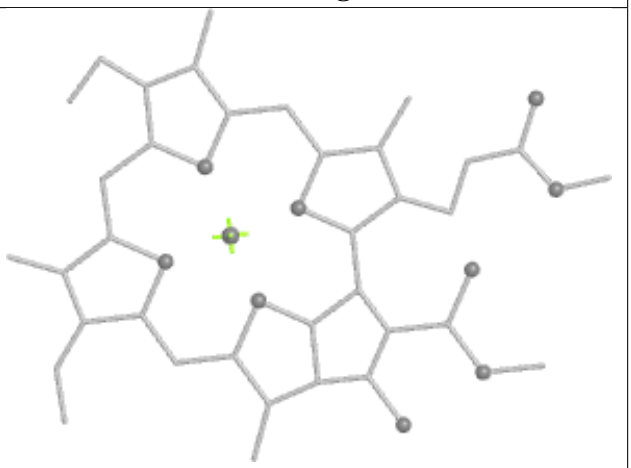
Bond lengths



Bond angles

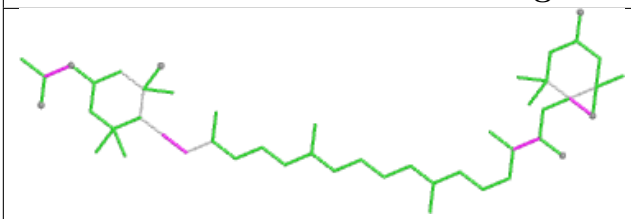


Torsions

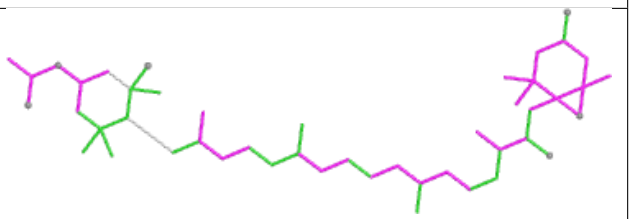


Rings

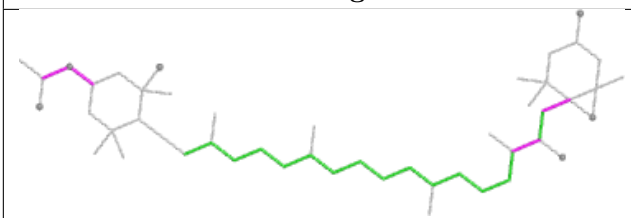
Ligand A86 9 304



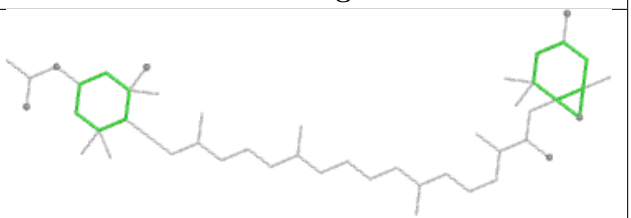
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

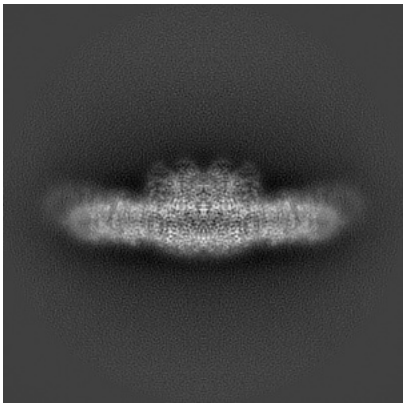
6 Map visualisation

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.

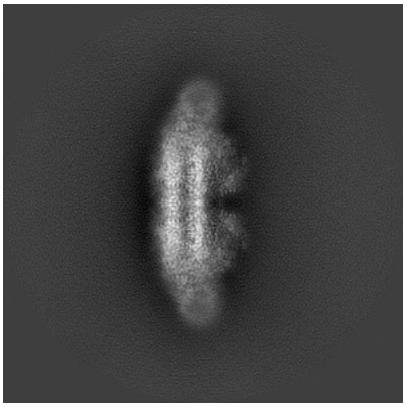
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

