Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:25 AM JST

PDB ID	:	6J3Z / pdb_00006j3z
EMDB ID	:	EMD-9776
Title	:	Structure of C2S1M1-type PSII-FCPII supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-01-07
Resolution	:	3.60 Å(reported)
Based on initial models	:	3WU2, 3JCU

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:

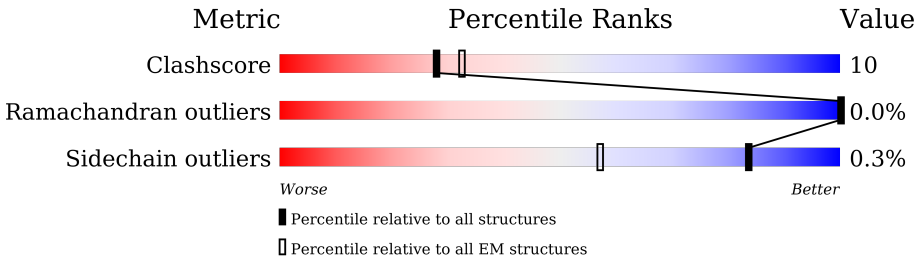
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

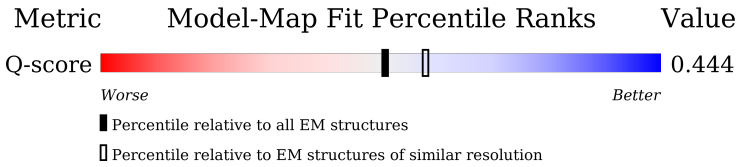
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	344	83% 14% .
1	a	344	84% 13% .
2	B	509	. 82% 13% 5%
2	b	509	. 81% 14% 5%

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Mol	Chain	Length	Quality of chain
3	C	471	81% 15%
3	c	471	81% 15%
4	D	351	84% 13%
4	d	351	84% 13%
5	E	84	6% 83% 6% 11%
5	e	84	83% 6% 11%
6	F	43	51% 14% 35%
6	f	43	51% 14% 35%
7	H	67	88% 10%
7	h	67	90% 9%
8	I	38	76% 16% 8%
8	i	38	74% 18% 8%
9	J	39	72% 15% 13%
9	j	39	5% 79% 8% 13%
10	K	44	73% 11% 16%
10	k	44	5% 73% 11% 16%
11	L	38	5% 84% 16%
11	l	38	5% 84% 16%
12	M	131	28% 68%
12	m	131	30% 68%
13	O	248	5% 79% 20%
13	o	248	8% 78% 21%
14	T	31	81% 16%
14	t	31	10% 81% 16%
15	U	93	85% 15%

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Mol	Chain	Length	Quality of chain
15	u	93	84% 16%
16	V	137	80% 19%
16	v	137	82% 17%
17	Y	34	6% 85% 15%
17	y	34	18% 85% 15%
18	X	38	8% 92% 5%
18	x	38	8% 97%
19	Z	61	87% 10%
19	z	61	84% 13%
20	Q	155	7% 76% 12% 12%
20	q	155	41% 75% 13% 12%
21	W	72	6% 64% 8% 28%
21	w	72	12% 60% 12% 28%
22	0	31	100%
22	5	31	97%
23	1	30	100%
23	6	30	97%
24	2	10	90% 10%
24	7	10	80% 20%
25	11	207	67% 18% 15%
25	12	207	68% 17% 15%
25	13	207	71% 14% 15%
25	14	207	71% 14% 15%
25	15	207	8% 66% 19% 15%
25	16	207	62% 23% 15%

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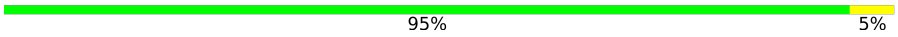
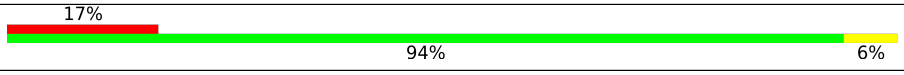
Mol	Chain	Length	Quality of chain
25	17	207	
25	18	207	
26	19	215	
27	20	143	
28	21	155	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	BCT	a	406	-	-	X	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 74619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II reaction center protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		

- Molecule 2 is a protein called Photosystem II chlorophyll protein CP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		
2	b	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		

- Molecule 3 is a protein called Photosystem II chlorophyll protein CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		
3	c	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		

- Molecule 4 is a protein called Photosystem II reaction center protein D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		
4	d	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 616	C 401	N 102	O 113	0	0
5	e	75	Total 616	C 401	N 102	O 113	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total 228	C 155	N 39	O 33	S 1	0	0
6	f	28	Total 228	C 155	N 39	O 33	S 1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	66	Total 513	C 340	N 83	O 88	S 2	0	0
7	h	66	Total 513	C 340	N 83	O 88	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total 287	C 194	N 45	O 47	S 1	0	0
8	i	35	Total 287	C 194	N 45	O 47	S 1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total 254	C 172	N 38	O 43	S 1	0	0
9	j	34	Total 254	C 172	N 38	O 43	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total 302	C 212	N 45	O 45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total 302	C 212	N 45	O 45	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total 310	C 208	N 48	O 53	S 1	0	0
11	l	38	Total 310	C 208	N 48	O 53	S 1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	42	Total 316	C 207	N 51	O 58	0	0
12	m	42	Total 316	C 207	N 51	O 58	0	0

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	245	Total 1845	C 1166	N 306	O 365	S 8	0	0
13	o	245	Total 1845	C 1166	N 306	O 365	S 8	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	93	Total 713	C 455	N 119	O 137	S 2	0	0
15	u	93	Total 713	C 455	N 119	O 137	S 2	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		
16	v	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		
17	y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	37	Total	C	N	O	S	0	0
			263	171	45	46	1		
18	x	37	Total	C	N	O	S	0	0
			263	171	45	46	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		
19	z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		
20	q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	52	Total	C	N	O	0	0
			422	273	65	84		
21	w	52	Total	C	N	O	0	0
			422	273	65	84		

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	0	31	Total	C	N	O	0	0
			155	93	31	31		
22	5	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	30	Total	C	N	O	0	0
			150	90	30	30		
23	6	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 24 is a protein called Unknown protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	10	Total	C	N	O	0	0
			50	30	10	10		
24	7	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	12	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	13	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	14	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	15	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	16	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	17	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	18	176	Total 1343	C 852	N 228	O 256	S 7	0	0

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	19	215	Total 1075	C 645	N 215	O 215	0	0

- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	20	143	Total 715	C 429	N 143	O 143	0	0

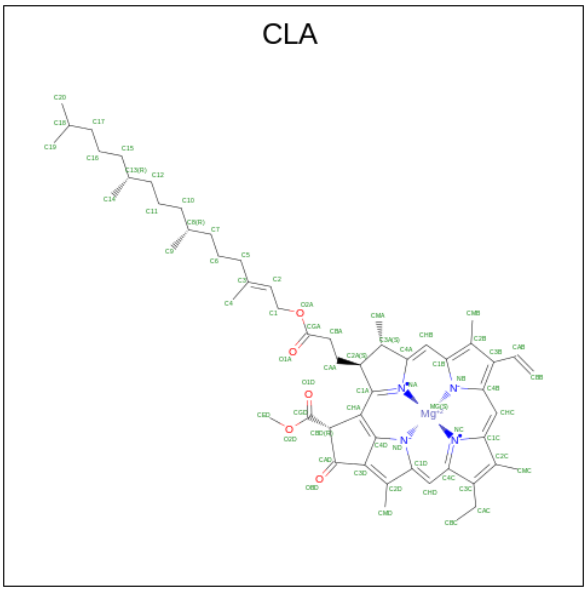
- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	21	155	Total 775	C 465	N 155	O 155	0	0

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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Mol	Chain	Residues	Atoms					AltConf
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
30	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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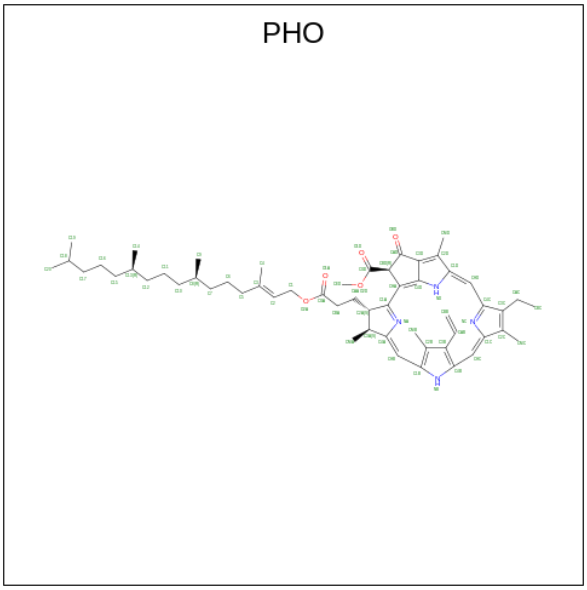
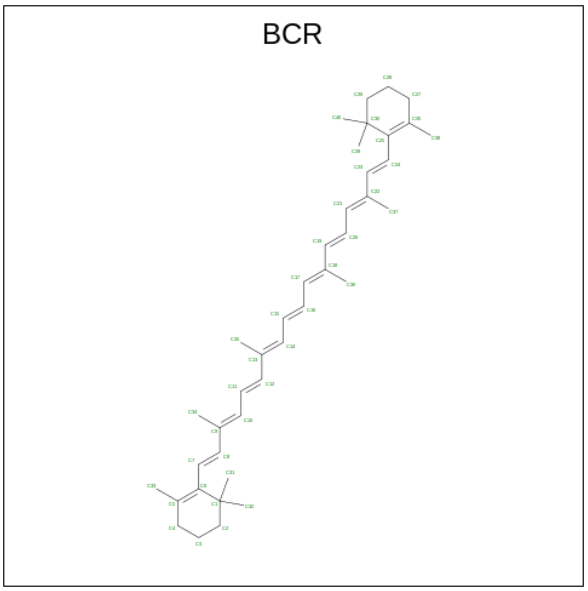
Mol	Chain	Residues	Atoms					AltConf
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	C	1	Total C 40 40	0
32	C	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	H	1	Total C 40 40	0
32	Y	1	Total C 40 40	0
32	Z	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0

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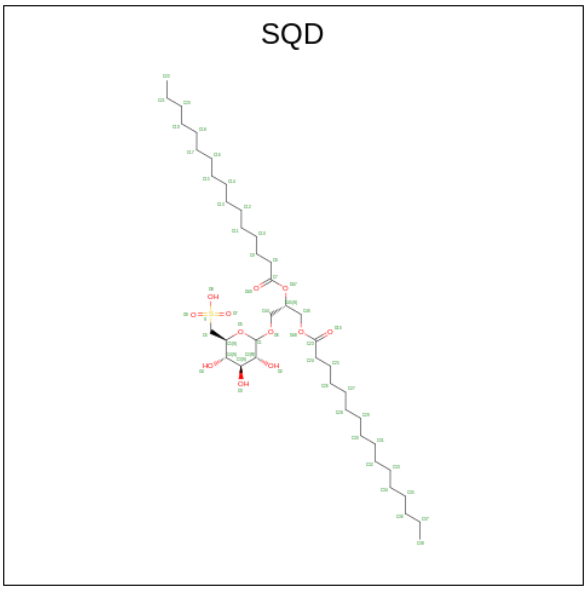
Mol	Chain	Residues	Atoms	AltConf
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	h	1	Total C 40 40	0
32	m	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O S 54 41 12 1	0

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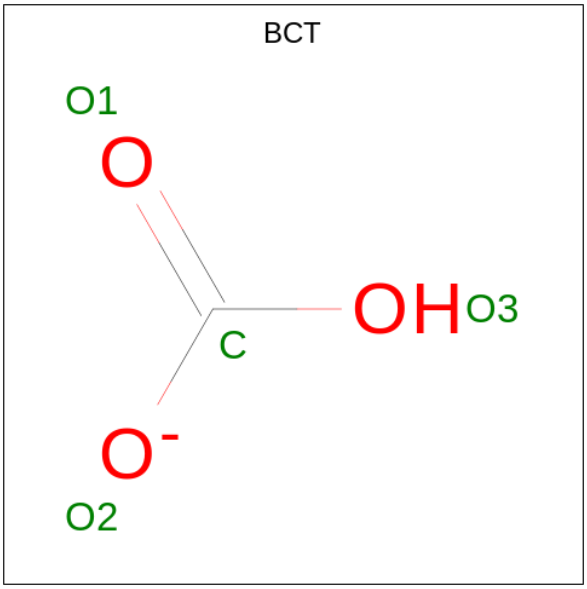
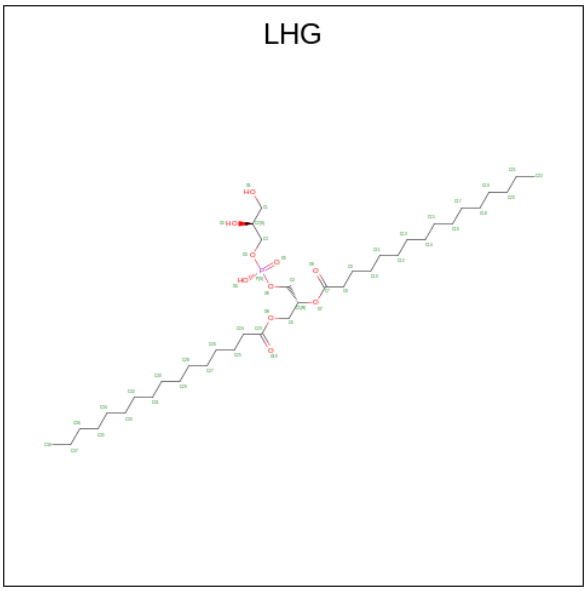
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



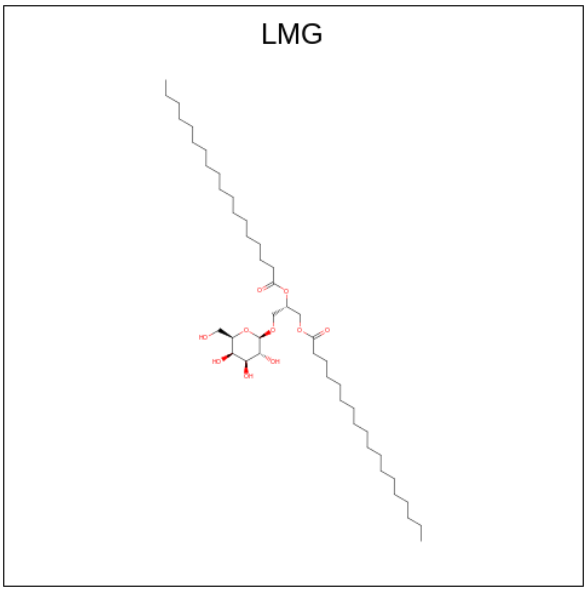
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	a	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



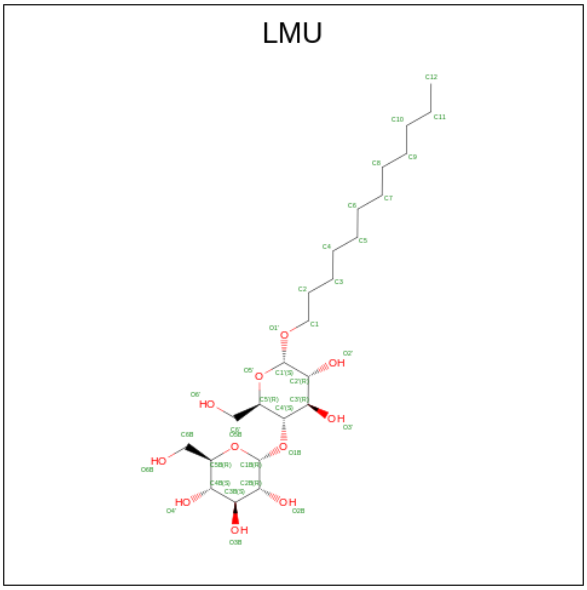
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	
35	B	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			46	35	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



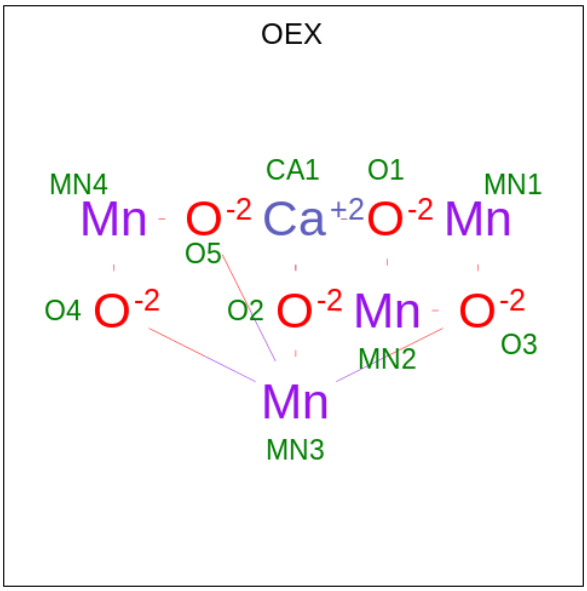
Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total C O 51 41 10	0
36	B	1	Total C O 51 41 10	0
36	D	1	Total C O 51 41 10	0
36	M	1	Total C O 40 30 10	0
36	Q	1	Total C O 51 41 10	0
36	W	1	Total C O 51 41 10	0
36	1	1	Total C O 39 29 10	0
36	b	1	Total C O 51 41 10	0
36	b	1	Total C O 51 41 10	0
36	c	1	Total C O 51 41 10	0
36	d	1	Total C O 51 41 10	0
36	m	1	Total C O 40 30 10	0
36	w	1	Total C O 51 41 10	0
36	12	1	Total C O 39 29 10	0

- Molecule 37 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			32	21	11	
37	12	1	Total	C	O	0
			32	21	11	

- Molecule 38 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	Ca	Mn	O	0
			10	1	4	5	

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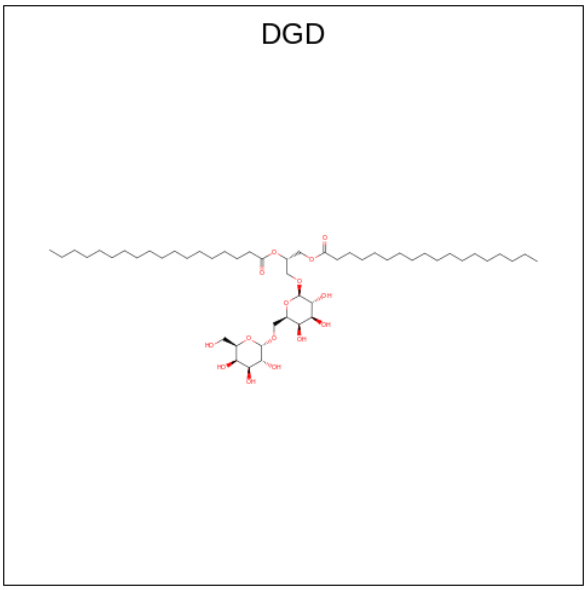
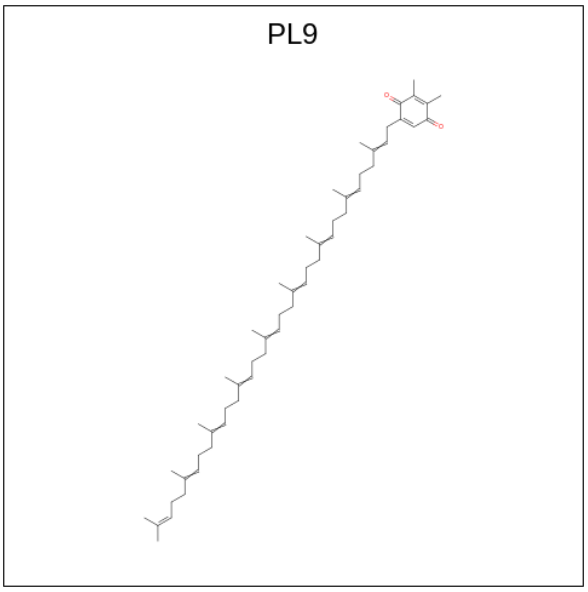
Mol	Chain	Residues	Atoms				AltConf
38	c	1	Total	Ca	Mn	O	0
			10	1	4	5	

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



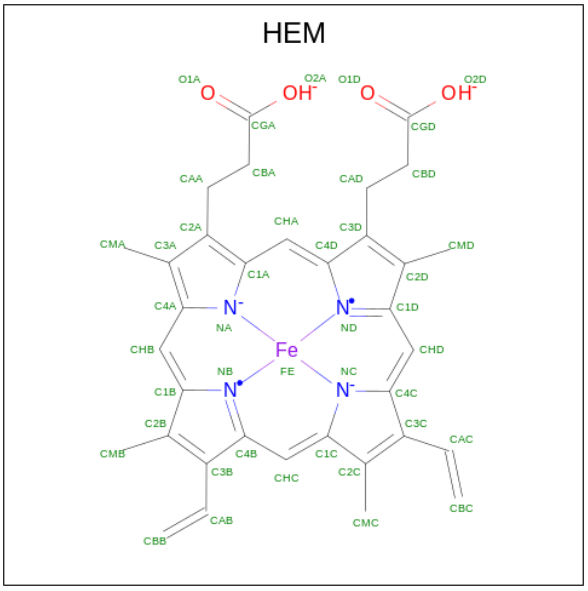
Mol	Chain	Residues	Atoms			AltConf
39	C	1	Total	C	O	0
			62	47	15	
39	C	1	Total	C	O	0
			62	47	15	
39	H	1	Total	C	O	0
			62	47	15	
39	J	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	h	1	Total	C	O	0
			62	47	15	
39	j	1	Total	C	O	0
			62	47	15	

- Molecule 40 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: $C_{53}H_{80}O_2$).