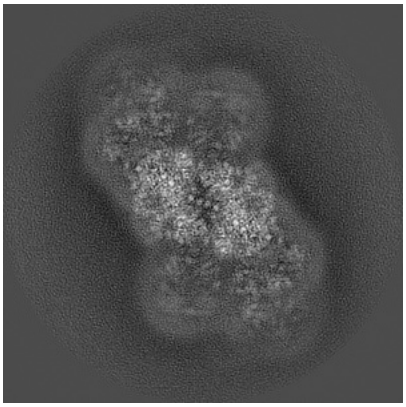
6.1.1 Primary map



X



Y

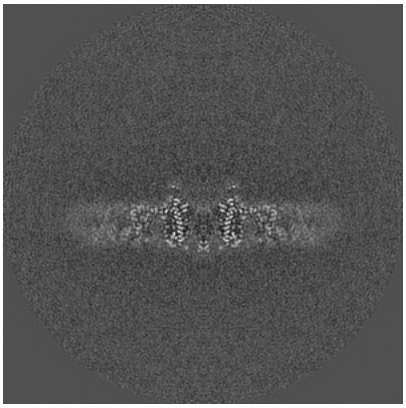


Z

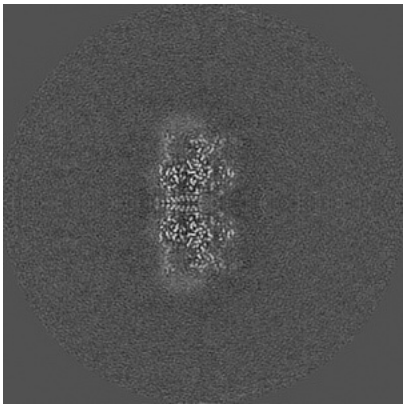
The images above show the map projected in three orthogonal directions.

6.2 Central slices

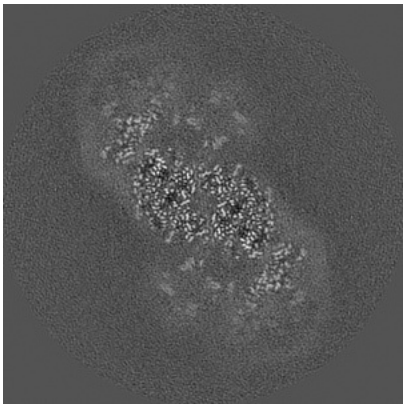
6.2.1 Primary map



X Index: 170



Y Index: 170

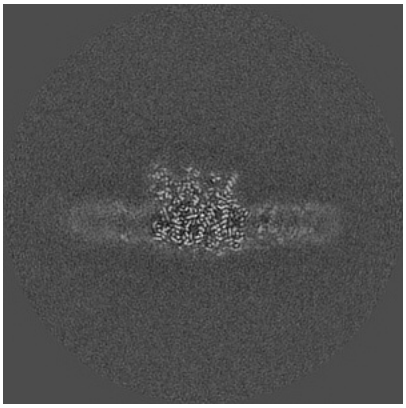


Z Index: 170

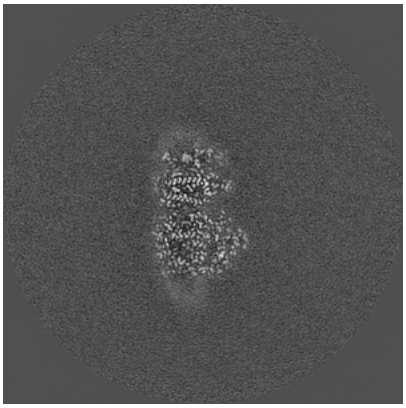
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

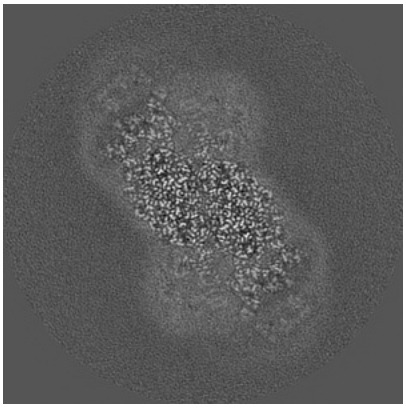
6.3.1 Primary map



X Index: 191



Y Index: 187

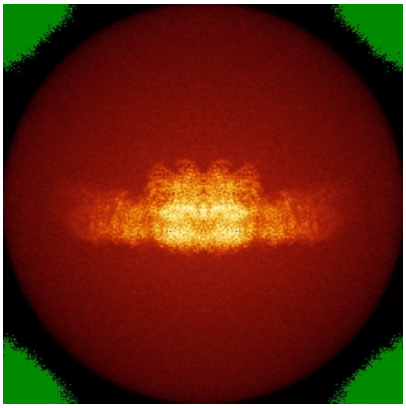


Z Index: 165

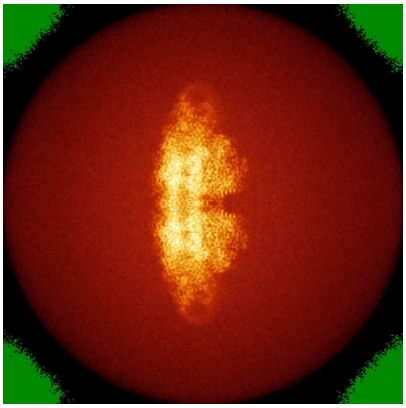
The images above show the largest variance slices of the map in three orthogonal directions.