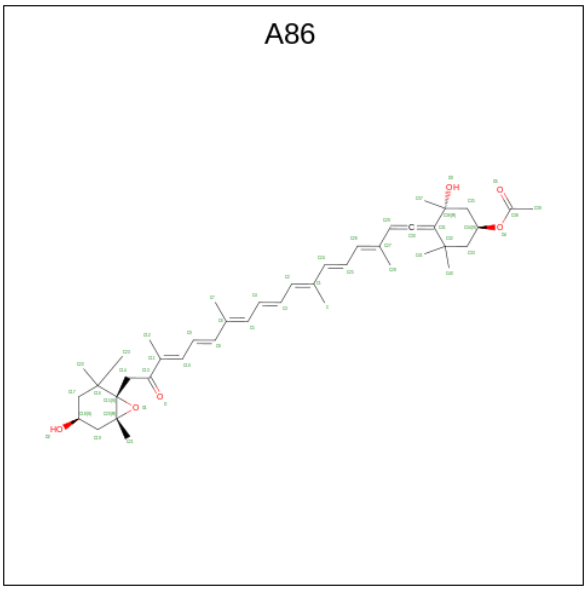
Mol	Chain	Residues	Atoms	AltConf
40	D	1	Total C O 55 53 2	0
40	D	1	Total C O 55 53 2	0
40	d	1	Total C O 55 53 2	0
40	d	1	Total C O 55 53 2	0

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



Mol	Chain	Residues	Atoms					AltConf
41	F	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	
41	f	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 (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
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	12	1	Total	C	O	0
			48	42	6	

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

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

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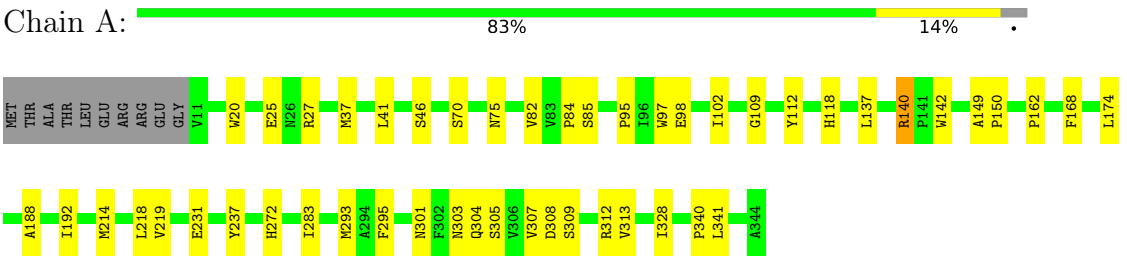
Mol	Chain	Residues	Atoms			AltConf
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	

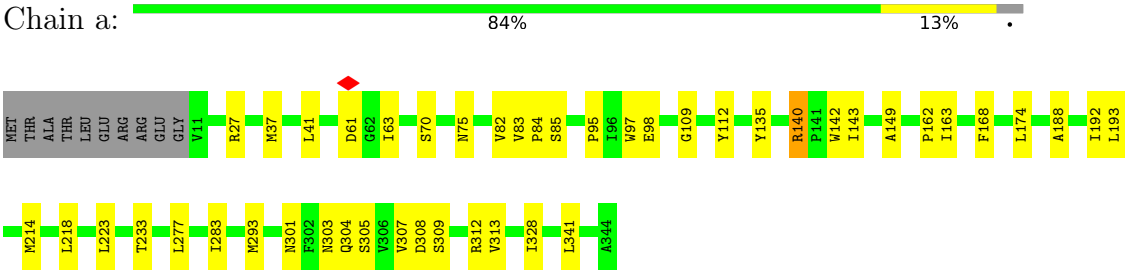
3 Residue-property plots (i)

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

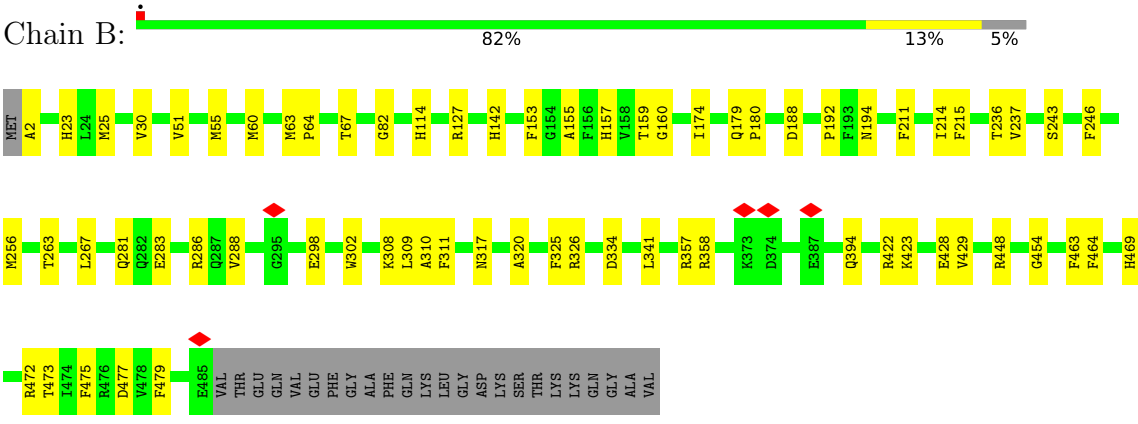
• Molecule 1: Photosystem II reaction center protein D1



• Molecule 1: Photosystem II reaction center protein D1

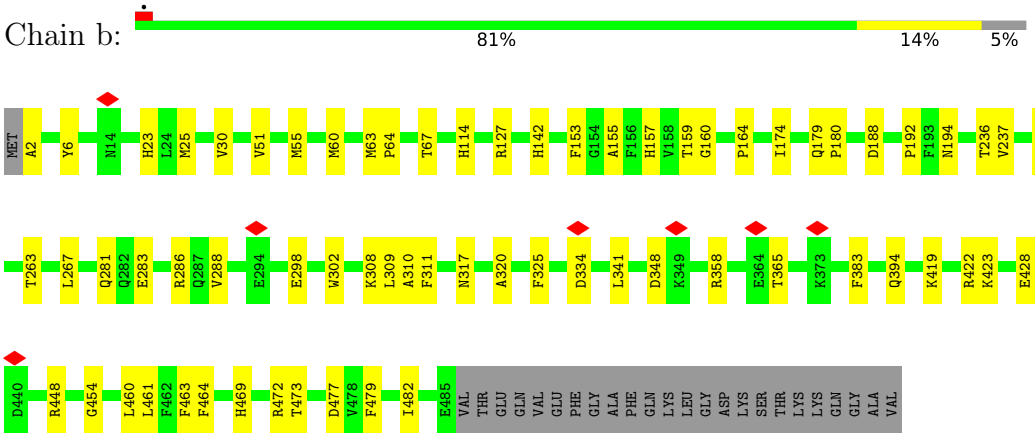


• Molecule 2: Photosystem II chlorophyll protein CP47



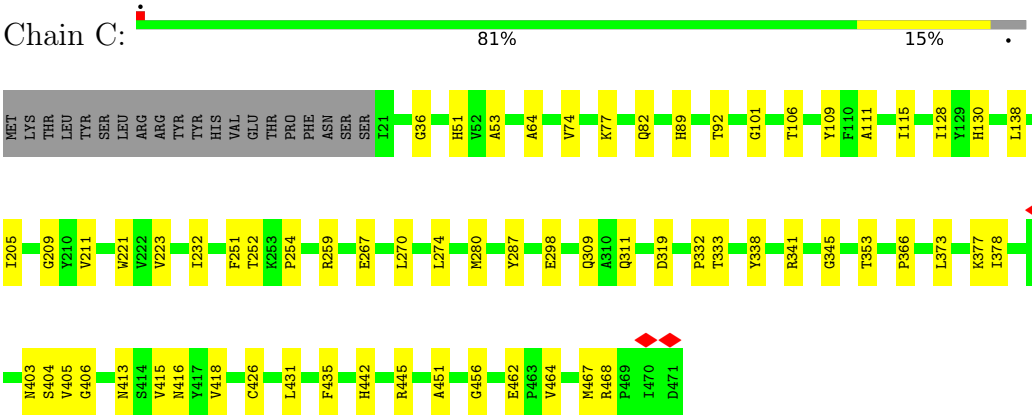
• Molecule 2: Photosystem II chlorophyll protein CP47

Chain b:



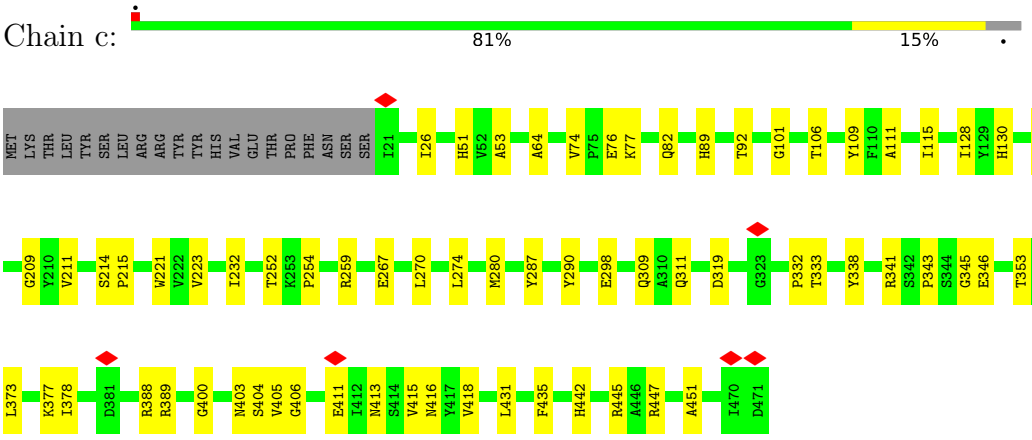
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain C:



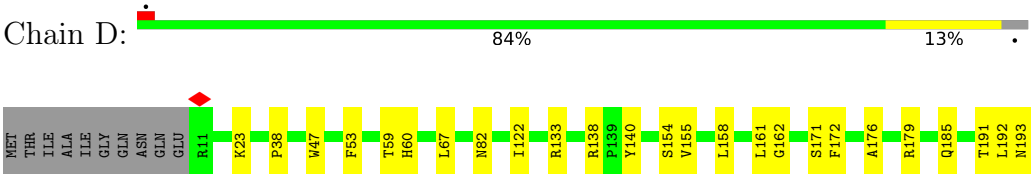
• Molecule 3: Photosystem II chlorophyll protein CP43

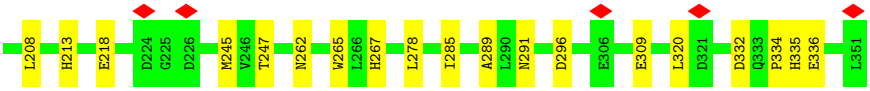
Chain c:



• Molecule 4: Photosystem II reaction center protein D2

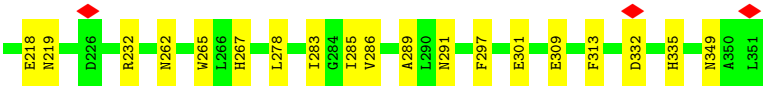
Chain D:





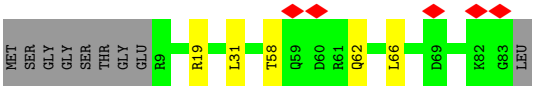
• Molecule 4: Photosystem II reaction center protein D2

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

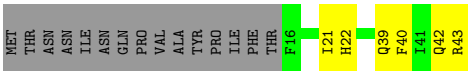
Chain e:

• Molecule 6: Cytochrome b559 subunit beta

Chain F:

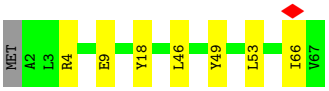
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



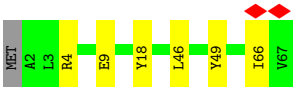
• Molecule 7: Photosystem II reaction center protein H

Chain H:



• Molecule 7: Photosystem II reaction center protein H

Chain h:

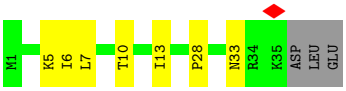


• Molecule 8: Photosystem II reaction center protein I

Chain I:

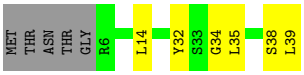
• Molecule 8: Photosystem II reaction center protein I

Chain i:



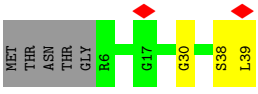
• Molecule 9: Photosystem II reaction center protein J

Chain J:



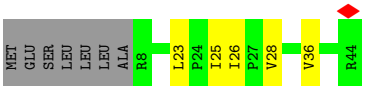
• Molecule 9: Photosystem II reaction center protein J

Chain j:



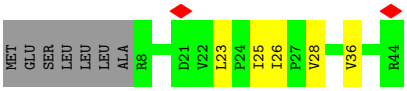
• Molecule 10: Photosystem II reaction center protein K

Chain K:



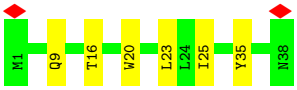
• Molecule 10: Photosystem II reaction center protein K

Chain k:



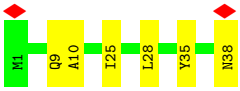
• Molecule 11: Photosystem II reaction center protein L

Chain L:



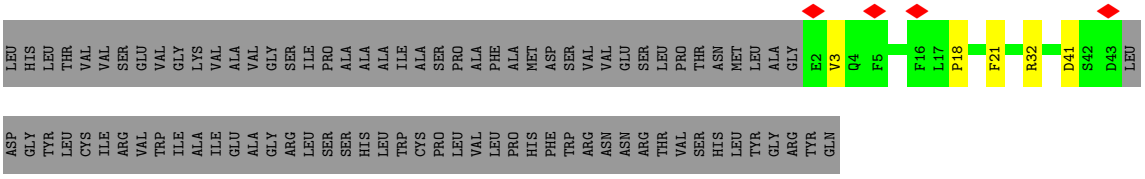
• Molecule 11: Photosystem II reaction center protein L

Chain l:



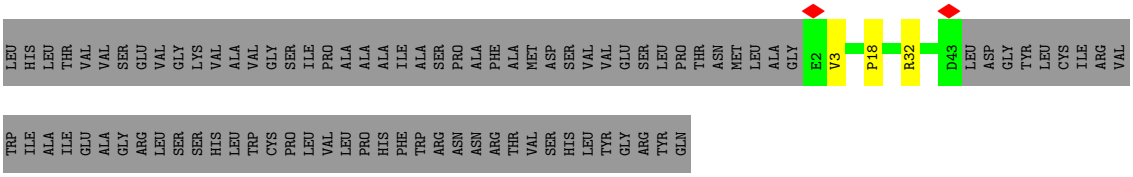
• Molecule 12: Photosystem II reaction center protein M

Chain M:



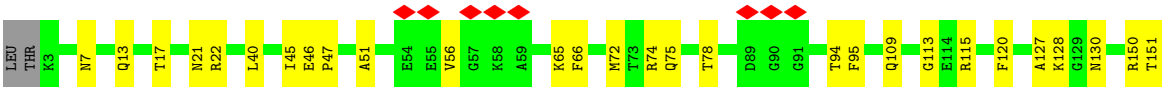
• Molecule 12: Photosystem II reaction center protein M

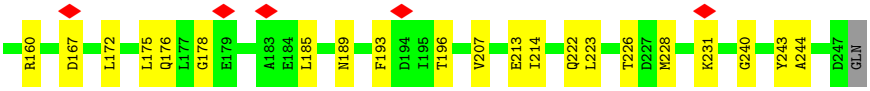
Chain m:



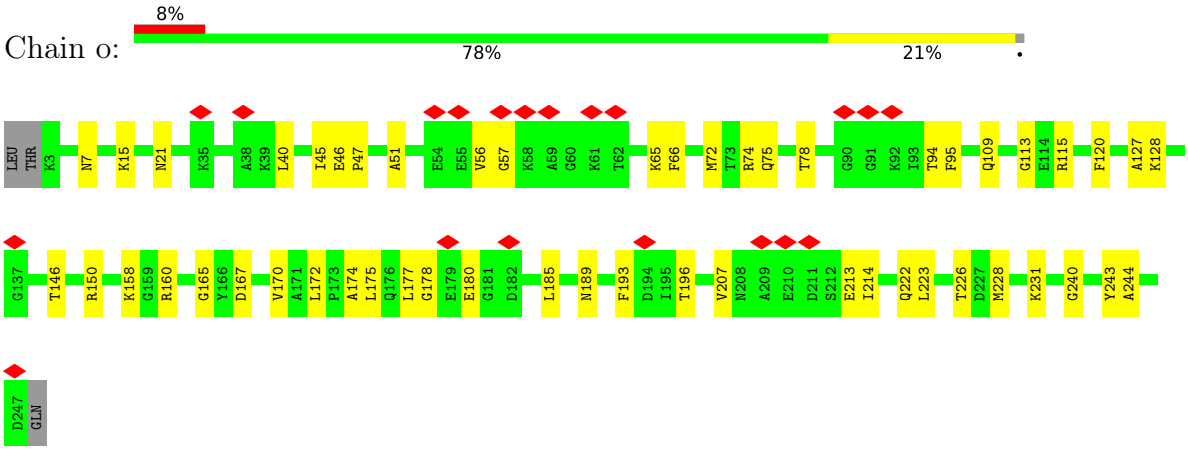
• Molecule 13: Extrinsic protein in photosystem II

Chain O:

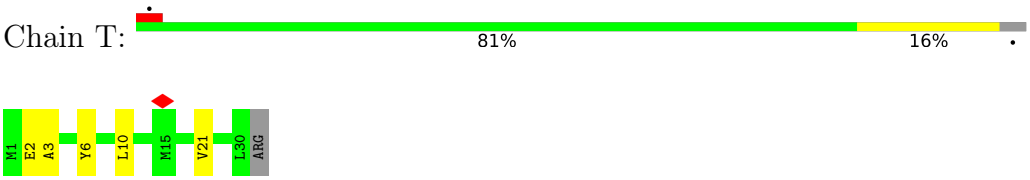




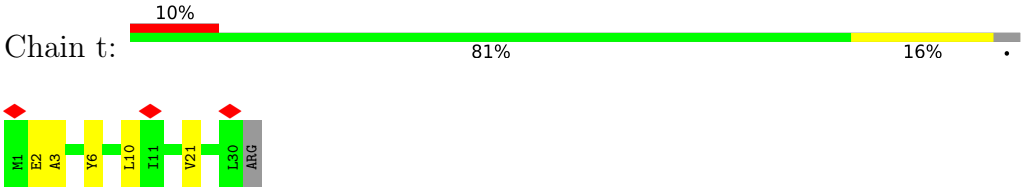
• Molecule 13: Extrinsic protein in photosystem II



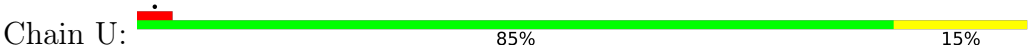
• Molecule 14: Photosystem II reaction center protein T

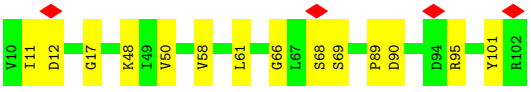


• Molecule 14: Photosystem II reaction center protein T

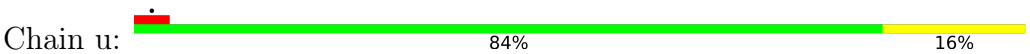


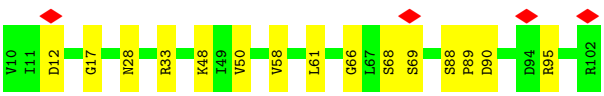
• Molecule 15: Extrinsic protein in photosystem II





• Molecule 15: Extrinsic protein in photosystem II



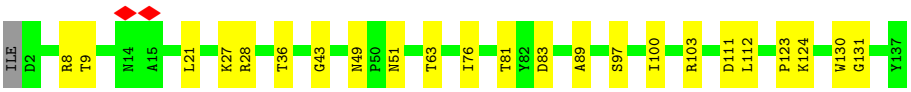


• Molecule 16: Cytochrome c-550

Chain V:

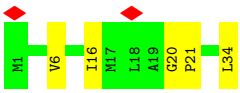
• Molecule 16: Cytochrome c-550

Chain v:



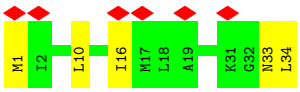
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



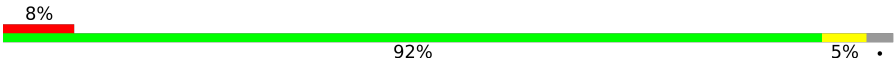
• Molecule 17: Photosystem II reaction center protein Ycf12

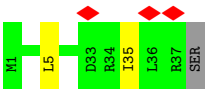
Chain y:



• Molecule 18: Photosystem II reaction center X protein

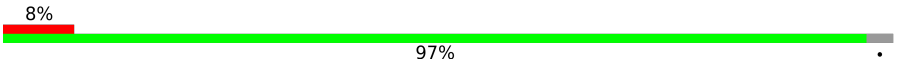
Chain X:

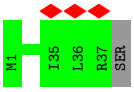




• Molecule 18: Photosystem II reaction center X protein

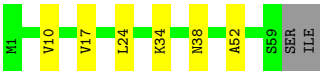
Chain x:





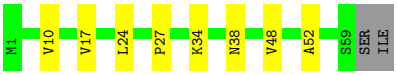
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



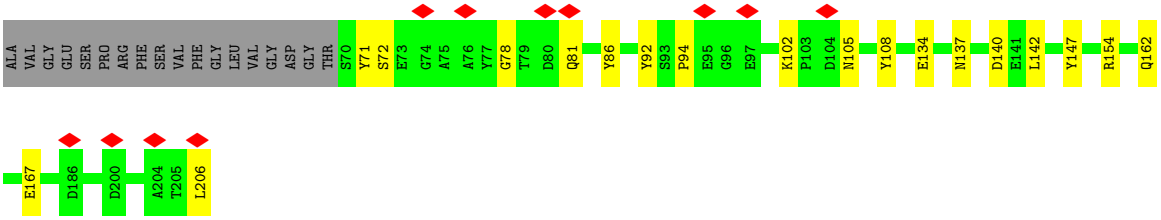
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



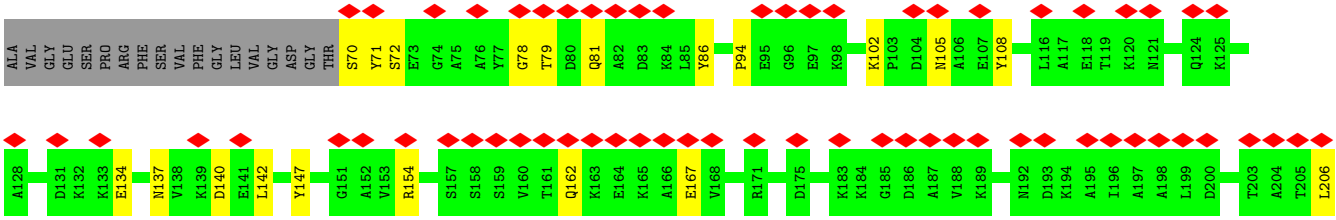
• Molecule 20: Extrinsic protein in photosystem II

Chain Q:



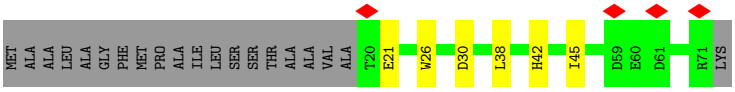
• Molecule 20: Extrinsic protein in photosystem II

Chain q:



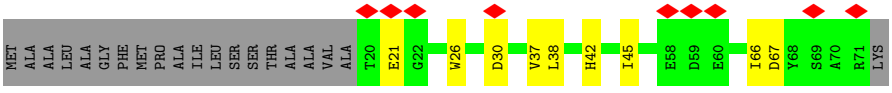
• Molecule 21: Photosystem II reaction center protein W

Chain W:



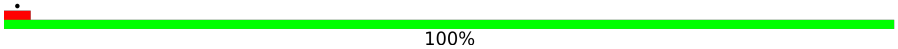
• Molecule 21: Photosystem II reaction center protein W

Chain w:



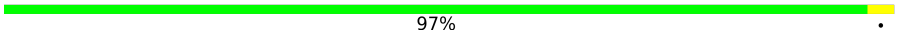
• Molecule 22: Unknown protein 0

Chain 0:



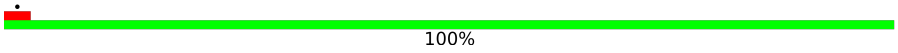
• Molecule 22: Unknown protein 0

Chain 5:



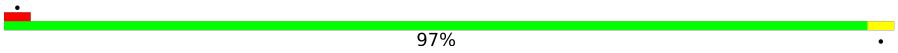
• Molecule 23: Unknown protein 1

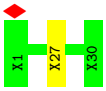
Chain 1:



• Molecule 23: Unknown protein 1

Chain 6:





• Molecule 24: Unknown protein 2

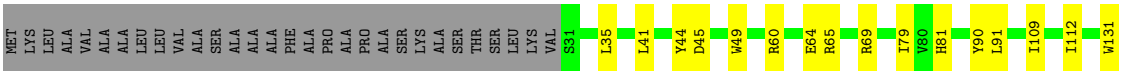
Chain 2:

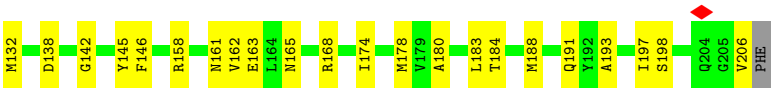
• Molecule 24: Unknown protein 2

Chain 7:

• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

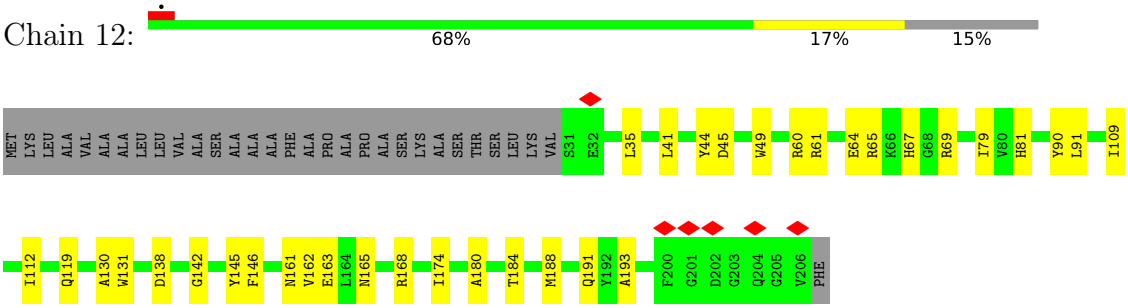
Chain 11:





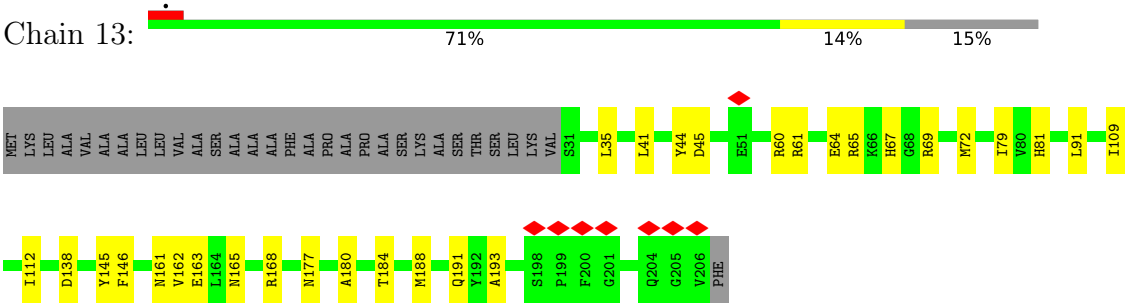
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:



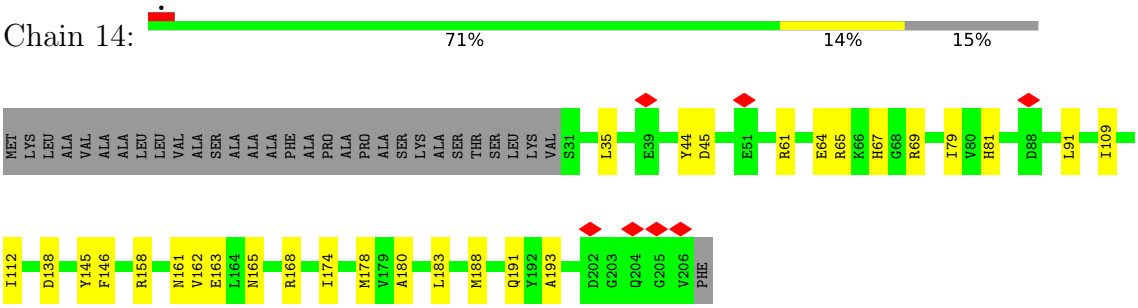
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13:



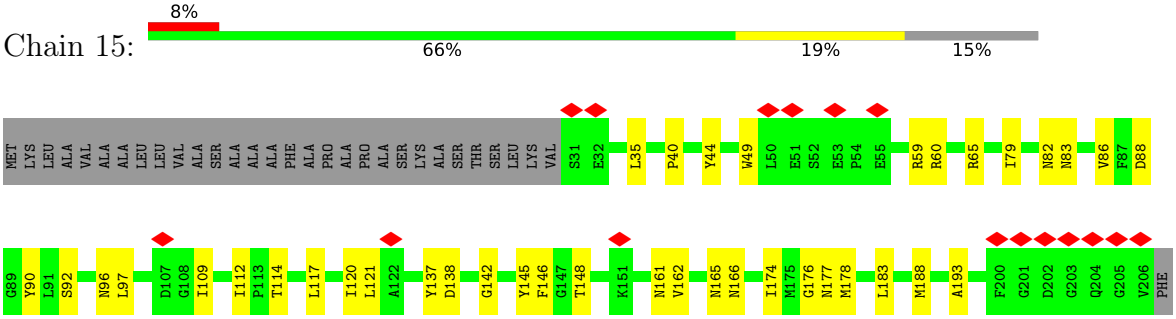
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14:



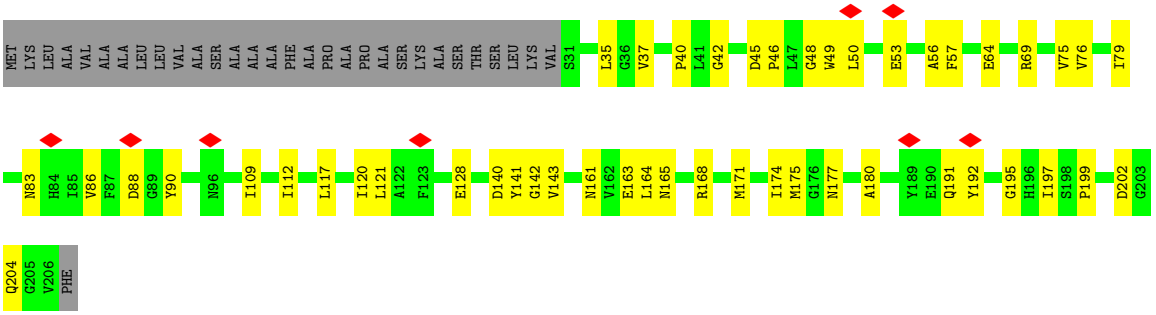
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 15:



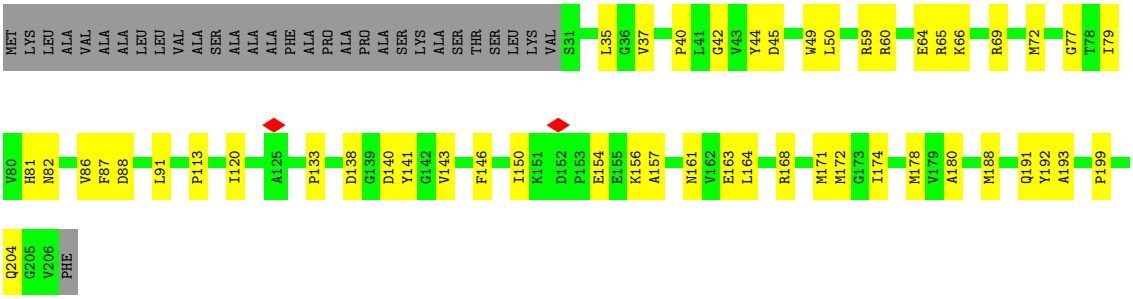
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 16:



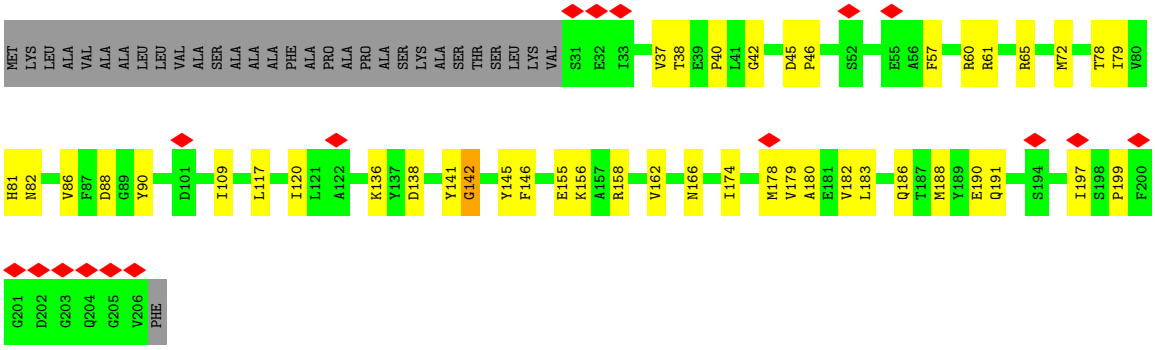
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 17:



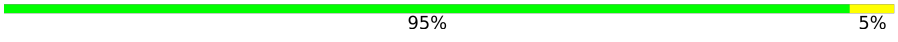
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

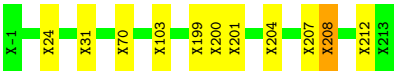
Chain 18:



• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1

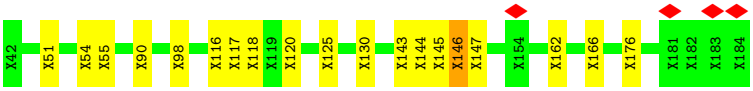
Chain 19:





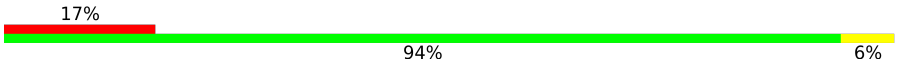
• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

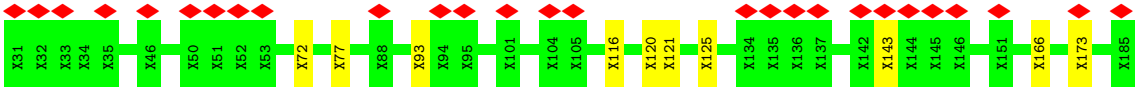
Chain 20:



• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

Chain 21:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	147981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2701	0.61	0/3682
1	a	0.53	0/2701	0.61	0/3682
2	B	0.51	0/3942	0.60	1/5362 (0.0%)
2	b	0.52	0/3942	0.60	1/5362 (0.0%)
3	C	0.52	0/3620	0.63	2/4933 (0.0%)
3	c	0.52	0/3620	0.63	2/4933 (0.0%)
4	D	0.52	0/2789	0.61	0/3803
4	d	0.52	0/2789	0.61	0/3803
5	E	0.36	0/634	0.55	0/864
5	e	0.36	0/634	0.55	0/864
6	F	0.45	0/235	0.80	0/316
6	f	0.45	0/235	0.80	0/316
7	H	0.44	0/523	0.60	0/714
7	h	0.43	0/523	0.60	0/714
8	I	0.55	0/294	0.78	0/397
8	i	0.55	0/294	0.77	0/397
9	J	0.35	0/260	0.52	0/351
9	j	0.35	0/260	0.52	0/351
10	K	0.49	0/313	1.00	2/429 (0.5%)
10	k	0.49	0/313	1.00	2/429 (0.5%)
11	L	0.52	0/319	0.53	0/433
11	l	0.52	0/319	0.53	0/433
12	M	0.46	0/321	0.67	0/433
12	m	0.46	0/321	0.67	0/433
13	O	0.37	0/1875	0.61	2/2528 (0.1%)
13	o	0.37	0/1875	0.61	2/2528 (0.1%)
14	T	0.38	0/256	0.54	0/346
14	t	0.38	0/256	0.54	0/346
15	U	0.32	0/728	0.62	0/989
15	u	0.32	0/728	0.62	0/989
16	V	0.39	0/1056	0.57	0/1435
16	v	0.39	0/1056	0.57	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.29	0/252	0.54	0/341
17	y	0.29	0/252	0.54	0/341
18	X	0.29	0/263	0.52	0/355
18	x	0.29	0/263	0.51	0/355
19	Z	0.34	0/456	0.55	0/624
19	z	0.35	0/456	0.55	0/624
20	Q	0.30	0/1099	0.56	0/1482
20	q	0.30	0/1099	0.56	0/1482
21	W	0.49	0/434	0.66	0/590
21	w	0.49	0/434	0.66	0/590
25	11	0.36	0/1373	0.58	0/1861
25	12	0.36	0/1373	0.58	0/1861
25	13	0.36	0/1373	0.58	0/1861
25	14	0.36	0/1373	0.58	0/1861
25	15	0.24	0/1373	0.50	0/1861
25	16	0.36	0/1373	0.66	0/1861
25	17	0.33	0/1373	0.59	0/1861
25	18	0.26	0/1373	0.53	0/1861
All	All	0.45	0/55724	0.61	14/75702 (0.0%)