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

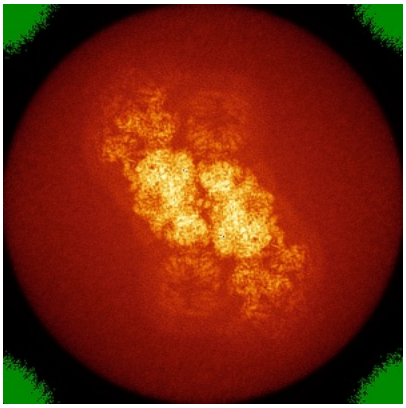
6.4.1 Primary map



X



Y

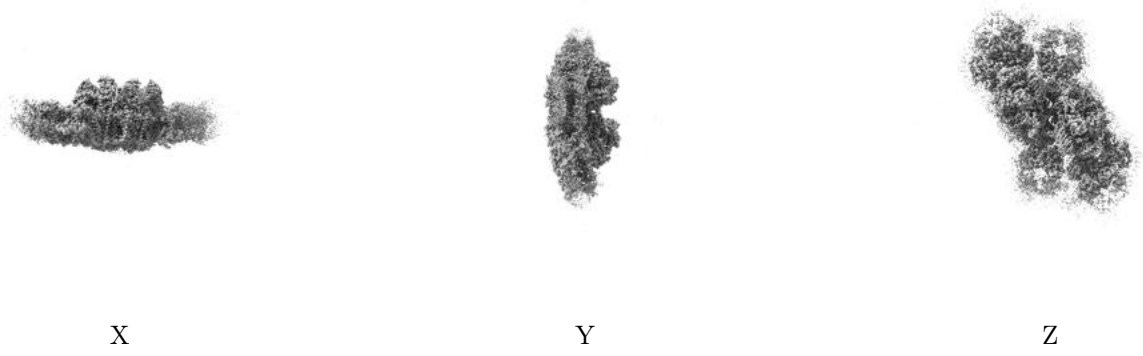


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

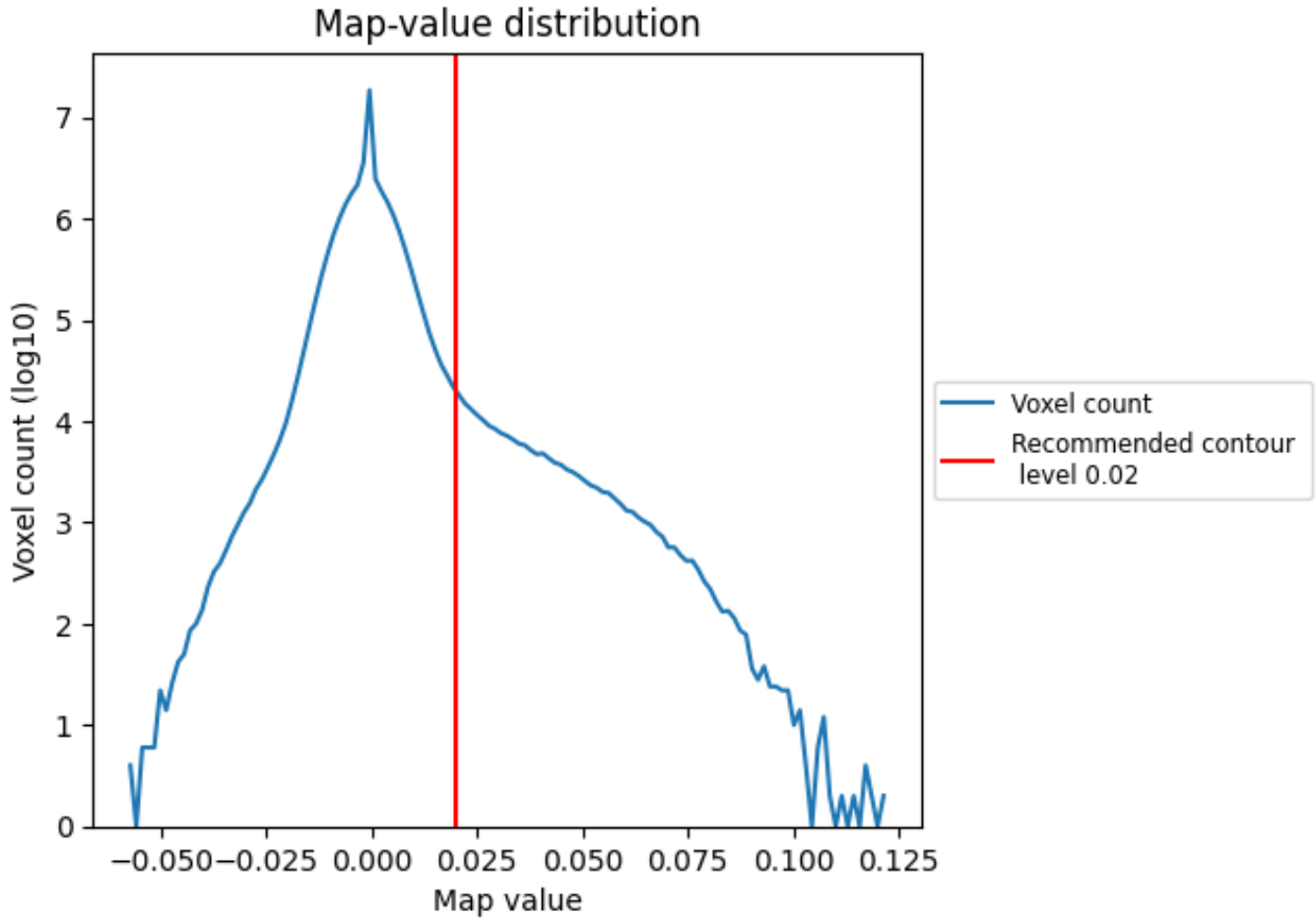
6.6 Mask visualisation (i)

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

7 Map analysis

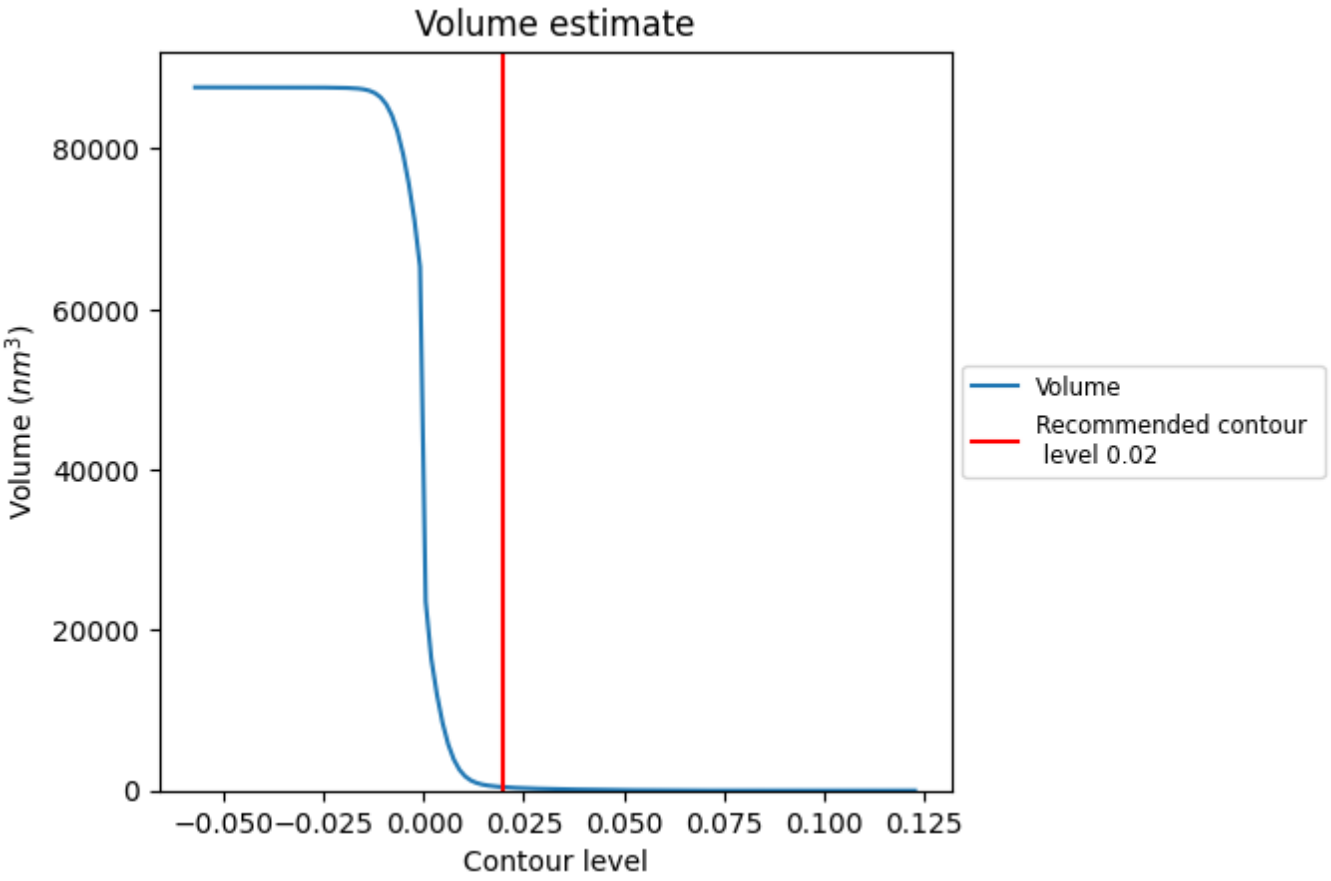
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