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
1	A	0	1
1	a	0	1
16	V	0	1
16	v	0	1
25	18	0	1
26	19	0	4
27	20	0	3
All	All	0	12

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	25	ILE	CA-C-N	8.78	125.77	120.24
10	k	25	ILE	C-N-CA	8.78	125.77	120.24
10	K	25	ILE	CA-C-N	8.77	125.76	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	25	ILE	C-N-CA	8.77	125.76	120.24
3	C	252	THR	CA-C-N	6.62	137.17	122.67
3	C	252	THR	C-N-CA	6.62	137.17	122.67
3	c	252	THR	CA-C-N	6.58	137.08	122.67
3	c	252	THR	C-N-CA	6.58	137.08	122.67
13	o	45	ILE	CA-C-N	-5.78	114.82	122.56
13	o	45	ILE	C-N-CA	-5.78	114.82	122.56
13	O	45	ILE	CA-C-N	-5.74	114.87	122.56
13	O	45	ILE	C-N-CA	-5.74	114.87	122.56
2	B	288	VAL	N-CA-C	-5.07	107.89	112.96
2	b	288	VAL	N-CA-C	-5.02	107.94	112.96

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	18	142	GLY	Peptide
26	19	200	UNK	Peptide
26	19	207	UNK	Peptide
26	19	208	UNK	Peptide
26	19	24	UNK	Peptide
27	20	146	UNK	Peptide
27	20	147	UNK	Peptide
27	20	55	UNK	Peptide
1	A	140	ARG	Peptide
16	V	63	THR	Peptide
1	a	140	ARG	Peptide
16	v	63	THR	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	2618	0	2520	45	0
1	a	2618	0	2520	37	0
2	B	3812	0	3690	55	0
2	b	3812	0	3690	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3504	0	3409	61	0
3	c	3504	0	3410	59	0
4	D	2697	0	2596	41	0
4	d	2697	0	2596	40	0
5	E	616	0	602	3	0
5	e	616	0	602	3	0
6	F	228	0	234	11	0
6	f	228	0	234	9	0
7	H	513	0	541	7	0
7	h	513	0	541	6	0
8	I	287	0	306	8	0
8	i	287	0	306	6	0
9	J	254	0	266	6	0
9	j	254	0	266	3	0
10	K	302	0	316	4	0
10	k	302	0	316	4	0
11	L	310	0	313	8	0
11	l	310	0	313	8	0
12	M	316	0	319	7	0
12	m	316	0	319	4	0
13	O	1845	0	1841	38	0
13	o	1845	0	1841	37	0
14	T	250	0	268	4	0
14	t	250	0	268	4	0
15	U	713	0	715	14	0
15	u	713	0	715	11	0
16	V	1037	0	1033	16	0
16	v	1037	0	1033	13	0
17	Y	250	0	287	8	0
17	y	250	0	287	6	0
18	X	263	0	301	3	0
18	x	263	0	301	0	0
19	Z	447	0	489	6	0
19	z	447	0	490	8	0
20	Q	1079	0	1068	15	0
20	q	1079	0	1068	16	0
21	W	422	0	377	5	0
21	w	422	0	377	9	0
22	0	155	0	34	0	0
22	5	155	0	34	1	0
23	1	150	0	34	0	0
23	6	150	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	2	50	0	12	4	0
24	7	50	0	12	2	0
25	11	1343	0	1306	43	0
25	12	1343	0	1305	39	0
25	13	1343	0	1306	37	0
25	14	1343	0	1306	27	0
25	15	1343	0	1306	41	0
25	16	1343	0	1306	45	0
25	17	1343	0	1306	53	0
25	18	1343	0	1305	57	0
26	19	1075	0	224	21	0
27	20	715	0	148	16	0
28	21	775	0	157	10	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	11	530	0	486	24	0
30	12	595	0	555	38	0
30	13	465	0	414	21	0
30	14	530	0	486	24	0
30	15	465	0	414	25	0
30	16	465	0	412	32	0
30	17	485	0	451	39	0
30	18	595	0	558	50	0
30	19	465	0	413	9	0
30	20	420	0	378	15	0
30	21	485	0	452	31	0
30	A	130	0	144	13	0
30	B	1040	0	1152	41	0
30	C	975	0	1080	51	0
30	D	260	0	288	12	0
30	M	65	0	67	1	0
30	W	130	0	144	9	0
30	Z	65	0	68	9	0
30	a	130	0	144	7	0
30	b	1040	0	1152	45	0
30	c	845	0	936	36	0
30	d	260	0	288	10	0
30	m	65	0	68	2	0
30	w	130	0	144	5	0
30	z	65	0	72	4	0
31	A	64	0	74	1	0
31	D	64	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	128	0	148	2	0
32	A	80	0	112	3	0
32	B	160	0	224	10	0
32	C	80	0	112	5	0
32	F	40	0	56	2	0
32	H	40	0	56	5	0
32	Y	40	0	56	4	0
32	Z	40	0	56	1	0
32	a	80	0	112	2	0
32	b	120	0	168	7	0
32	c	160	0	224	8	0
32	f	40	0	56	1	0
32	h	40	0	56	3	0
32	m	40	0	56	3	0
33	A	54	0	77	0	0
33	B	37	0	37	0	0
33	L	54	0	77	3	0
33	a	54	0	78	0	0
33	b	37	0	37	2	0
33	l	54	0	77	3	0
34	A	4	0	0	1	0
34	a	4	0	0	2	0
35	A	46	0	65	4	0
35	B	49	0	74	1	0
35	L	98	0	148	6	0
35	a	46	0	65	6	0
35	b	49	0	74	2	0
35	d	49	0	74	3	0
35	l	49	0	74	3	0
36	1	39	0	48	0	0
36	12	39	0	46	8	0
36	B	102	0	143	5	0
36	D	51	0	72	2	0
36	M	40	0	50	5	0
36	Q	51	0	72	2	0
36	W	51	0	72	8	0
36	b	102	0	143	5	0
36	c	51	0	72	1	0
36	d	51	0	72	1	0
36	m	40	0	50	2	0
36	w	51	0	72	6	0
37	12	32	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	B	32	0	37	0	0
38	C	10	0	0	0	0
38	c	10	0	0	1	0
39	C	124	0	162	0	0
39	H	62	0	82	5	0
39	J	62	0	82	1	0
39	c	124	0	162	0	0
39	h	62	0	82	3	0
39	j	62	0	82	1	0
40	D	110	0	157	7	0
40	d	110	0	157	8	0
41	F	43	0	30	3	0
41	V	43	0	30	2	0
41	f	43	0	30	4	0
41	v	43	0	30	2	0
42	11	288	0	0	31	0
42	12	288	0	0	26	0
42	13	288	0	0	36	0
42	14	288	0	0	18	0
42	15	336	0	0	40	0
42	16	192	0	0	21	0
42	17	336	0	0	61	0
42	18	192	0	0	33	0
42	19	144	0	0	22	0
42	20	240	0	0	42	0
42	21	240	0	0	44	0
All	All	74619	0	69551	1379	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 (1379) 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)
36:12:301:LMG:C16	30:12:308:CLA:CED	1.75	1.65
30:21:303:CLA:H11	42:21:314:A86:C4	1.35	1.55
30:18:303:CLA:H61	42:18:314:A86:C29	1.28	1.55
30:16:308:CLA:CAB	42:17:302:A86:C3	1.86	1.53
30:21:309:CLA:HAB	42:21:312:A86:C7	1.39	1.53
30:16:308:CLA:HAB	42:17:302:A86:C3	0.97	1.45
25:13:188:MET:HE3	42:13:315:A86:O	1.26	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:15:146:PHE:HB3	42:15:316:A86:O5	1.20	1.34
30:16:308:CLA:HAB	42:17:302:A86:C2	1.56	1.33
30:18:303:CLA:H121	42:18:314:A86:C28	1.63	1.29
30:17:303:CLA:H122	42:17:312:A86:C28	1.65	1.26
25:18:146:PHE:HB3	42:18:302:A86:O5	1.32	1.25
25:11:146:PHE:HB3	42:11:316:A86:O5	1.36	1.21
30:16:308:CLA:CAB	42:17:302:A86:C2	2.13	1.21
28:21:93:UNK:CB	42:21:314:A86:C40	2.20	1.20
30:C:514:CLA:CED	30:Z:102:CLA:H152	1.71	1.20
25:17:193:ALA:HA	42:17:316:A86:C39	1.72	1.20
30:18:303:CLA:C6	42:18:314:A86:C29	2.20	1.20
25:18:146:PHE:O	42:18:302:A86:O5	1.59	1.19
30:C:514:CLA:HED2	30:Z:102:CLA:H152	1.26	1.18
30:18:303:CLA:C12	42:18:314:A86:C28	2.23	1.16
25:12:146:PHE:HB3	42:12:304:A86:O5	1.45	1.15
13:O:13:GLN:NE2	26:19:204:UNK:O	1.80	1.14
30:17:305:CLA:H93	42:17:315:A86:C9	1.77	1.14
25:13:146:PHE:O	42:13:301:A86:O5	1.63	1.14
30:21:303:CLA:C1	42:21:314:A86:C4	2.25	1.14
25:13:146:PHE:HB3	42:13:301:A86:O5	1.44	1.12
25:11:146:PHE:O	42:11:316:A86:O5	1.62	1.12
30:13:302:CLA:H72	42:13:312:A86:C28	1.80	1.11
42:15:316:A86:O	25:18:188:MET:HE3	1.50	1.09
25:13:188:MET:CE	42:13:315:A86:O	2.02	1.08
30:20:203:CLA:HMA3	42:20:212:A86:C29	1.83	1.07
25:15:146:PHE:CB	42:15:316:A86:O5	2.02	1.06
25:13:109:ILE:HG13	42:13:312:A86:O2	1.51	1.06
30:21:309:CLA:CAB	42:21:312:A86:C7	2.34	1.06
30:C:514:CLA:HED2	30:Z:102:CLA:C15	1.85	1.05
13:O:22:ARG:NH2	26:19:212:UNK:O	1.90	1.04
3:C:205:ILE:HD11	26:19:199:UNK:C	1.87	1.04
30:21:302:CLA:HMB1	42:21:311:A86:C28	1.87	1.04
25:11:146:PHE:CB	42:11:316:A86:O5	2.05	1.03
25:18:179:VAL:HG21	30:18:312:CLA:HBC3	1.39	1.03
25:12:188:MET:HE3	42:13:301:A86:O	1.56	1.03
25:15:188:MET:HE3	42:15:315:A86:O	1.57	1.03
25:18:146:PHE:CB	42:18:302:A86:O5	2.05	1.02
30:21:303:CLA:H93	42:21:314:A86:C9	1.89	1.02
25:12:193:ALA:HA	42:12:319:A86:C39	1.90	1.01
25:15:60:ARG:NH2	42:15:313:A86:O3	1.92	1.01
30:18:303:CLA:H72	42:18:314:A86:C28	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:13:302:CLA:H61	42:13:312:A86:C29	1.90	1.00
25:17:66:LYS:HE3	42:17:315:A86:O2	1.61	1.00
25:13:79:ILE:HG23	42:13:315:A86:C12	1.92	1.00
25:11:188:MET:HE3	42:12:304:A86:O	1.62	0.98
25:16:121:LEU:HD11	42:20:201:A86:C21	1.94	0.98
30:21:303:CLA:C9	42:21:314:A86:C8	2.41	0.98
28:21:143:UNK:CB	42:21:310:A86:C39	2.42	0.97
25:11:146:PHE:HB3	42:11:316:A86:C38	1.96	0.95
25:18:179:VAL:HG21	30:18:312:CLA:CBC	1.97	0.95
3:C:205:ILE:HD11	26:19:199:UNK:CA	1.95	0.95
25:13:146:PHE:CB	42:13:301:A86:O5	2.16	0.94
30:21:303:CLA:H12	42:21:314:A86:C7	1.96	0.94
25:18:146:PHE:HB3	42:18:302:A86:C38	1.97	0.94
30:16:308:CLA:C3B	42:17:302:A86:C2	2.46	0.94
25:16:40:PRO:HG2	42:16:312:A86:O2	1.68	0.93
30:11:301:CLA:H122	42:11:311:A86:C28	1.99	0.93
25:15:193:ALA:HA	42:16:313:A86:C39	1.98	0.93
3:C:205:ILE:HD11	26:19:199:UNK:HA	1.49	0.92
42:11:316:A86:O	25:14:188:MET:HE3	1.70	0.91
30:12:305:CLA:H122	42:12:316:A86:C28	2.01	0.91
25:15:146:PHE:O	42:15:316:A86:O5	1.89	0.91
25:18:199:PRO:HB3	30:18:312:CLA:HBD	1.51	0.91
25:17:192:TYR:O	42:17:316:A86:C39	2.19	0.91
42:15:316:A86:C2	30:18:311:CLA:HAB	2.00	0.91
25:11:193:ALA:HA	42:11:314:A86:C39	2.00	0.90
30:17:305:CLA:H12	42:17:315:A86:C4	2.02	0.89
42:13:315:A86:O5	25:14:146:PHE:HB3	1.72	0.88
30:12:305:CLA:H72	42:12:316:A86:C28	2.03	0.88
25:18:199:PRO:HD3	30:18:312:CLA:HBA1	1.54	0.86
30:20:202:CLA:H41	42:20:211:A86:C29	2.06	0.86
25:15:146:PHE:HB3	42:15:316:A86:C38	2.06	0.85
25:18:199:PRO:HB3	30:18:312:CLA:CBD	2.06	0.85
30:21:302:CLA:CMB	42:21:311:A86:C28	2.54	0.85
2:b:394:GLN:HE21	15:u:17:GLY:HA2	1.42	0.85
23:6:27:UNK:O	25:11:198:SER:OG	1.93	0.85
30:21:304:CLA:HMB2	42:21:314:A86:C25	2.05	0.84
30:17:305:CLA:C1	42:17:315:A86:C4	2.56	0.84
30:16:302:CLA:H43	42:16:311:A86:C29	2.07	0.83
30:15:301:CLA:H41	42:15:311:A86:C29	2.07	0.83
26:19:103:UNK:CB	42:19:311:A86:C39	2.57	0.83
25:15:44:TYR:OH	42:15:311:A86:O5	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:11:301:CLA:C12	42:11:311:A86:C28	2.56	0.83
25:15:90:TYR:O	42:15:314:A86:O3	1.96	0.83
3:C:205:ILE:CD1	26:19:199:UNK:C	2.56	0.83
25:13:146:PHE:HB3	42:13:301:A86:C38	2.08	0.83
30:C:514:CLA:HED2	30:Z:102:CLA:C14	2.09	0.83
3:C:205:ILE:CD1	26:19:199:UNK:HA	2.08	0.82
30:18:303:CLA:H102	42:18:314:A86:C28	2.09	0.82
30:20:203:CLA:CMA	42:20:212:A86:C29	2.57	0.82
30:14:303:CLA:H122	42:14:313:A86:C28	2.09	0.82
25:15:177:ASN:ND2	42:15:310:A86:O1	2.12	0.82
30:12:305:CLA:C12	42:12:316:A86:C28	2.58	0.82
30:13:302:CLA:H41	42:13:312:A86:C29	2.10	0.81
30:15:301:CLA:H61	42:15:311:A86:C29	2.10	0.81
31:d:404:PHO:H3A	30:d:406:CLA:H142	1.61	0.81
25:13:193:ALA:HA	42:14:316:A86:C39	2.10	0.81
30:C:514:CLA:HED1	30:Z:102:CLA:H152	1.63	0.81
30:13:302:CLA:H122	42:13:312:A86:C28	2.10	0.81
25:11:146:PHE:C	42:11:316:A86:O5	2.23	0.81
25:13:146:PHE:C	42:13:301:A86:O5	2.24	0.80
30:17:303:CLA:H41	42:17:312:A86:C29	2.12	0.80
1:a:140:ARG:NH2	35:a:407:LHG:O5	2.14	0.80
4:d:192:LEU:O	11:l:35:TYR:OH	1.99	0.80
25:18:179:VAL:CG2	30:18:312:CLA:HBC3	2.11	0.80
30:12:305:CLA:H61	42:12:316:A86:C29	2.12	0.80
2:b:157:HIS:HE1	30:b:606:CLA:NA	1.79	0.79
30:21:303:CLA:C9	42:21:314:A86:C9	2.60	0.79
30:20:203:CLA:HBB1	42:20:211:A86:C3	2.13	0.79
2:B:157:HIS:HE1	30:B:606:CLA:NA	1.79	0.79
30:17:303:CLA:C4	42:17:312:A86:C29	2.61	0.78
30:14:303:CLA:C12	42:14:313:A86:C28	2.62	0.78
30:18:303:CLA:H122	42:18:314:A86:C28	2.14	0.77
30:17:303:CLA:C12	42:17:312:A86:C28	2.56	0.77
30:11:301:CLA:H72	42:11:311:A86:C28	2.14	0.77
25:17:72:MET:HE2	42:17:311:A86:C2	2.15	0.77
25:12:146:PHE:CB	42:12:304:A86:O5	2.29	0.77
25:17:193:ALA:CA	42:17:316:A86:C39	2.60	0.76
2:B:320:ALA:HB1	4:D:291:ASN:HD22	1.49	0.76
30:17:305:CLA:H93	42:17:315:A86:C10	2.14	0.76
25:18:199:PRO:CB	30:18:312:CLA:HBD	2.16	0.76
30:14:303:CLA:H72	42:14:313:A86:C28	2.16	0.75
30:b:622:CLA:HAC1	30:12:310:CLA:HBB1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:12:301:LMG:C15	30:12:308:CLA:CED	2.64	0.75
30:13:306:CLA:HBA1	42:13:314:A86:C10	2.15	0.75
30:20:202:CLA:H72	42:20:211:A86:C28	2.16	0.75
30:21:303:CLA:H92	42:21:314:A86:C8	2.15	0.75
30:a:403:CLA:H2	36:w:101:LMG:H132	1.69	0.75
25:18:146:PHE:C	42:18:302:A86:O5	2.29	0.75
30:18:303:CLA:C10	42:18:314:A86:C28	2.65	0.75
36:12:301:LMG:C16	30:12:308:CLA:HED1	2.10	0.75
25:12:188:MET:CE	42:13:301:A86:O	2.35	0.74
25:16:90:TYR:O	42:16:313:A86:O3	2.03	0.74
27:20:118:UNK:HA	42:20:201:A86:C22	2.18	0.74
25:14:193:ALA:HA	42:14:301:A86:C39	2.18	0.73
30:13:302:CLA:C12	42:13:312:A86:C28	2.66	0.73
42:11:316:A86:C12	25:14:79:ILE:HG23	2.19	0.73
5:e:24:HIS:CD2	41:f:102:HEM:NC	2.57	0.72