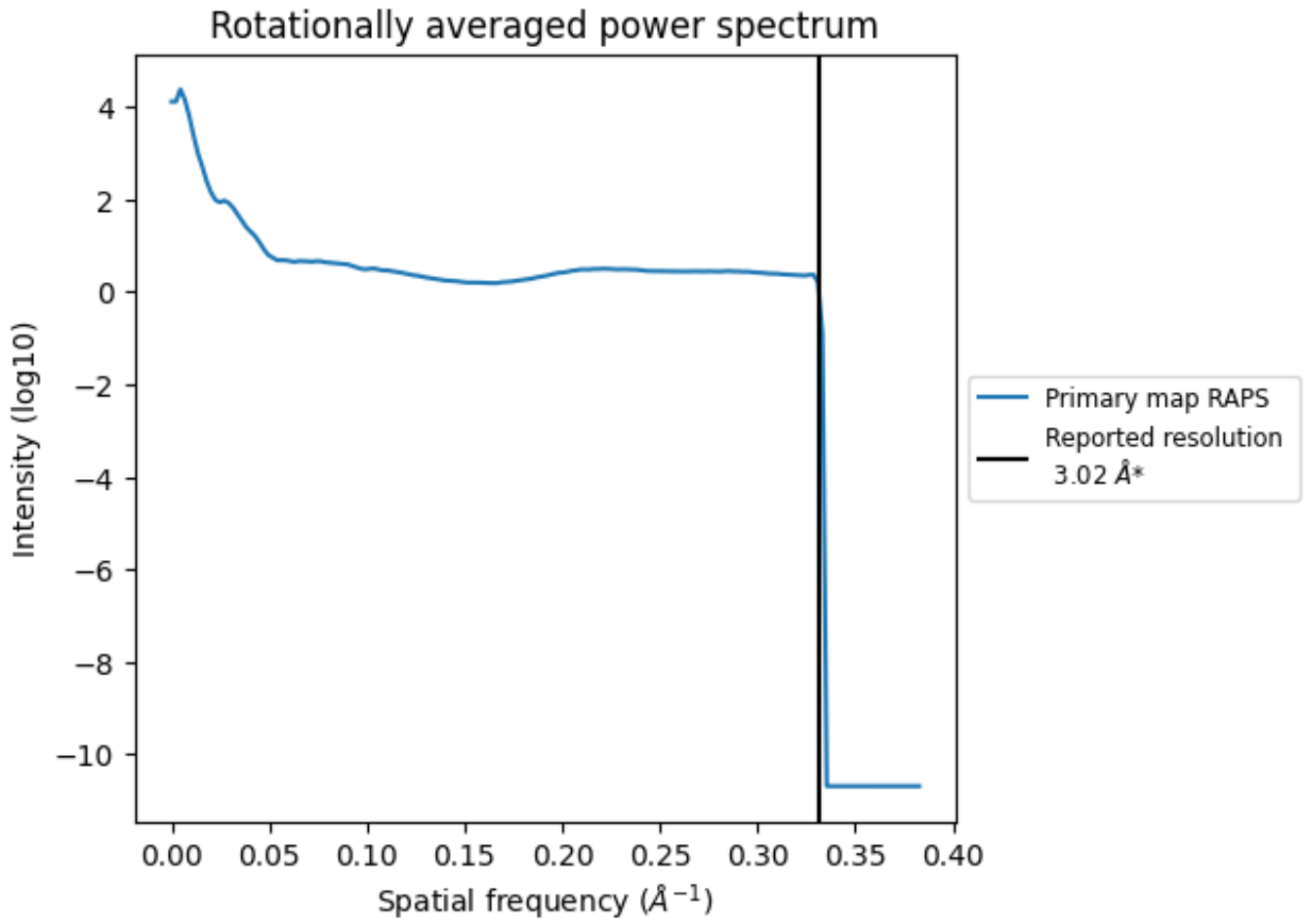
7.2 Volume estimate



The volume at the recommended contour level is 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}

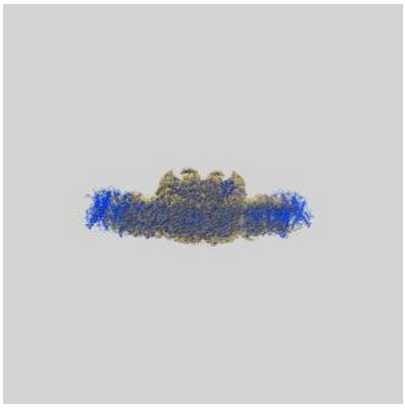
8 Fourier-Shell correlation

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

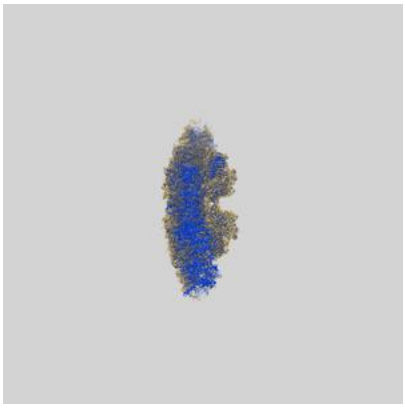
9 Map-model fit

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 47.