42:15:316:A86:C12	25:18:79:ILE:HG23	2.18	0.72
25:18:199:PRO:HD3	30:18:312:CLA:CBA	2.19	0.72
30:19:303:CLA:CHB	42:19:311:A86:C40	2.67	0.71
25:12:109:ILE:HG13	42:12:316:A86:O2	1.90	0.71
4:d:309:GLU:OE2	13:o:231:LYS:NZ	2.23	0.71
34:a:406:BCT:O3	4:d:267:HIS:CE1	2.44	0.71
30:20:203:CLA:O1A	42:20:212:A86:C35	2.38	0.71
19:Z:52:ALA:HB2	32:Z:101:BCR:HC7	1.72	0.70
30:21:303:CLA:H93	42:21:314:A86:C8	2.17	0.70
30:18:303:CLA:C7	42:18:314:A86:C28	2.68	0.70
30:13:306:CLA:HBA1	42:13:314:A86:C9	2.21	0.70
25:17:188:MET:SD	42:17:311:A86:C22	2.80	0.70
4:D:196:HIS:HE1	30:D:405:CLA:NC	1.89	0.70
1:a:140:ARG:HH22	35:a:407:LHG:HC41	1.57	0.70
30:14:307:CLA:HBA1	42:14:315:A86:C9	2.22	0.70
3:C:462:GLU:OE2	4:D:247:THR:OG1	2.10	0.69
1:A:307:VAL:HG21	6:F:43:ARG:HH21	1.56	0.69
25:14:109:ILE:HG13	42:14:313:A86:O2	1.91	0.69
42:16:312:A86:O	30:17:301:CLA:HAC2	1.93	0.69
30:A:404:CLA:H2	36:W:101:LMG:H132	1.75	0.69
30:11:301:CLA:H61	42:11:311:A86:C29	2.23	0.69
4:d:196:HIS:HE1	30:d:406:CLA:NC	1.89	0.69
25:15:146:PHE:C	42:15:316:A86:O5	2.36	0.68
25:17:66:LYS:CE	42:17:315:A86:O2	2.40	0.68
30:C:514:CLA:CED	30:Z:102:CLA:C14	2.71	0.68
42:17:316:A86:O3	25:18:90:TYR:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:12:119:GLN:NE2	36:12:301:LMG:HC8	2.08	0.68
42:15:316:A86:C1	30:18:311:CLA:HAB	2.23	0.68
31:D:403:PHO:H3A	30:D:405:CLA:H142	1.74	0.68
25:12:193:ALA:CA	42:12:319:A86:C39	2.70	0.68
30:14:303:CLA:H61	42:14:313:A86:C29	2.23	0.68
3:C:274:LEU:HD21	30:C:509:CLA:HAB	1.75	0.67
30:17:303:CLA:HMC2	42:17:312:A86:C25	2.24	0.67
3:c:161:ILE:HD13	30:c:513:CLA:HBB1	1.76	0.67
13:O:193:PHE:CD2	15:U:89:PRO:HB2	2.30	0.67
36:12:301:LMG:C16	30:12:308:CLA:O2D	2.42	0.67
30:16:308:CLA:CBB	42:17:302:A86:C3	2.70	0.67
25:16:192:TYR:HB3	42:17:315:A86:C33	2.23	0.67
25:16:121:LEU:CD1	42:20:201:A86:C21	2.73	0.67
25:16:35:LEU:O	25:16:161:ASN:ND2	2.27	0.67
3:c:274:LEU:HD21	30:c:509:CLA:HAB	1.75	0.66
34:A:407:BCT:O3	4:D:267:HIS:CE1	2.44	0.66
3:C:161:ILE:HD13	30:C:513:CLA:HBB1	1.76	0.66
1:A:305:SER:HA	9:J:38:SER:HB3	1.78	0.66
3:C:130:HIS:HE1	30:C:514:CLA:NA	1.93	0.66
3:c:130:HIS:HE1	30:c:514:CLA:NA	1.93	0.66
25:11:44:TYR:OH	42:11:311:A86:O5	2.12	0.66
25:11:188:MET:CE	42:12:304:A86:O	2.43	0.66
42:15:316:A86:O	25:18:188:MET:CE	2.36	0.66
30:17:305:CLA:H101	42:17:315:A86:C10	2.26	0.66
30:16:302:CLA:C4	42:16:311:A86:C29	2.73	0.66
25:17:60:ARG:NH2	42:17:314:A86:O3	2.29	0.66
30:C:507:CLA:H172	30:W:102:CLA:H72	1.77	0.66
13:O:109:GLN:HE21	13:O:113:GLY:HA2	1.61	0.66
25:17:146:PHE:HB3	42:17:302:A86:O5	1.96	0.66
3:c:209:GLY:HA2	21:w:26:TRP:HE1	1.62	0.65
25:11:109:ILE:HG13	42:11:311:A86:O2	1.97	0.65
25:18:199:PRO:HB3	30:18:312:CLA:CGD	2.26	0.65
30:21:301:CLA:H41	42:21:311:A86:C29	2.26	0.65
25:17:188:MET:HE3	42:18:302:A86:O	1.96	0.65
4:d:185:GLN:HB2	30:d:406:CLA:HBC1	1.79	0.65
25:12:79:ILE:HG23	42:13:301:A86:C12	2.27	0.65
26:19:103:UNK:HA	42:19:311:A86:C39	2.27	0.64
1:A:309:SER:HA	6:F:43:ARG:HB3	1.78	0.64
25:16:49:TRP:HE1	30:16:302:CLA:H2	1.62	0.64
25:16:79:ILE:HD13	42:17:302:A86:C9	2.28	0.64
25:16:53:GLU:HB3	25:16:56:ALA:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:512:CLA:H151	19:z:17:VAL:HG13	1.80	0.64
8:I:5:LYS:NZ	21:W:30:ASP:OD2	2.32	0.63
3:c:332:PRO:HG2	4:d:349:ASN:HD21	1.62	0.63
25:17:163:GLU:HA	30:17:308:CLA:HBB1	1.80	0.63
2:B:142:HIS:HE1	30:B:614:CLA:ND	1.96	0.63
3:c:404:SER:O	3:c:416:ASN:ND2	2.31	0.63
30:c:514:CLA:H193	30:z:101:CLA:H201	1.78	0.63
13:o:109:GLN:HE21	13:o:113:GLY:HA2	1.61	0.63
30:14:303:CLA:H121	42:14:313:A86:C28	2.28	0.63
1:a:85:SER:HA	1:a:109:GLY:HA3	1.81	0.63
25:18:86:VAL:HG12	25:18:88:ASP:H	1.63	0.63
30:21:301:CLA:C4	42:21:311:A86:C29	2.77	0.63
3:c:377:LYS:NZ	20:q:140:ASP:OD2	2.32	0.63
1:a:305:SER:HA	9:j:38:SER:HB3	1.80	0.63
33:L:103:SQD:H102	30:M:101:CLA:H43	1.80	0.63
25:11:79:ILE:HG23	42:12:304:A86:C12	2.29	0.63
25:13:177:ASN:OD1	42:13:311:A86:O1	2.15	0.63
26:19:31:UNK:N	30:19:301:CLA:OBD	2.32	0.63
3:C:404:SER:O	3:C:416:ASN:ND2	2.31	0.62
13:o:7:ASN:HB3	20:q:134:GLU:HG2	1.81	0.62
25:11:90:TYR:O	42:14:301:A86:O3	2.17	0.62
30:11:301:CLA:H121	42:11:311:A86:C28	2.27	0.62
25:15:86:VAL:HG12	25:15:88:ASP:H	1.64	0.62
1:a:233:THR:HG21	4:d:138:ARG:HH12	1.64	0.62
30:d:402:CLA:H122	40:d:405:PL9:H23	1.82	0.62
1:A:140:ARG:NH2	35:A:408:LHG:O5	2.31	0.62
4:D:185:GLN:HB2	30:D:405:CLA:HBC1	1.79	0.62
2:b:142:HIS:HE1	30:b:614:CLA:ND	1.96	0.62
25:12:146:PHE:HB3	42:12:304:A86:C38	2.25	0.62
25:16:199:PRO:O	25:16:204:GLN:NE2	2.32	0.62
27:20:51:UNK:CB	42:20:212:A86:C39	2.78	0.62
30:15:302:CLA:HMA3	42:15:313:A86:C27	2.29	0.62
1:A:85:SER:HA	1:A:109:GLY:HA3	1.81	0.62
4:D:179:ARG:NH1	4:D:332:ASP:OD1	2.32	0.62
4:d:179:ARG:NH1	4:d:332:ASP:OD1	2.32	0.62
30:D:402:CLA:H122	40:D:404:PL9:H23	1.82	0.62
30:B:601:CLA:H2	32:B:624:BCR:H323	1.81	0.61
30:17:309:CLA:HMD2	30:18:301:CLA:H2	1.82	0.61
30:14:307:CLA:HBA1	42:14:315:A86:C10	2.30	0.61
25:17:168:ARG:HB3	30:17:303:CLA:HBC3	1.82	0.61
30:b:604:CLA:H93	30:b:605:CLA:HAB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:18:197:ILE:O	30:18:312:CLA:HBA1	2.00	0.61
30:C:507:CLA:H161	30:W:102:CLA:H102	1.83	0.61
25:17:64:GLU:OE2	25:17:168:ARG:NE	2.32	0.61
30:12:305:CLA:H41	42:12:316:A86:C29	2.30	0.61
30:16:309:CLA:HMD3	42:16:312:A86:C29	2.30	0.61
2:b:311:PHE:O	2:b:317:ASN:ND2	2.34	0.61
2:B:311:PHE:O	2:B:317:ASN:ND2	2.34	0.61
32:b:623:BCR:H312	30:12:309:CLA:CAD	2.31	0.61
3:c:106:THR:HA	3:c:109:TYR:HD2	1.65	0.61
30:c:510:CLA:H91	30:c:513:CLA:HBD	1.82	0.61
30:12:309:CLA:HBA1	42:12:318:A86:C9	2.31	0.61
30:B:604:CLA:H93	30:B:605:CLA:HAB	1.82	0.61
30:B:604:CLA:HBB1	30:B:613:CLA:HBC2	1.83	0.60
3:C:377:LYS:NZ	20:Q:140:ASP:OD2	2.33	0.60
27:20:146:UNK:HA	42:20:210:A86:C35	2.31	0.60
6:F:42:GLN:HB2	20:Q:72:SER:HB3	1.84	0.60
2:b:422:ARG:NH2	13:o:167:ASP:OD2	2.34	0.60
13:O:13:GLN:HE21	26:19:204:UNK:C	2.06	0.60
25:13:60:ARG:NH2	42:13:314:A86:O3	2.33	0.60
30:12:305:CLA:H121	42:12:316:A86:C28	2.30	0.60
25:15:145:TYR:HB2	30:15:307:CLA:HAA1	1.84	0.60
30:17:305:CLA:C2	42:17:315:A86:C4	2.79	0.60
30:17:303:CLA:H43	42:17:312:A86:C29	2.32	0.60
30:C:503:CLA:H11	30:C:504:CLA:H171	1.83	0.60
2:b:469:HIS:HE1	30:b:611:CLA:NA	2.00	0.60
25:15:40:PRO:HB3	30:16:301:CLA:HBB1	1.83	0.60
25:17:199:PRO:O	25:17:204:GLN:NE2	2.31	0.60
30:C:510:CLA:H91	30:C:513:CLA:HBD	1.82	0.60
2:b:153:PHE:HB2	30:b:606:CLA:HBB1	1.83	0.60
25:12:44:TYR:OH	42:12:316:A86:O5	2.15	0.60
1:A:27:ARG:NH2	14:T:21:VAL:O	2.34	0.59
4:d:208:LEU:HD13	30:d:401:CLA:H42	1.83	0.59
30:15:301:CLA:C12	42:15:311:A86:C28	2.80	0.59
30:15:301:CLA:HMC2	42:15:311:A86:C25	2.31	0.59
2:B:153:PHE:HB2	30:B:606:CLA:HBB1	1.83	0.59
30:C:514:CLA:HED2	30:Z:102:CLA:C13	2.32	0.59
1:a:142:TRP:HZ2	3:c:445:ARG:HB2	1.67	0.59
30:21:301:CLA:H61	42:21:311:A86:C29	2.32	0.59
3:C:106:THR:HA	3:C:109:TYR:HD2	1.65	0.59
30:11:305:CLA:HBA1	42:11:313:A86:C9	2.32	0.59
26:19:70:UNK:CA	42:19:312:A86:C23	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:GLN:HE22	7:H:66:ILE:HB	1.66	0.59
35:a:407:LHG:H202	30:c:511:CLA:H52	1.85	0.59
2:b:320:ALA:HB1	4:d:291:ASN:HD22	1.65	0.59
30:c:503:CLA:H11	30:c:504:CLA:H171	1.83	0.59
3:C:128:ILE:HG22	19:Z:24:LEU:HD12	1.85	0.59
3:C:431:LEU:HD21	30:C:509:CLA:H191	1.84	0.59
13:O:13:GLN:NE2	26:19:204:UNK:C	2.64	0.59
16:V:27:LYS:HE2	20:Q:71:TYR:HA	1.85	0.59
30:20:202:CLA:H61	42:20:211:A86:C29	2.32	0.59
42:11:316:A86:O	25:14:188:MET:CE	2.48	0.59
25:15:109:ILE:HG13	42:15:311:A86:O2	2.03	0.59
4:D:23:LYS:HZ2	18:X:35:ILE:HD11	1.67	0.59
30:16:309:CLA:HAB	42:16:312:A86:C7	2.33	0.59
1:a:27:ARG:NH2	14:t:21:VAL:O	2.36	0.59
25:17:40:PRO:HG2	42:17:313:A86:O2	2.03	0.59
2:B:469:HIS:HE1	30:B:611:CLA:NA	2.00	0.58
25:18:146:PHE:O	42:18:302:A86:C38	2.45	0.58
30:C:514:CLA:H193	30:C:519:CLA:H201	1.85	0.58
30:b:604:CLA:HBB1	30:b:613:CLA:HBC2	1.83	0.58
25:18:145:TYR:HB2	30:18:309:CLA:HAA1	1.84	0.58
25:14:35:LEU:O	25:14:161:ASN:ND2	2.37	0.58
26:19:103:UNK:CA	42:19:311:A86:C39	2.82	0.58
30:21:304:CLA:CMB	42:21:314:A86:C25	2.79	0.58
25:12:35:LEU:O	25:12:161:ASN:ND2	2.37	0.58
25:17:72:MET:HE1	30:17:308:CLA:HHC	1.86	0.58
27:20:118:UNK:CA	42:20:201:A86:C22	2.81	0.58
2:B:127:ARG:NH2	7:H:18:TYR:O	2.37	0.58
11:L:9:GLN:O	36:M:102:LMG:O3	2.20	0.58
3:c:431:LEU:HD21	30:c:509:CLA:H191	1.84	0.58
42:17:302:A86:O2	42:17:315:A86:C35	2.51	0.58
30:A:404:CLA:H171	30:C:507:CLA:H41	1.85	0.58
25:17:35:LEU:O	25:17:161:ASN:ND2	2.37	0.58
3:C:205:ILE:HG21	26:19:201:UNK:HA	1.83	0.58
25:16:64:GLU:OE2	25:16:168:ARG:NE	2.29	0.58
25:18:174:ILE:HG22	25:18:178:MET:HE2	1.86	0.58
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.86	0.58
30:11:304:CLA:HAA2	30:11:315:CLA:H192	1.86	0.58
30:17:305:CLA:C9	42:17:315:A86:C9	2.70	0.58
30:20:203:CLA:HMA3	42:20:212:A86:C30	2.34	0.58
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.86	0.57
30:A:404:CLA:HBB2	8:I:15:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:503:CLA:HBB2	30:C:511:CLA:H151	1.86	0.57
13:o:172:LEU:HB3	13:o:175:LEU:HD23	1.86	0.57
25:15:183:LEU:HD21	42:15:313:A86:C21	2.34	0.57
30:15:301:CLA:H121	42:15:311:A86:C28	2.34	0.57
32:a:408:BCR:H342	35:d:409:LHG:H362	1.85	0.57
42:11:312:A86:O	30:12:303:CLA:HAC2	2.05	0.57
30:13:304:CLA:HBB1	42:13:312:A86:C21	2.34	0.57
30:15:303:CLA:HBB1	42:15:311:A86:C21	2.35	0.57
25:16:75:VAL:HG11	42:16:310:A86:C8	2.34	0.57
30:18:303:CLA:C7	42:18:314:A86:C29	2.83	0.57
33:L:103:SQD:H101	32:m:103:BCR:H24C	1.87	0.57
13:o:120:PHE:HA	13:o:222:GLN:HE22	1.69	0.57
30:13:302:CLA:C6	42:13:312:A86:C29	2.76	0.57
1:A:140:ARG:HH22	35:A:408:LHG:HC41	1.70	0.57
13:O:172:LEU:HB3	13:O:175:LEU:HD23	1.86	0.57
30:16:302:CLA:HMC1	42:16:311:A86:C24	2.35	0.57
25:18:179:VAL:HG21	30:18:312:CLA:HBC1	1.86	0.57
32:B:616:BCR:H24C	33:l:101:SQD:H101	1.87	0.57
1:a:301:ASN:H	3:c:403:ASN:HD21	1.53	0.57
3:C:77:LYS:HB2	3:C:82:GLN:HE21	1.70	0.57
4:D:334:PRO:HG2	5:E:66:LEU:HD21	1.87	0.57
3:c:366:PRO:HA	20:q:140:ASP:HB2	1.87	0.57
25:16:86:VAL:HG12	25:16:88:ASP:H	1.70	0.57
6:f:40:PHE:O	24:7:13:UNK:HA	2.05	0.56
25:11:146:PHE:CA	42:11:316:A86:O5	2.53	0.56
26:19:70:UNK:CB	42:19:312:A86:C23	2.83	0.56
30:C:506:CLA:H201	36:W:101:LMG:H321	1.87	0.56
30:17:303:CLA:HMC2	42:17:312:A86:C26	2.35	0.56
30:c:503:CLA:HBB2	30:c:511:CLA:H151	1.86	0.56
4:d:194:PRO:HG3	11:l:35:TYR:CE2	2.40	0.56
25:13:35:LEU:O	25:13:161:ASN:ND2	2.37	0.56
26:19:70:UNK:HA	42:19:312:A86:C23	2.35	0.56
25:11:35:LEU:O	25:11:161:ASN:ND2	2.37	0.56
25:12:146:PHE:O	42:12:304:A86:O5	2.24	0.56
25:18:162:VAL:O	25:18:166:ASN:N	2.36	0.56
2:B:214:ILE:HG21	30:B:623:CLA:HAA2	1.87	0.56
3:c:77:LYS:HB2	3:c:82:GLN:HE21	1.70	0.56
13:o:213:GLU:OE1	13:o:243:TYR:OH	2.23	0.56
25:13:79:ILE:CG2	42:13:315:A86:C12	2.76	0.56
42:13:315:A86:O5	25:14:146:PHE:O	2.22	0.56
25:17:37:VAL:HG13	25:17:42:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:7:ASN:HB3	20:Q:134:GLU:HG2	1.88	0.56
13:O:213:GLU:OE1	13:O:243:TYR:OH	2.23	0.56
4:D:53:PHE:HA	4:D:67:LEU:HD13	1.88	0.56
1:a:341:LEU:H	3:c:311:GLN:HE22	1.53	0.56
14:t:3:ALA:HA	14:t:6:TYR:HD2	1.71	0.56
2:b:127:ARG:NH2	7:h:18:TYR:O	2.39	0.56
3:c:74:VAL:O	3:c:82:GLN:NE2	2.32	0.56
25:12:41:LEU:CD1	42:12:317:A86:C22	2.83	0.56
25:17:69:ARG:NE	25:17:163:GLU:OE2	2.34	0.56
4:d:53:PHE:HA	4:d:67:LEU:HD13	1.88	0.56
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.88	0.55
25:15:121:LEU:HB3	30:15:306:CLA:HBB2	1.87	0.55
12:M:32:ARG:HH22	36:M:102:LMG:HO4	1.53	0.55
25:15:146:PHE:CA	42:15:316:A86:O5	2.54	0.55
3:c:333:THR:O	13:o:150:ARG:NH2	2.40	0.55
7:h:4:ARG:HH11	7:h:9:GLU:HG2	1.72	0.55
27:20:176:UNK:CB	42:20:210:A86:C10	2.84	0.55
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.88	0.55
30:C:512:CLA:H151	19:Z:17:VAL:HG13	1.89	0.55
14:T:3:ALA:HA	14:T:6:TYR:HD2	1.71	0.55
2:b:383:PHE:CE1	13:o:165:GLY:HA2	2.41	0.55
25:18:109:ILE:HG13	42:18:314:A86:O2	2.07	0.55
6:f:42:GLN:HB2	20:q:72:SER:HB3	1.88	0.55
25:13:162:VAL:HG11	30:13:309:CLA:HAA2	1.89	0.55
30:15:301:CLA:HMC2	42:15:311:A86:C26	2.36	0.55
25:15:165:ASN:ND2	30:16:301:CLA:O1D	2.39	0.55
25:18:46:PRO:HG2	42:18:314:A86:O5	2.07	0.55
8:i:5:LYS:NZ	21:w:30:ASP:OD2	2.39	0.55
13:o:146:THR:HG1	13:o:196:THR:HG1	1.55	0.55
17:y:1:MET:SD	20:q:79:THR:HA	2.47	0.55
25:14:162:VAL:HG11	30:14:310:CLA:HAA2	1.89	0.55
30:19:303:CLA:HHB	42:19:311:A86:C40	2.36	0.55
32:A:409:BCR:H342	35:L:101:LHG:H362	1.89	0.55
35:b:621:LHG:O4	4:d:140:TYR:OH	2.24	0.55
25:17:192:TYR:C	42:17:316:A86:C39	2.80	0.55
25:18:199:PRO:CD	30:18:312:CLA:CGA	2.85	0.55
13:O:120:PHE:HA	13:O:222:GLN:HE22	1.69	0.55
30:13:302:CLA:H121	42:13:312:A86:C28	2.36	0.55
42:19:311:A86:C21	42:19:311:A86:C13	2.85	0.55
27:20:130:UNK:CB	42:20:201:A86:C28	2.85	0.55
42:21:310:A86:C23	42:21:310:A86:C13	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:188:ASP:OD2	2:b:194:ASN:ND2	2.40	0.55
25:12:162:VAL:HG11	30:12:313:CLA:HAA2	1.88	0.55
25:15:79:ILE:HG23	42:15:315:A86:C12	2.37	0.55
25:16:37:VAL:HG13	25:16:42:GLY:HA2	1.88	0.55
42:21:311:A86:C28	42:21:311:A86:C24	2.85	0.55
42:21:311:A86:C23	42:21:311:A86:C13	2.85	0.55
42:21:314:A86:C21	42:21:314:A86:C13	2.85	0.55
35:B:622:LHG:O4	4:D:140:TYR:OH	2.24	0.54
3:C:451:ALA:O	8:I:33:ASN:ND2	2.40	0.54
25:15:35:LEU:O	25:15:161:ASN:ND2	2.40	0.54
30:19:303:CLA:C2B	42:19:311:A86:C41	2.85	0.54
42:20:210:A86:C37	42:20:210:A86:C40	2.86	0.54
42:20:213:A86:C13	42:20:213:A86:C21	2.85	0.54
17:y:10:LEU:HD11	24:7:19:UNK:CB	2.37	0.54
25:13:41:LEU:CD1	42:13:313:A86:C22	2.86	0.54
25:13:44:TYR:OH	42:13:312:A86:O5	2.19	0.54
42:19:310:A86:C28	42:19:310:A86:C24	2.85	0.54
4:D:23:LYS:NZ	18:X:35:ILE:HD11	2.23	0.54
32:c:515:BCR:HC7	19:z:52:ALA:HB2	1.88	0.54
30:14:303:CLA:H41	42:14:313:A86:C29	2.38	0.54
42:19:310:A86:C39	42:19:310:A86:C33	2.86	0.54
20:q:134:GLU:OE1	20:q:137:ASN:ND2	2.39	0.54
25:15:188:MET:CE	42:15:315:A86:O	2.45	0.54
42:17:302:A86:C8	42:17:302:A86:C12	2.86	0.54
42:20:210:A86:C10	42:20:210:A86:C23	2.86	0.54
42:21:313:A86:C23	42:21:313:A86:C13	2.85	0.54
30:a:403:CLA:HAA2	36:w:101:LMG:H111	1.88	0.54
25:15:65:ARG:NH1	25:15:138:ASP:O	2.41	0.54
25:17:171:MET:HB2	42:17:312:A86:C3	2.37	0.54
42:19:310:A86:C10	42:19:310:A86:C23	2.86	0.54
42:19:310:A86:C23	42:19:310:A86:C13	2.85	0.54
42:19:310:A86:C40	42:19:310:A86:C37	2.86	0.54
42:20:212:A86:C10	42:20:212:A86:C17	2.86	0.54
42:20:212:A86:C8	42:20:212:A86:C12	2.86	0.54
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.40	0.54
36:D:408:LMG:H401	6:F:24:LEU:HG	1.89	0.54
25:15:117:LEU:HD23	25:15:120:ILE:HD12	1.89	0.54
25:16:45:ASP:HB2	25:16:48:GLY:HA2	1.88	0.54
42:17:315:A86:C23	42:17:315:A86:C13	2.85	0.54
2:B:423:LYS:HE3	13:O:176:GLN:O	2.08	0.54
25:12:41:LEU:HD11	42:12:317:A86:C22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:17:315:A86:C12	42:17:315:A86:C8	2.85	0.54
42:20:201:A86:C37	42:20:201:A86:C39	2.86	0.54
42:20:212:A86:C41	42:20:212:A86:C37	2.85	0.54
3:C:74:VAL:O	3:C:82:GLN:NE2	2.32	0.54
30:C:506:CLA:H201	36:W:101:LMG:H291	1.89	0.54
11:l:9:GLN:O	36:m:102:LMG:O3	2.23	0.54
42:20:211:A86:C28	42:20:211:A86:C24	2.85	0.54
42:20:211:A86:C23	42:20:211:A86:C13	2.85	0.54
42:21:312:A86:C24	42:21:312:A86:C28	2.86	0.54
1:A:140:ARG:NH1	4:D:218:GLU:O	2.40	0.54
4:D:171:SER:HB2	4:D:176:ALA:HB1	1.90	0.54
2:B:215:PHE:HB2	32:B:624:BCR:H272	1.89	0.53
7:H:4:ARG:HH11	7:H:9:GLU:HG2	1.72	0.53
30:18:304:CLA:O1A	42:18:315:A86:C37	2.56	0.53
42:19:311:A86:C21	42:19:311:A86:C12	2.85	0.53
42:19:311:A86:C4	42:19:311:A86:C	2.86	0.53
42:20:210:A86:C23	42:20:210:A86:C13	2.85	0.53
33:l:101:SQD:H102	30:m:101:CLA:H43	1.89	0.53
25:11:183:LEU:HD21	42:11:313:A86:C21	2.38	0.53
30:18:304:CLA:O1A	42:18:315:A86:C30	2.56	0.53
30:18:310:CLA:H2	30:18:311:CLA:HMD2	1.89	0.53
42:19:311:A86:C7	42:19:311:A86:C3	2.85	0.53
42:20:201:A86:C37	42:20:201:A86:C41	2.85	0.53
42:21:310:A86:C24	42:21:310:A86:C28	2.86	0.53
3:C:309:GLN:OE1	3:C:353:THR:OG1	2.27	0.53
30:b:607:CLA:H42	36:b:618:LMG:H152	1.90	0.53
25:11:162:VAL:HG11	30:11:308:CLA:HAA2	1.89	0.53
25:14:65:ARG:NH1	25:14:138:ASP:O	2.42	0.53
42:16:310:A86:C23	42:16:310:A86:C13	2.85	0.53
1:a:140:ARG:NH1	4:d:218:GLU:O	2.41	0.53
30:15:301:CLA:H122	42:15:311:A86:C28	2.38	0.53
42:17:311:A86:C17	42:17:311:A86:C12	2.85	0.53
28:21:72:UNK:O	42:21:310:A86:C	2.56	0.53
17:Y:6:VAL:HG11	24:2:19:UNK:CA	2.38	0.53
42:11:314:A86:O3	25:12:90:TYR:O	2.26	0.53
25:13:65:ARG:NH1	25:13:138:ASP:O	2.42	0.53
30:21:304:CLA:HMB2	42:21:314:A86:C2	2.37	0.53
2:B:23:HIS:CD2	30:B:612:CLA:NA	2.77	0.53
13:O:46:GLU:HB3	13:O:78:THR:HG23	1.90	0.53
25:12:65:ARG:NH1	25:12:138:ASP:O	2.42	0.53
28:21:166:UNK:HA	30:21:307:CLA:HMD1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:6:VAL:HG11	24:2:19:UNK:HA	1.91	0.53
2:b:423:LYS:HE2	13:o:178:GLY:O	2.09	0.53
30:b:608:CLA:HBB2	4:d:122:ILE:HG12	1.90	0.53
1:A:137:LEU:HD23	3:C:467:MET:HE1	1.91	0.53
16:V:36:THR:HA	16:V:103:ARG:HD3	1.91	0.53
20:Q:134:GLU:OE1	20:Q:137:ASN:ND2	2.39	0.53
3:c:309:GLN:OE1	3:c:353:THR:OG1	2.26	0.53
32:c:515:BCR:H343	19:z:48:VAL:HG12	1.90	0.53
25:11:197:ILE:HD13	30:12:308:CLA:HMD3	1.91	0.53
25:14:44:TYR:OH	42:14:313:A86:O5	2.25	0.53
25:17:49:TRP:HH2	42:17:314:A86:C39	2.22	0.53
30:16:308:CLA:HBB1	42:16:310:A86:C3	2.39	0.53
25:18:136:LYS:O	25:18:141:TYR:OH	2.23	0.53
1:A:341:LEU:H	3:C:311:GLN:HE22	1.57	0.52
30:B:607:CLA:H42	36:B:619:LMG:H152	1.90	0.52
30:18:303:CLA:H72	42:18:314:A86:C27	2.37	0.52
13:O:207:VAL:HG13	13:O:214:ILE:HG22	1.91	0.52
30:11:301:CLA:H41	42:11:311:A86:C29	2.39	0.52
25:11:65:ARG:NH1	25:11:138:ASP:O	2.42	0.52
25:17:86:VAL:HG12	25:17:88:ASP:H	1.75	0.52
25:17:172:MET:HE2	42:17:312:A86:C	2.40	0.52
30:A:404:CLA:HAA2	36:W:101:LMG:H111	1.91	0.52
25:17:143:VAL:HG21	42:17:311:A86:C39	2.40	0.52
2:B:211:PHE:CZ	30:B:623:CLA:H61	2.43	0.52
3:c:26:ILE:HD13	4:d:232:ARG:NH1	2.24	0.52
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.92	0.52
8:I:13:ILE:HD12	21:W:38:LEU:HD22	1.91	0.52
5:e:58:THR:O	5:e:62:GLN:NE2	2.43	0.52
30:12:309:CLA:HBA1	42:12:318:A86:C10	2.40	0.52
3:C:51:HIS:CD2	30:C:510:CLA:NA	2.77	0.52
36:M:102:LMG:O2	30:m:101:CLA:OBD	2.27	0.52
35:a:407:LHG:H281	35:a:407:LHG:H181	1.91	0.52
25:17:140:ASP:HB2	30:17:308:CLA:H42	1.90	0.52
2:b:334:ASP:HB3	13:o:174:ALA:HB1	1.92	0.52
25:18:199:PRO:HG3	30:18:312:CLA:HBD	1.92	0.52
28:21:116:UNK:O	28:21:120:UNK:N	2.42	0.52
1:A:231:GLU:HA	2:B:2:ALA:O	2.10	0.52
30:12:312:CLA:HAC2	42:12:317:A86:O	2.09	0.52
30:15:302:CLA:HBC1	30:15:306:CLA:HBC2	1.92	0.52
25:17:44:TYR:OH	42:17:312:A86:O5	2.23	0.52
25:18:199:PRO:CG	30:18:312:CLA:HBD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD12	33:b:620:SQD:H2	1.92	0.51
16:V:8:ARG:NH1	16:V:21:LEU:O	2.39	0.51
4:d:171:SER:HB2	4:d:176:ALA:HB1	1.90	0.51
13:o:46:GLU:HB3	13:o:78:THR:HG23	1.91	0.51
25:18:199:PRO:HB3	30:18:312:CLA:O1D	2.09	0.51
5:E:58:THR:O	5:E:62:GLN:NE2	2.43	0.51
2:b:23:HIS:CD2	30:b:612:CLA:NA	2.77	0.51
2:b:55:MET:HE1	2:b:67:THR:HG21	1.92	0.51
2:b:482:ILE:HG21	4:d:137:ILE:HA	1.92	0.51
13:o:207:VAL:HG13	13:o:214:ILE:HG22	1.92	0.51
16:v:27:LYS:HE2	20:q:71:TYR:HA	1.91	0.51
25:16:50:LEU:HD22	30:16:302:CLA:HBD	1.92	0.51
30:C:509:CLA:H192	36:Q:301:LMG:H412	1.92	0.51
3:c:389:ARG:NH2	20:q:147:TYR:OH	2.37	0.51
30:c:509:CLA:H192	36:c:519:LMG:H412	1.92	0.51
15:u:48:LYS:NZ	15:u:66:GLY:O	2.38	0.51
25:11:206:VAL:O	36:12:301:LMG:H151	2.10	0.51
25:13:41:LEU:HD12	42:13:313:A86:C22	2.40	0.51
25:17:87:PHE:HZ	30:17:305:CLA:H42	1.76	0.51
30:21:309:CLA:HMD3	42:21:312:A86:C37	2.40	0.51
3:c:51:HIS:CD2	30:c:510:CLA:NA	2.78	0.51
25:16:180:ALA:O	25:16:191:GLN:NE2	2.42	0.51
35:A:408:LHG:H181	35:A:408:LHG:H281	1.91	0.51
13:O:189:ASN:CB	15:U:11:ILE:HD11	2.41	0.51
1:a:301:ASN:ND2	3:c:411:GLU:O	2.38	0.51
2:b:454:GLY:HA2	36:b:618:LMG:H212	1.92	0.51
4:d:47:TRP:NE1	4:d:172:PHE:O	2.32	0.51
16:v:36:THR:HA	16:v:103:ARG:HD3	1.91	0.51
25:13:146:PHE:CA	42:13:301:A86:O5	2.59	0.51
25:16:109:ILE:HA	25:16:112:ILE:HD12	1.92	0.51
25:16:143:VAL:HA	30:16:307:CLA:HBD	1.92	0.51
2:B:55:MET:HE1	2:B:67:THR:HG21	1.92	0.51
16:V:28:ARG:NH1	16:V:111:ASP:OD1	2.44	0.51
4:d:278:LEU:HD22	31:d:404:PHO:HBC3	1.93	0.51
25:15:142:GLY:HA3	25:18:158:ARG:HH21	1.76	0.51
25:17:65:ARG:NH1	25:17:138:ASP:O	2.43	0.51
9:J:32:TYR:CZ	39:J:101:DGD:HG32	2.46	0.51
30:b:607:CLA:H43	36:b:618:LMG:H311	1.93	0.51
25:16:142:GLY:N	30:16:307:CLA:OBD	2.44	0.51
30:16:309:CLA:CMD	42:16:312:A86:C29	2.89	0.51
30:11:315:CLA:HAC2	42:14:314:A86:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:309:GLU:OE2	13:O:231:LYS:NZ	2.41	0.51
3:c:26:ILE:HG21	4:d:232:ARG:HH12	1.76	0.51
30:c:509:CLA:H193	30:c:511:CLA:H112	1.93	0.51
16:v:28:ARG:NH1	16:v:111:ASP:OD1	2.44	0.51
30:20:203:CLA:HAB	42:20:212:A86:C2	2.39	0.51
1:A:70:SER:O	1:A:75:ASN:ND2	2.43	0.50
3:C:333:THR:O	13:O:150:ARG:NH2	2.44	0.50
42:20:201:A86:C7	42:20:201:A86:C3	2.89	0.50
2:B:211:PHE:HB3	32:B:624:BCR:H381	1.92	0.50
3:C:197:ILE:HG13	3:C:232:ILE:HG13	1.93	0.50
4:D:208:LEU:HD13	30:D:401:CLA:H42	1.93	0.50
16:V:36:THR:HG1	20:Q:92:TYR:HH	1.55	0.50
25:13:81:HIS:HE1	30:13:304:CLA:NB	2.09	0.50
25:14:81:HIS:HE1	30:14:305:CLA:NB	2.08	0.50
25:18:199:PRO:HD2	30:18:312:CLA:O1A	2.11	0.50
42:20:212:A86:C10	42:20:212:A86:C23	2.89	0.50
15:U:12:ASP:OD1	15:U:12:ASP:N	2.42	0.50
1:a:70:SER:O	1:a:75:ASN:ND2	2.43	0.50
16:v:8:ARG:NH1	16:v:21:LEU:O	2.39	0.50
42:15:316:A86:C4	30:18:310:CLA:H162	2.42	0.50
2:B:454:GLY:HA2	36:B:619:LMG:H212	1.92	0.50
30:b:602:CLA:H203	39:h:102:DGD:HA72	1.94	0.50
25:11:158:ARG:NH1	25:12:142:GLY:O	2.44	0.50
25:11:193:ALA:CA	42:11:314:A86:C39	2.82	0.50
3:C:251:PHE:CE1	30:C:520:CLA:C4C	2.94	0.50
12:M:32:ARG:NH2	36:M:102:LMG:O4	2.40	0.50
30:C:509:CLA:H193	30:C:511:CLA:H112	1.93	0.50
35:b:621:LHG:H192	11:l:28:LEU:HD11	1.94	0.50
25:12:119:GLN:HE21	36:12:301:LMG:HC8	1.72	0.50
25:16:69:ARG:NE	25:16:163:GLU:OE2	2.45	0.50
27:20:90:UNK:HA	27:20:98:UNK:HA	1.94	0.50
3:C:406:GLY:H	3:C:415:VAL:HG23	1.77	0.50
2:b:341:LEU:HD12	2:b:429:VAL:HG12	1.94	0.50
30:b:614:CLA:H91	30:b:614:CLA:H171	1.94	0.50
25:11:81:HIS:HE1	30:11:303:CLA:NB	2.08	0.50
25:16:79:ILE:HG12	42:17:302:A86:C10	2.41	0.50
28:21:173:UNK:CB	42:21:310:A86:C10	2.90	0.50
1:A:142:TRP:HZ2	3:C:445:ARG:HB2	1.77	0.50
1:A:214:MET:HE3	1:A:218:LEU:HD11	1.93	0.50
30:b:602:CLA:H71	7:h:46:LEU:HD12	1.94	0.50
25:11:69:ARG:NE	25:11:163:GLU:OE2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:69:ARG:NE	25:13:163:GLU:OE2	2.38	0.50
27:20:143:UNK:CB	42:20:210:A86:C39	2.89	0.50
30:B:604:CLA:H112	30:B:614:CLA:H42	1.94	0.49
1:a:214:MET:HE3	1:a:218:LEU:HD11	1.93	0.49
25:12:60:ARG:NH2	42:12:318:A86:O3	2.45	0.49
30:21:304:CLA:C2B	42:21:314:A86:C25	2.90	0.49
40:D:407:PL9:H401	35:L:101:LHG:H223	1.94	0.49
17:y:33:ASN:ND2	19:z:27:PRO:HG3	2.27	0.49
27:20:117:UNK:C	42:20:201:A86:C22	2.90	0.49
3:c:197:ILE:HG13	3:c:232:ILE:HG13	1.93	0.49
40:d:408:PL9:H401	35:d:409:LHG:H223	1.94	0.49
30:16:303:CLA:HBC1	30:16:306:CLA:HBC2	1.93	0.49
4:D:162:GLY:HA3	4:D:289:ALA:HB1	1.94	0.49