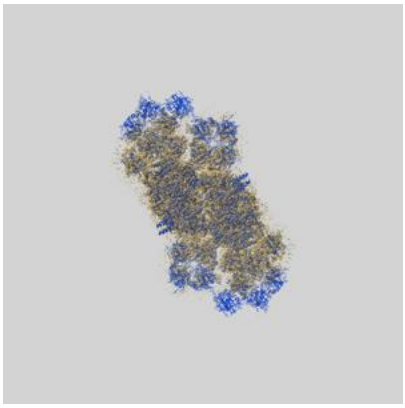
9.1 Map-model overlay



X



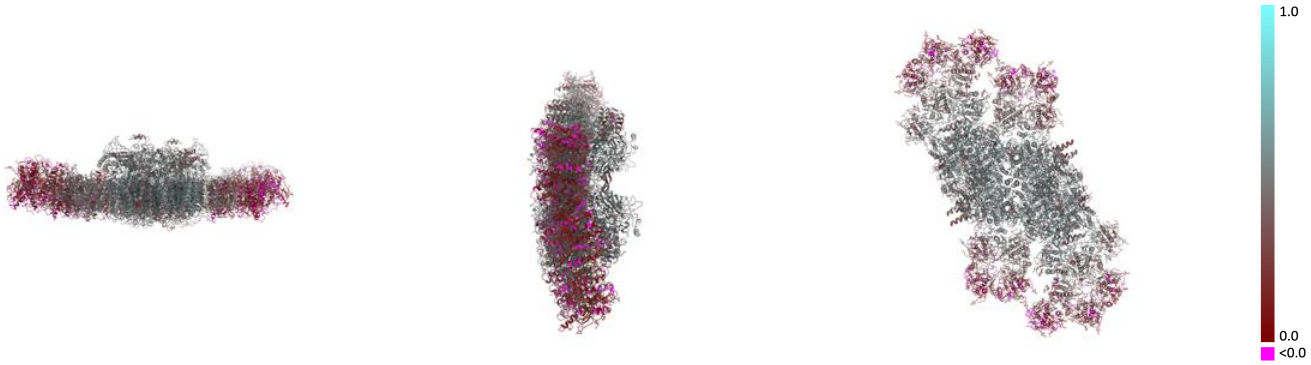
Y



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.