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.93	0.49
25:12:81:HIS:HE1	30:12:307:CLA:NB	2.08	0.49
25:15:176:GLY:C	42:15:310:A86:C21	2.85	0.49
25:18:182:VAL:CG1	42:18:315:A86:C19	2.90	0.49
2:B:60:MET:HB3	2:B:63:MET:HB3	1.94	0.49
30:b:604:CLA:H112	30:b:614:CLA:H42	1.94	0.49
25:14:61:ARG:NH2	30:14:303:CLA:O1D	2.36	0.49
25:15:49:TRP:HH2	42:15:313:A86:C39	2.25	0.49
30:17:308:CLA:C2C	42:17:311:A86:C28	2.90	0.49
13:O:150:ARG:HB2	13:O:228:MET:HE3	1.94	0.49
3:c:64:ALA:HB1	10:k:23:LEU:HB3	1.94	0.49
16:v:89:ALA:O	16:v:97:SER:OG	2.31	0.49
25:11:146:PHE:HB3	42:11:316:A86:C39	2.42	0.49
25:17:81:HIS:HE1	30:17:305:CLA:NB	2.10	0.49
2:b:60:MET:HB3	2:b:63:MET:HB3	1.94	0.49
25:11:41:LEU:CD1	42:11:312:A86:C22	2.91	0.49
30:B:602:CLA:H71	7:H:46:LEU:HD12	1.94	0.49
2:b:179:GLN:NE2	7:h:66:ILE:O	2.46	0.49
13:o:150:ARG:HB2	13:o:228:MET:HE3	1.94	0.49
15:u:58:VAL:HA	15:u:61:LEU:HD23	1.95	0.49
30:21:304:CLA:CMB	42:21:314:A86:C2	2.91	0.49
1:A:140:ARG:HD2	3:C:456:GLY:HA2	1.95	0.49
2:B:155:ALA:O	2:B:159:THR:OG1	2.31	0.49
30:B:607:CLA:H43	36:B:619:LMG:H311	1.93	0.49
15:U:58:VAL:HA	15:U:61:LEU:HD23	1.95	0.49
32:b:623:BCR:H312	30:12:309:CLA:OBD	2.13	0.49
3:c:406:GLY:H	3:c:415:VAL:HG23	1.77	0.49
25:13:72:MET:HE2	42:13:311:A86:C2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:601:CLA:HBB2	32:H:101:BCR:H16C	1.95	0.48
32:B:617:BCR:H19C	33:l:101:SQD:H222	1.95	0.48
3:C:77:LYS:HE3	3:C:82:GLN:HG2	1.95	0.48
3:C:254:PRO:O	3:C:259:ARG:NH1	2.47	0.48
30:a:403:CLA:H3A	36:w:101:LMG:H131	1.95	0.48
3:c:101:GLY:HA3	3:c:298:GLU:HB3	1.95	0.48
42:17:302:A86:C17	42:17:315:A86:C35	2.91	0.48
27:20:145:UNK:O	42:20:210:A86:C35	2.61	0.48
2:b:2:ALA:N	11:l:10:ALA:O	2.46	0.48
25:18:182:VAL:HG11	42:18:315:A86:C19	2.41	0.48
30:B:614:CLA:H91	30:B:614:CLA:H171	1.94	0.48
3:C:64:ALA:HB1	10:K:23:LEU:HB3	1.94	0.48
30:C:520:CLA:H162	30:C:520:CLA:H71	1.95	0.48
4:d:154:SER:HA	4:d:158:LEU:HB2	1.94	0.48
4:d:162:GLY:HA3	4:d:289:ALA:HB1	1.94	0.48
25:18:146:PHE:CA	42:18:302:A86:O5	2.60	0.48
2:B:325:PHE:CG	11:L:35:TYR:HB3	2.48	0.48
30:B:601:CLA:CBB	32:H:101:BCR:H16C	2.44	0.48
2:b:64:PRO:HB3	2:b:267:LEU:HB3	1.96	0.48
16:v:9:THR:O	16:v:124:LYS:NZ	2.46	0.48
25:14:145:TYR:HB2	30:14:309:CLA:HAA1	1.96	0.48
2:B:334:ASP:N	2:B:334:ASP:OD1	2.47	0.48
2:b:157:HIS:HE1	30:b:606:CLA:C1A	2.27	0.48
30:b:612:CLA:H102	30:b:612:CLA:H61	1.59	0.48
25:13:145:TYR:OH	42:13:315:A86:C40	2.62	0.48
2:B:341:LEU:HD12	2:B:429:VAL:HG12	1.94	0.48
4:D:154:SER:HA	4:D:158:LEU:HB2	1.94	0.48
2:b:155:ALA:O	2:b:159:THR:OG1	2.31	0.48
3:c:77:LYS:HE3	3:c:82:GLN:HG2	1.95	0.48
25:18:180:ALA:O	25:18:191:GLN:NE2	2.46	0.48
16:V:49:ASN:ND2	41:V:201:HEM:O1D	2.47	0.48
3:c:274:LEU:HD22	3:c:435:PHE:HD1	1.79	0.48
3:c:343:PRO:HB3	13:o:74:ARG:HD3	1.96	0.48
25:11:142:GLY:O	25:14:158:ARG:NH1	2.47	0.48
25:11:145:TYR:HB2	30:11:307:CLA:HAA1	1.95	0.48
25:12:41:LEU:HD12	42:12:317:A86:C22	2.44	0.48
30:17:308:CLA:H62	30:17:308:CLA:H41	1.66	0.48
33:L:103:SQD:H222	32:b:616:BCR:H19C	1.95	0.48
16:V:9:THR:O	16:V:124:LYS:NZ	2.46	0.48
16:V:89:ALA:O	16:V:97:SER:OG	2.30	0.48
1:a:309:SER:HA	6:f:43:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:15:316:A86:C3	30:18:311:CLA:HAB	2.43	0.48
13:O:72:MET:HE1	13:O:115:ARG:HG2	1.95	0.48
13:o:72:MET:HE1	13:o:115:ARG:HG2	1.95	0.48
25:15:59:ARG:HH11	25:15:137:TYR:HE1	1.62	0.48
25:16:164:LEU:O	25:16:168:ARG:N	2.45	0.48
25:17:77:GLY:O	25:17:81:HIS:ND1	2.47	0.48
13:O:47:PRO:HA	13:O:240:GLY:HA3	1.96	0.48
3:c:211:VAL:O	3:c:221:TRP:NE1	2.38	0.48
42:15:316:A86:C40	30:18:311:CLA:HMA2	2.43	0.48
42:17:302:A86:C37	42:17:302:A86:C40	2.91	0.48
30:A:404:CLA:H193	30:C:507:CLA:H193	1.96	0.47
30:C:511:CLA:H191	10:K:28:VAL:HG22	1.96	0.47
4:D:194:PRO:HG3	11:L:35:TYR:CE2	2.49	0.47
3:c:254:PRO:O	3:c:259:ARG:NH1	2.46	0.47
30:11:304:CLA:HBA1	30:11:315:CLA:H151	1.96	0.47
25:12:145:TYR:HB2	30:12:311:CLA:HAA1	1.95	0.47
25:16:64:GLU:OE1	30:16:302:CLA:C4A	2.58	0.47
25:17:164:LEU:O	25:17:168:ARG:N	2.39	0.47
5:E:19:ARG:NH1	41:F:102:HEM:O2A	2.47	0.47
11:L:25:ILE:HD13	12:M:18:PRO:HB2	1.95	0.47
20:Q:102:LYS:O	20:Q:105:ASN:ND2	2.47	0.47
34:a:406:BCT:O3	4:d:213:HIS:CE1	2.67	0.47
25:18:78:THR:O	25:18:82:ASN:ND2	2.47	0.47
1:A:328:ILE:HG23	4:D:320:LEU:HD22	1.97	0.47
3:C:101:GLY:HA3	3:C:298:GLU:HB3	1.95	0.47
3:C:254:PRO:HA	30:C:507:CLA:HED3	1.96	0.47
13:O:189:ASN:HB2	15:U:11:ILE:HD11	1.96	0.47
16:V:73:VAL:HG12	16:V:77:LYS:HZ2	1.78	0.47
30:W:103:CLA:H162	30:W:103:CLA:H122	1.53	0.47
30:c:507:CLA:H203	30:c:507:CLA:H122	1.96	0.47
41:v:201:HEM:HBC2	41:v:201:HEM:HHD	1.96	0.47
25:12:69:ARG:NE	25:12:163:GLU:OE2	2.38	0.47
30:15:308:CLA:HAB	42:15:315:A86:C3	2.44	0.47
25:17:40:PRO:HG3	30:18:301:CLA:C3B	2.44	0.47
25:17:174:ILE:HG22	25:17:178:MET:HE2	1.96	0.47
30:C:506:CLA:H201	36:W:101:LMG:C29	2.43	0.47
30:c:513:CLA:H3A	30:c:513:CLA:HBA1	1.55	0.47
36:d:410:LMG:H352	32:f:101:BCR:H19C	1.97	0.47
25:12:45:ASP:OD1	25:12:45:ASP:N	2.48	0.47
30:21:306:CLA:CHD	42:21:310:A86:C37	2.92	0.47
2:B:64:PRO:HB3	2:B:267:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:610:CLA:H43	30:B:612:CLA:H51	1.97	0.47
30:C:504:CLA:H102	30:C:504:CLA:H62	1.64	0.47
30:C:507:CLA:H203	30:C:507:CLA:H122	1.96	0.47
2:b:334:ASP:OD1	2:b:334:ASP:N	2.47	0.47
3:c:451:ALA:O	8:i:33:ASN:ND2	2.48	0.47
30:16:307:CLA:CBB	30:16:308:CLA:H3A	2.45	0.47
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.47
2:B:157:HIS:HE1	30:B:606:CLA:C1A	2.27	0.47
16:v:49:ASN:ND2	41:v:201:HEM:O1D	2.47	0.47
20:q:105:ASN:HB2	20:q:108:TYR:HD2	1.79	0.47
25:13:145:TYR:HB2	30:13:308:CLA:HAA1	1.96	0.47
25:15:59:ARG:HH22	30:15:306:CLA:HBA2	1.79	0.47
25:16:171:MET:SD	42:16:311:A86:C2	3.03	0.47
27:20:118:UNK:N	42:20:201:A86:C22	2.77	0.47
28:21:93:UNK:CA	42:21:314:A86:C40	2.89	0.47
2:b:464:PHE:HD2	30:b:611:CLA:HAC2	1.80	0.47
4:d:155:VAL:HG22	4:d:285:ILE:HG12	1.97	0.47
15:u:50:VAL:HG13	15:u:95:ARG:HB3	1.97	0.47
25:15:145:TYR:N	25:15:148:THR:O	2.47	0.47
30:15:308:CLA:HBA2	42:15:315:A86:C40	2.44	0.47
25:16:171:MET:HB3	42:16:311:A86:C3	2.45	0.47
42:19:310:A86:C23	42:19:310:A86:C11	2.93	0.47
3:C:274:LEU:HD22	3:C:435:PHE:HD1	1.79	0.47
32:Y:101:BCR:HC21	19:Z:10:VAL:HG13	1.97	0.47
25:15:83:ASN:ND2	42:15:315:A86:O1	2.48	0.47
2:B:422:ARG:NH2	13:O:167:ASP:OD2	2.47	0.47
30:B:602:CLA:H202	39:H:102:DGD:HB82	1.97	0.47
3:C:89:HIS:O	3:C:92:THR:OG1	2.32	0.47
39:H:102:DGD:HB91	39:H:102:DGD:HB62	1.71	0.47
41:V:201:HEM:HBC2	41:V:201:HEM:HHD	1.96	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.97	0.47
30:b:610:CLA:H43	30:b:612:CLA:H51	1.97	0.47
3:c:214:SER:HB2	36:w:101:LMG:HC72	1.97	0.47
15:u:33:ARG:NH1	16:v:51:ASN:OD1	2.48	0.47
2:B:30:VAL:HG11	30:B:612:CLA:H112	1.97	0.47
11:L:16:THR:HG23	35:L:101:LHG:HC62	1.97	0.47
2:b:243:SER:HA	2:b:246:PHE:CE1	2.50	0.47
6:f:22:HIS:CE1	41:f:102:HEM:C4D	3.03	0.47
8:i:28:PRO:O	21:w:66:ILE:HD11	2.14	0.47
20:q:102:LYS:O	20:q:105:ASN:ND2	2.47	0.47
25:16:83:ASN:ND2	42:17:302:A86:C20	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:17:306:CLA:CHB	42:17:315:A86:C25	2.93	0.47
2:B:357:ARG:HH21	4:D:336:GLU:HG3	1.79	0.46
2:B:464:PHE:HD2	30:B:611:CLA:HAC2	1.80	0.46
13:O:74:ARG:NH1	21:W:21:GLU:OE2	2.48	0.46
2:b:192:PRO:HG3	7:h:49:TYR:CD1	2.50	0.46
2:b:434:ARG:NH1	13:o:180:GLU:OE2	2.46	0.46
5:e:19:ARG:NH1	41:f:102:HEM:O2A	2.47	0.46
30:11:302:CLA:HBC1	30:11:306:CLA:HBC2	1.97	0.46
25:12:165:ASN:ND2	30:12:312:CLA:O1D	2.39	0.46
30:B:604:CLA:H91	30:B:604:CLA:H111	1.76	0.46
4:D:278:LEU:HD22	31:D:403:PHO:HBC3	1.95	0.46
15:U:50:VAL:HG13	15:U:95:ARG:HB3	1.97	0.46
2:b:30:VAL:HG11	30:b:612:CLA:H112	1.97	0.46
30:c:504:CLA:H193	30:c:511:CLA:HBB2	1.97	0.46
30:12:306:CLA:HBC1	30:12:310:CLA:HBC2	1.97	0.46
25:13:45:ASP:OD1	25:13:45:ASP:N	2.48	0.46
30:21:303:CLA:H43	42:21:314:A86:C4	2.45	0.46
3:C:366:PRO:HA	20:Q:140:ASP:HB2	1.97	0.46
1:a:188:ALA:HB2	1:a:328:ILE:HB	1.98	0.46
20:q:162:GLN:HE21	20:q:206:LEU:HD13	1.80	0.46
25:11:45:ASP:N	25:11:45:ASP:OD1	2.48	0.46
30:13:303:CLA:HBC1	30:13:307:CLA:HBC2	1.97	0.46
30:17:303:CLA:H3A	30:17:303:CLA:HBA2	1.35	0.46
30:19:301:CLA:H3A	30:19:301:CLA:HBA2	1.57	0.46
1:A:309:SER:HA	6:F:43:ARG:HD3	1.98	0.46
2:B:192:PRO:HG3	7:H:49:TYR:CD1	2.51	0.46
20:Q:162:GLN:HE21	20:Q:206:LEU:HD13	1.80	0.46
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.46
6:f:43:ARG:NH2	9:j:39:LEU:OXT	2.49	0.46
2:B:256:MET:O	2:B:448:ARG:NH1	2.45	0.46
20:Q:105:ASN:HB2	20:Q:108:TYR:HD2	1.79	0.46
40:d:405:PL9:H28	40:d:405:PL9:H322	1.77	0.46
13:o:47:PRO:HA	13:o:240:GLY:HA3	1.96	0.46
15:u:12:ASP:OD1	15:u:12:ASP:N	2.42	0.46
30:11:315:CLA:O1D	25:14:165:ASN:ND2	2.40	0.46
25:15:92:SER:HG	25:15:97:LEU:H	1.59	0.46
30:15:308:CLA:HBC1	30:16:301:CLA:HBC2	1.96	0.46
25:16:202:ASP:OD1	25:16:202:ASP:N	2.48	0.46
25:17:146:PHE:HB3	42:17:302:A86:C38	2.46	0.46
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.97	0.46
30:A:402:CLA:H52	30:D:401:CLA:HAB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:GLY:HA3	30:C:512:CLA:HMD2	1.98	0.46
3:C:209:GLY:HA2	21:W:26:TRP:HE1	1.80	0.46
3:C:211:VAL:O	3:C:221:TRP:NE1	2.38	0.46
3:C:267:GLU:OE2	3:C:442:HIS:ND1	2.40	0.46
4:D:262:ASN:HB3	4:D:265:TRP:HB3	1.98	0.46
30:b:602:CLA:H41	30:b:602:CLA:H62	1.66	0.46
13:o:51:ALA:HB1	13:o:66:PHE:HB3	1.98	0.46
30:18:303:CLA:C8	42:18:314:A86:C28	2.93	0.46
3:C:205:ILE:HD13	26:19:201:UNK:HA	1.98	0.46
4:D:191:THR:HG23	30:D:405:CLA:HBC2	1.98	0.46
2:b:256:MET:O	2:b:448:ARG:NH1	2.45	0.46
30:b:609:CLA:H92	30:b:609:CLA:H62	1.82	0.46
3:c:254:PRO:HA	30:c:507:CLA:HED3	1.96	0.46
30:c:502:CLA:H122	30:c:508:CLA:H61	1.98	0.46
25:11:41:LEU:HD11	42:11:312:A86:C22	2.45	0.46
25:16:53:GLU:O	25:16:57:PHE:N	2.48	0.46
27:20:116:UNK:O	27:20:120:UNK:N	2.49	0.46
28:21:77:UNK:CB	42:21:311:A86:C21	2.94	0.46
1:A:97:TRP:NE1	36:W:101:LMG:O3	2.36	0.46
2:B:243:SER:HA	2:B:246:PHE:CE1	2.50	0.46
30:C:502:CLA:H122	30:C:508:CLA:H61	1.98	0.46
13:O:51:ALA:HB1	13:O:66:PHE:HB3	1.98	0.46
21:W:42:HIS:CD2	30:W:102:CLA:ND	2.83	0.46
30:W:103:CLA:H2	30:W:103:CLA:HAA1	1.98	0.46
32:a:404:BCR:H24C	32:a:404:BCR:H371	1.76	0.46
25:16:141:TYR:N	30:16:307:CLA:OBD	2.49	0.46
30:19:303:CLA:C1B	42:19:311:A86:C40	2.93	0.46
4:D:155:VAL:HG22	4:D:285:ILE:HG12	1.97	0.46
30:b:608:CLA:CBB	4:d:122:ILE:HG12	2.46	0.46
40:d:405:PL9:HC8	40:d:405:PL9:H121	1.74	0.46
25:11:64:GLU:OE2	25:11:168:ARG:NE	2.49	0.46
25:16:177:ASN:OD1	42:16:310:A86:O1	2.33	0.46
25:17:146:PHE:O	42:17:302:A86:O5	2.34	0.46
27:20:162:UNK:O	27:20:166:UNK:N	2.49	0.46
1:A:188:ALA:HB2	1:A:328:ILE:HB	1.98	0.46
1:A:237:TYR:OH	4:D:245:MET:HG2	2.16	0.46
2:B:326:ARG:NH2	4:D:296:ASP:OD1	2.48	0.46
10:K:26:ILE:HD11	17:Y:16:ILE:HD13	1.98	0.46
1:a:135:TYR:CE1	3:c:447:ARG:HG3	2.51	0.46
3:c:267:GLU:OE2	3:c:442:HIS:ND1	2.40	0.46
32:c:520:BCR:HC21	19:z:10:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:w:103:CLA:H162	30:w:103:CLA:H122	1.53	0.46
30:16:308:CLA:HMD2	30:17:301:CLA:H2	1.98	0.46
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.97	0.45
2:B:114:HIS:CE1	30:B:615:CLA:ND	2.83	0.45
30:C:502:CLA:HBB1	32:C:515:BCR:H21C	1.97	0.45
30:C:507:CLA:H202	30:W:102:CLA:H61	1.98	0.45
13:o:193:PHE:HB2	15:u:90:ASP:HB3	1.96	0.45
25:13:64:GLU:OE2	25:13:168:ARG:NE	2.49	0.45
25:14:45:ASP:N	25:14:45:ASP:OD1	2.48	0.45
25:17:82:ASN:HD22	25:17:188:MET:HE2	1.80	0.45
25:18:38:THR:HG22	25:18:40:PRO:HD2	1.97	0.45
25:18:199:PRO:HD3	30:18:312:CLA:CGA	2.46	0.45
30:B:615:CLA:H142	30:B:615:CLA:H112	1.78	0.45
17:Y:6:VAL:CG1	24:2:19:UNK:CB	2.95	0.45