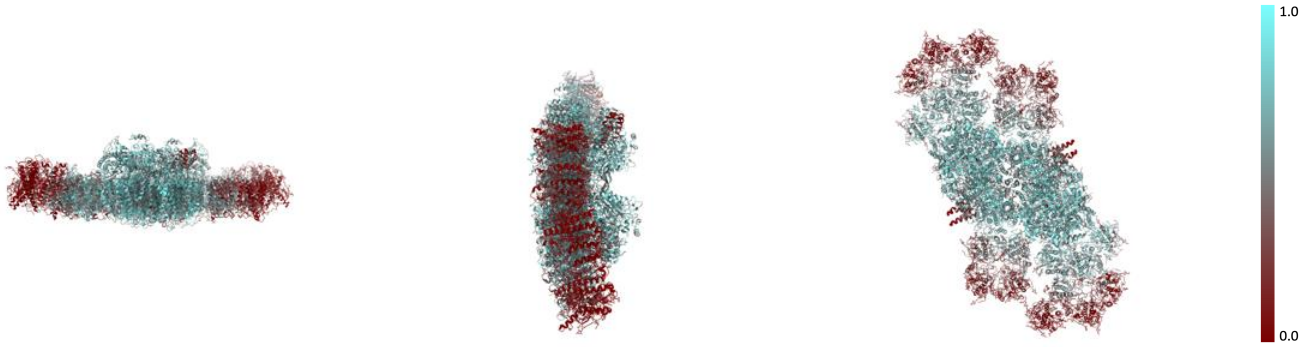
9.2 Q-score mapped to coordinate model



X Y Z

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

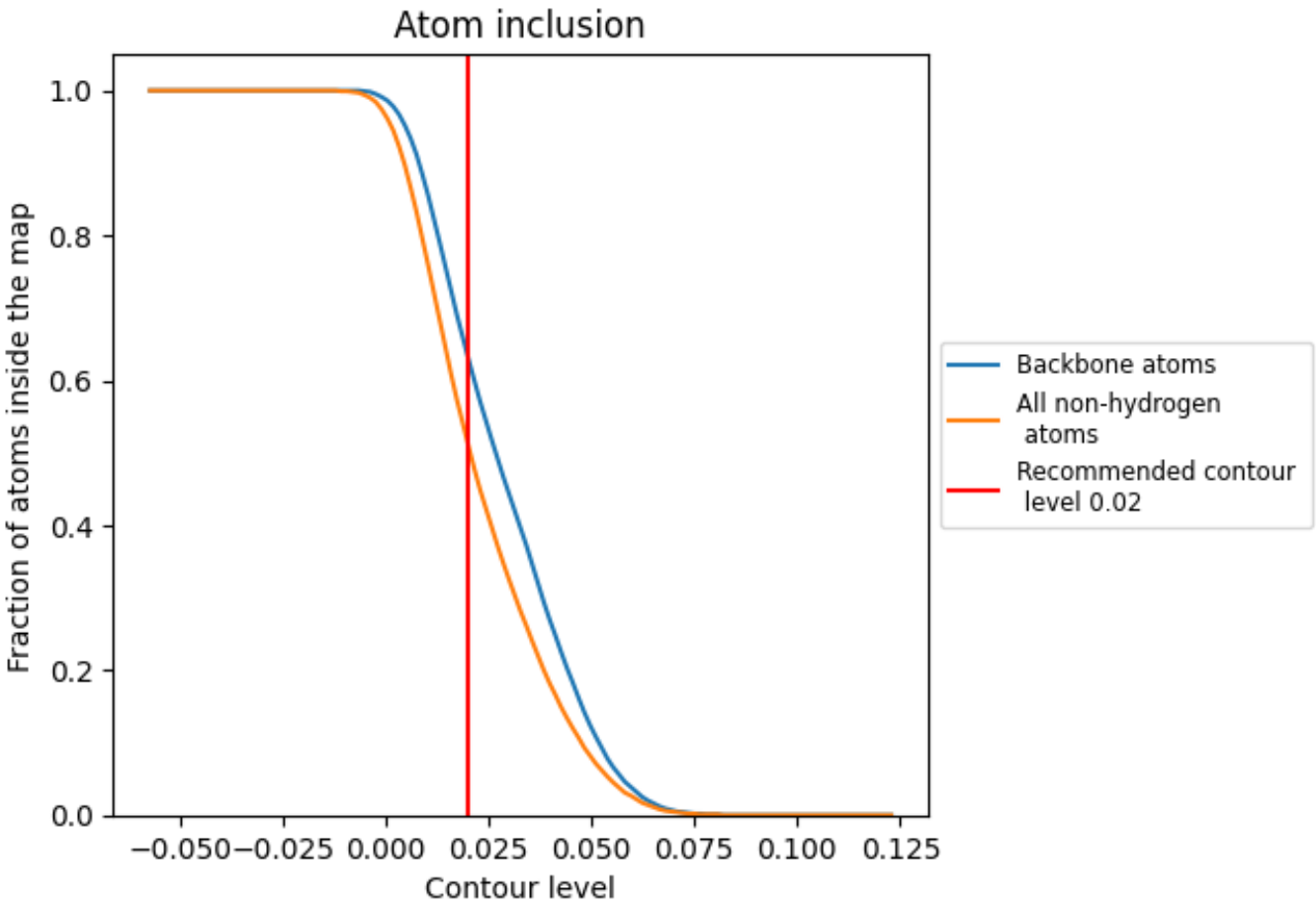
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

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	Q-score
All	0.5130	0.3850
0	0.5870	0.3810
1	0.3470	0.2950
10	0.5900	0.3960
11	0.3310	0.2880
12	0.0900	0.1210
13	0.0840	0.1180
14	0.4270	0.3380
15	0.4080	0.2930
16	0.0380	0.1490
17	0.0840	0.1710
18	0.5780	0.3840
19	0.0060	0.0800
2	0.0910	0.1220
3	0.0880	0.1170
4	0.4240	0.3460
5	0.4000	0.2960
6	0.0350	0.1540
7	0.0820	0.1720
8	0.5890	0.3800
9	0.0050	0.0870
A	0.7640	0.5220
B	0.7290	0.5140
C	0.7560	0.5300
D	0.7530	0.5220
E	0.6500	0.4390
F	0.5790	0.4350
G	0.2400	0.3790
H	0.7270	0.4870
I	0.7470	0.5030
J	0.5510	0.4140
K	0.6550	0.4860
L	0.6270	0.5090
M	0.5940	0.4760
N	0.7580	0.4700



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Chain	Atom inclusion	Q-score
O	0.6790	0.4660
P	0.6380	0.4460
Q	0.6190	0.4260
R	0.6270	0.4430
T	0.6530	0.4970
U	0.6900	0.4650
V	0.7300	0.4920
W	0.5480	0.4210
X	0.4670	0.4270
Y	0.5190	0.3660
Z	0.6110	0.4460
a	0.7710	0.5220
b	0.7290	0.5140
c	0.7560	0.5280
d	0.7550	0.5240
e	0.6530	0.4420
f	0.5790	0.4530
g	0.2390	0.3770
h	0.7290	0.4920
i	0.6740	0.5100
j	0.5820	0.4360
k	0.6550	0.4750
l	0.6370	0.5090
m	0.5940	0.4720
n	0.7810	0.4780
o	0.6820	0.4700
p	0.6380	0.4490
q	0.6230	0.4290
r	0.6300	0.4490
t	0.6610	0.4960
u	0.6950	0.4680
v	0.7350	0.4920
w	0.5290	0.4240
x	0.4830	0.4400
y	0.5220	0.3540
z	0.6340	0.4460