2:b:114:HIS:CE1	30:b:615:CLA:ND	2.83	0.45
25:12:64:GLU:OE2	25:12:168:ARG:NE	2.49	0.45
25:14:69:ARG:NE	25:14:163:GLU:OE2	2.38	0.45
30:17:304:CLA:HBC1	30:17:307:CLA:HBC2	1.98	0.45
30:14:304:CLA:HBC1	30:14:308:CLA:HBC2	1.98	0.45
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.98	0.45
2:B:211:PHE:O	32:B:624:BCR:H381	2.17	0.45
30:C:504:CLA:H193	30:C:511:CLA:HBB2	1.98	0.45
13:O:21:ASN:ND2	13:O:75:GLN:OE1	2.44	0.45
13:O:40:LEU:HD11	13:O:244:ALA:HB1	1.99	0.45
1:a:95:PRO:HD2	1:a:98:GLU:HB2	1.97	0.45
1:a:223:LEU:O	2:b:482:ILE:HG12	2.16	0.45
2:b:237:VAL:HG22	30:b:610:CLA:HBC2	1.98	0.45
30:b:615:CLA:H142	30:b:615:CLA:H112	1.78	0.45
3:c:319:ASP:OD2	3:c:338:TYR:OH	2.34	0.45
25:16:79:ILE:CD1	42:17:302:A86:C9	2.95	0.45
25:16:112:ILE:HD11	30:16:304:CLA:H3A	1.99	0.45
30:16:307:CLA:HBA2	30:16:307:CLA:H3A	1.63	0.45
30:18:309:CLA:H142	30:18:309:CLA:H112	1.84	0.45
30:A:404:CLA:H172	30:C:507:CLA:H52	1.97	0.45
2:b:325:PHE:CG	11:l:35:TYR:HB3	2.51	0.45
2:b:383:PHE:CZ	13:o:165:GLY:HA2	2.52	0.45
30:c:502:CLA:HBB1	32:c:516:BCR:H21C	1.97	0.45
30:11:301:CLA:HMC1	42:11:311:A86:C24	2.45	0.45
25:15:142:GLY:O	25:18:158:ARG:NE	2.37	0.45
25:18:146:PHE:HB3	42:18:302:A86:C39	2.47	0.45
30:21:303:CLA:C1	42:21:314:A86:C5	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PHE:HB2	3:C:426:CYS:SG	2.56	0.45
2:B:179:GLN:NE2	7:H:66:ILE:O	2.50	0.45
2:B:237:VAL:HG22	30:B:610:CLA:HBC2	1.98	0.45
2:B:283:GLU:OE2	2:B:286:ARG:NH2	2.46	0.45
30:B:602:CLA:H203	39:H:102:DGD:HA72	1.99	0.45
3:C:205:ILE:CD1	26:19:199:UNK:CA	2.72	0.45
12:M:41:ASP:O	12:m:32:ARG:NH1	2.49	0.45
40:d:408:PL9:H512	14:t:10:LEU:HD13	1.98	0.45
20:q:154:ARG:NH2	20:q:167:GLU:OE2	2.47	0.45
21:w:42:HIS:CD2	30:w:102:CLA:ND	2.83	0.45
30:21:306:CLA:C4C	42:21:310:A86:C37	2.95	0.45
6:F:41:ILE:O	9:J:35:LEU:HG	2.17	0.45
30:c:511:CLA:H191	10:k:28:VAL:HG22	1.98	0.45
30:12:305:CLA:HMC1	42:12:316:A86:C24	2.47	0.45
25:14:64:GLU:OE2	25:14:168:ARG:NE	2.49	0.45
42:20:212:A86:C21	42:20:212:A86:C13	2.94	0.45
30:C:507:CLA:H192	30:C:507:CLA:H102	1.99	0.45
30:C:514:CLA:H143	30:C:514:CLA:H111	1.82	0.45
3:c:53:ALA:HB1	32:c:521:BCR:H373	1.99	0.45
30:c:502:CLA:H41	30:c:502:CLA:H61	1.74	0.45
25:17:172:MET:CE	42:17:312:A86:C	2.95	0.45
25:18:65:ARG:NH1	25:18:138:ASP:O	2.50	0.45
2:B:423:LYS:HE2	13:O:178:GLY:O	2.17	0.45
4:D:192:LEU:O	11:L:35:TYR:OH	2.24	0.45
25:13:41:LEU:HD11	42:13:313:A86:C22	2.46	0.45
30:17:305:CLA:H62	42:17:315:A86:C5	2.47	0.45
30:21:302:CLA:HBC1	30:21:305:CLA:HBC2	1.99	0.45
1:A:301:ASN:OD1	1:A:303:ASN:ND2	2.50	0.45
30:B:602:CLA:H92	30:B:602:CLA:H62	1.80	0.45
6:F:42:GLN:HB3	9:J:34:GLY:HA2	2.00	0.45
12:M:21:PHE:HB2	36:M:102:LMG:H362	1.99	0.45
2:b:461:LEU:HD21	4:d:283:ILE:HD11	1.99	0.45
30:c:507:CLA:H102	30:c:507:CLA:H192	1.99	0.45
30:c:512:CLA:H42	17:y:34:LEU:HA	1.99	0.45
11:l:25:ILE:HD13	12:m:18:PRO:HB2	1.98	0.45
25:11:49:TRP:HH2	42:11:313:A86:C39	2.30	0.45
25:13:165:ASN:ND2	30:14:302:CLA:O1D	2.39	0.45
25:16:175:MET:HG3	30:16:309:CLA:HBC2	1.99	0.45
25:17:180:ALA:O	25:17:191:GLN:NE2	2.50	0.45
30:21:308:CLA:HMC1	42:21:310:A86:C9	2.47	0.45
6:F:21:ILE:HD12	41:F:102:HEM:HBD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:193:PHE:HB2	15:U:90:ASP:HB3	1.99	0.44
13:O:196:THR:HG21	13:O:223:LEU:HD23	1.99	0.44
30:Z:102:CLA:CAC	42:20:210:A86:C28	2.95	0.44
2:b:283:GLU:OE2	2:b:286:ARG:NH2	2.46	0.44
4:d:262:ASN:HB3	4:d:265:TRP:HB3	1.98	0.44
13:o:95:PHE:HB3	13:o:127:ALA:HB3	1.99	0.44
30:17:306:CLA:C1B	42:17:315:A86:C26	2.95	0.44
1:A:37:MET:SD	1:A:41:LEU:HD12	2.57	0.44
2:B:281:GLN:HB2	2:B:358:ARG:HH12	1.82	0.44
30:B:613:CLA:H92	30:B:613:CLA:H61	1.84	0.44
30:C:507:CLA:H143	30:W:102:CLA:H142	1.99	0.44
1:a:163:ILE:O	3:c:290:TYR:OH	2.36	0.44
1:a:301:ASN:OD1	1:a:303:ASN:ND2	2.50	0.44
30:b:604:CLA:H91	30:b:604:CLA:H111	1.76	0.44
13:o:94:THR:HG22	13:o:128:LYS:HG2	1.99	0.44
30:w:103:CLA:H2	30:w:103:CLA:HAA1	1.98	0.44
25:11:165:ASN:ND2	30:12:303:CLA:O1D	2.39	0.44
25:13:180:ALA:O	25:13:191:GLN:NE2	2.51	0.44
3:C:405:VAL:HG21	3:C:413:ASN:HA	2.00	0.44
19:Z:34:LYS:O	19:Z:38:ASN:N	2.46	0.44
1:a:307:VAL:HG21	6:f:43:ARG:HH21	1.81	0.44
3:c:89:HIS:NE2	30:c:503:CLA:O1D	2.44	0.44
30:14:303:CLA:HMC1	42:14:313:A86:C24	2.47	0.44
4:D:82:ASN:HD22	4:D:335:HIS:CD2	2.36	0.44
30:Z:102:CLA:HAC2	42:20:210:A86:C28	2.48	0.44
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.98	0.44
30:b:604:CLA:H193	32:b:617:BCR:HC8	1.99	0.44
30:12:312:CLA:H71	30:12:312:CLA:H112	1.83	0.44
25:16:163:GLU:HB2	30:16:307:CLA:C1B	2.47	0.44
25:16:174:ILE:HG21	42:16:311:A86:C8	2.47	0.44
30:21:302:CLA:HMB3	42:21:311:A86:C28	2.46	0.44
35:L:102:LHG:H312	12:M:18:PRO:HB3	2.00	0.44
13:O:167:ASP:HB2	15:U:11:ILE:HG12	2.00	0.44
17:Y:20:GLY:HA3	32:Y:101:BCR:C15	2.47	0.44
2:b:179:GLN:HE22	7:h:66:ILE:HB	1.82	0.44
3:c:26:ILE:HD13	4:d:232:ARG:HH11	1.81	0.44
3:c:405:VAL:HG21	3:c:413:ASN:HA	2.00	0.44
4:d:82:ASN:HD22	4:d:335:HIS:CD2	2.35	0.44
6:f:21:ILE:HD12	41:f:102:HEM:HBD2	2.00	0.44
13:o:21:ASN:ND2	13:o:75:GLN:OE1	2.44	0.44
19:z:34:LYS:O	19:z:38:ASN:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:11:131:TRP:HH2	30:14:310:CLA:HAC2	1.82	0.44
25:14:180:ALA:O	25:14:191:GLN:NE2	2.51	0.44
3:C:400:GLY:HA3	3:C:418:VAL:HG22	2.00	0.44
39:H:102:DGD:O5D	39:H:102:DGD:O4D	2.25	0.44
32:b:617:BCR:H24C	32:b:617:BCR:H371	1.77	0.44
4:d:191:THR:HG23	30:d:406:CLA:HBC2	1.98	0.44
13:o:146:THR:OG1	13:o:196:THR:OG1	2.27	0.44
25:11:180:ALA:O	25:11:191:GLN:NE2	2.51	0.44
25:12:180:ALA:O	25:12:191:GLN:NE2	2.50	0.44
25:18:60:ARG:NH2	42:18:315:A86:O3	2.51	0.44
30:20:209:CLA:H202	30:20:209:CLA:H162	1.83	0.44
1:A:307:VAL:HG23	6:F:43:ARG:HE	1.82	0.44
3:C:319:ASP:OD2	3:C:338:TYR:OH	2.34	0.44
3:C:442:HIS:HE1	30:C:509:CLA:NA	2.12	0.44
30:C:512:CLA:H42	17:Y:34:LEU:HA	1.98	0.44
32:H:101:BCR:H361	32:H:101:BCR:H20C	1.77	0.44
32:Y:101:BCR:C34	19:Z:17:VAL:HG11	2.48	0.44
20:Q:154:ARG:NH2	20:Q:167:GLU:OE2	2.47	0.44
30:a:403:CLA:H193	30:c:507:CLA:H193	2.00	0.44
2:b:281:GLN:HB2	2:b:358:ARG:HH12	1.82	0.44
30:c:504:CLA:C4B	30:z:101:CLA:H162	2.48	0.44
30:18:312:CLA:H2A	30:18:312:CLA:HED2	2.00	0.44
3:C:464:VAL:HG21	4:D:247:THR:HG23	1.99	0.44
40:D:404:PL9:H322	40:D:404:PL9:H28	1.77	0.44
25:15:174:ILE:HG22	25:15:178:MET:HE2	2.00	0.44
25:16:197:ILE:HG23	30:16:309:CLA:HMA2	1.99	0.44
30:18:303:CLA:C11	42:18:314:A86:C28	2.92	0.44
1:A:25:GLU:HB3	3:C:468:ARG:HD2	2.00	0.44
1:A:303:ASN:O	3:C:413:ASN:ND2	2.51	0.44
30:A:404:CLA:CBB	8:I:15:PHE:HB2	2.48	0.44
30:C:506:CLA:C20	36:W:101:LMG:H321	2.48	0.44
13:O:94:THR:HG22	13:O:128:LYS:HG2	1.99	0.44
15:U:48:LYS:NZ	15:U:66:GLY:O	2.37	0.44
2:b:256:MET:HA	2:b:263:THR:HG21	2.00	0.44
30:c:513:CLA:H162	30:z:101:CLA:H142	2.00	0.44
16:v:43:GLY:O	16:v:131:GLY:N	2.44	0.44
25:16:76:VAL:HG21	42:16:310:A86:C	2.48	0.44
30:17:305:CLA:H161	30:17:305:CLA:H122	1.69	0.44
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.43
6:F:43:ARG:NH2	9:J:39:LEU:OXT	2.51	0.43
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:68:SER:OG	15:U:69:SER:N	2.51	0.43
15:U:101:TYR:CD1	16:V:50:PRO:HG2	2.53	0.43
1:a:37:MET:SD	1:a:41:LEU:HD12	2.57	0.43
30:a:403:CLA:H112	30:c:506:CLA:H202	2.00	0.43
35:a:407:LHG:H281	35:a:407:LHG:H212	2.00	0.43
4:d:138:ARG:NH2	4:d:140:TYR:OH	2.51	0.43
8:i:13:ILE:HD12	21:w:38:LEU:HD22	1.99	0.43
25:15:82:ASN:HD22	25:15:188:MET:HE2	1.83	0.43
30:19:301:CLA:H141	30:19:301:CLA:H161	1.83	0.43
32:A:409:BCR:H15C	32:A:409:BCR:H351	1.84	0.43
2:B:357:ARG:NH2	4:D:336:GLU:HG3	2.33	0.43
4:d:38:PRO:HB2	30:d:407:CLA:HAB	2.01	0.43
21:w:21:GLU:O	36:w:101:LMG:O5	2.18	0.43
25:15:162:VAL:HG11	30:15:308:CLA:HAA2	2.00	0.43
25:16:161:ASN:O	25:16:165:ASN:N	2.48	0.43
25:17:45:ASP:OD1	25:17:45:ASP:N	2.51	0.43
25:17:113:PRO:HD2	30:17:306:CLA:HBB2	2.00	0.43
25:17:133:PRO:O	25:17:141:TYR:OH	2.36	0.43
3:C:89:HIS:NE2	30:C:503:CLA:O1D	2.44	0.43
4:D:38:PRO:HB2	30:D:406:CLA:HAB	2.01	0.43
11:L:20:TRP:HH2	35:L:101:LHG:H101	1.83	0.43
2:b:460:LEU:HD22	4:d:286:VAL:HG21	2.00	0.43
30:c:507:CLA:H203	30:c:507:CLA:H162	1.85	0.43
30:18:303:CLA:H142	30:18:303:CLA:H112	1.85	0.43
30:21:306:CLA:C1D	42:21:310:A86:C37	2.95	0.43
4:D:138:ARG:NH2	4:D:140:TYR:OH	2.51	0.43
30:b:602:CLA:H202	39:h:102:DGD:HB82	2.01	0.43
3:c:89:HIS:O	3:c:92:THR:OG1	2.33	0.43
30:12:303:CLA:H71	30:12:303:CLA:H112	1.82	0.43
30:15:305:CLA:HBA2	30:15:305:CLA:H3A	1.67	0.43
30:18:304:CLA:HBC1	30:18:308:CLA:HBC2	2.00	0.43
2:B:310:ALA:HB1	2:B:428:GLU:HG3	2.01	0.43
30:C:509:CLA:H193	30:C:509:CLA:H161	1.81	0.43
10:K:36:VAL:HG21	32:Y:101:BCR:H19C	2.00	0.43
13:o:40:LEU:HD11	13:o:244:ALA:HB1	1.99	0.43
25:11:132:MET:HG3	30:11:315:CLA:H12	2.01	0.43
30:11:301:CLA:H3A	30:11:301:CLA:HBA2	1.38	0.43
25:14:67:HIS:HE1	30:14:304:CLA:ND	2.16	0.43
25:15:183:LEU:CD2	42:15:313:A86:C21	2.97	0.43
25:17:79:ILE:HG23	42:18:302:A86:C12	2.48	0.43
25:17:171:MET:SD	42:17:312:A86:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:18:186:GLN:HB3	25:18:190:GLU:HB2	2.00	0.43
13:O:160:ARG:NH1	13:O:189:ASN:OD1	2.51	0.43
30:a:403:CLA:H93	30:a:403:CLA:H111	1.82	0.43
36:b:618:LMG:H332	36:b:618:LMG:H361	1.79	0.43
3:c:111:ALA:O	3:c:115:ILE:HG12	2.19	0.43
32:c:520:BCR:H19C	10:k:36:VAL:HG21	2.00	0.43
30:13:307:CLA:HBC1	42:13:312:A86:C12	2.49	0.43
25:15:109:ILE:HA	25:15:112:ILE:HD12	1.99	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
1:A:304:GLN:HG2	1:A:313:VAL:HG11	2.01	0.43
30:B:612:CLA:H102	30:B:612:CLA:H61	1.59	0.43
2:b:365:THR:HG21	13:o:170:VAL:HG22	2.00	0.43
2:b:477:ASP:OD1	2:b:477:ASP:N	2.51	0.43
3:c:400:GLY:HA3	3:c:418:VAL:HG22	2.00	0.43
30:w:102:CLA:H202	30:w:102:CLA:H162	1.82	0.43
30:12:305:CLA:H3A	30:12:305:CLA:HBA2	1.38	0.43
32:B:618:BCR:H371	32:B:618:BCR:H24C	1.77	0.43
6:F:22:HIS:CE1	41:F:102:HEM:C4D	3.07	0.43
2:b:310:ALA:HB1	2:b:428:GLU:HG3	2.01	0.43
30:b:614:CLA:H152	30:b:614:CLA:H112	1.85	0.43
30:d:401:CLA:H41	40:d:408:PL9:H162	2.00	0.43
25:11:112:ILE:HD11	30:11:303:CLA:H3A	2.01	0.43
30:11:305:CLA:HBA1	42:11:313:A86:C10	2.49	0.43
25:13:61:ARG:NH2	30:13:302:CLA:O1D	2.40	0.43
25:13:112:ILE:HD11	30:13:304:CLA:H3A	2.01	0.43
25:17:64:GLU:HB2	30:17:303:CLA:C1B	2.49	0.43
35:A:408:LHG:H281	35:A:408:LHG:H212	2.00	0.43
2:B:394:GLN:HE21	15:U:17:GLY:HA2	1.84	0.43
30:B:604:CLA:H193	32:B:618:BCR:HC8	2.00	0.43
30:B:613:CLA:H62	30:B:613:CLA:H41	1.72	0.43
3:C:332:PRO:HA	13:O:151:THR:HB	2.01	0.43
30:b:601:CLA:H151	30:b:601:CLA:HBB1	2.00	0.43
4:d:301:GLU:OE1	13:o:158:LYS:NZ	2.51	0.43
30:14:303:CLA:H71	30:14:304:CLA:HMA1	2.01	0.43
30:D:401:CLA:H41	40:D:407:PL9:H162	2.00	0.43
10:k:26:ILE:HD11	17:y:16:ILE:HD13	2.00	0.43
13:o:196:THR:HG21	13:o:223:LEU:HD23	1.99	0.43
25:13:193:ALA:CA	42:14:316:A86:C39	2.92	0.43
25:17:59:ARG:HH21	30:17:304:CLA:HED3	1.84	0.43
25:17:150:ILE:O	25:17:156:LYS:NZ	2.48	0.43
1:A:46:SER:OG	33:b:620:SQD:H121	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PRO:HG3	15:U:101:TYR:CD2	2.54	0.42
3:C:223:VAL:HA	3:C:287:TYR:CE1	2.54	0.42
25:17:143:VAL:HG11	42:17:311:A86:C34	2.49	0.42
30:20:207:CLA:HMC1	42:20:210:A86:C26	2.49	0.42
36:B:620:LMG:H391	36:B:620:LMG:H421	1.86	0.42
3:C:341:ARG:NH1	3:C:345:GLY:O	2.52	0.42
36:D:408:LMG:H352	32:F:101:BCR:H19C	2.00	0.42
16:V:5:GLU:O	16:V:9:THR:OG1	2.34	0.42
1:a:83:VAL:HG22	4:d:313:PHE:CE2	2.54	0.42
3:c:341:ARG:NH1	3:c:345:GLY:O	2.52	0.42
25:11:112:ILE:HD11	30:11:303:CLA:HAA2	2.01	0.42
25:12:112:ILE:HD11	30:12:307:CLA:HAA2	2.01	0.42
30:17:310:CLA:HBD	30:17:310:CLA:HBA1	2.01	0.42
25:18:199:PRO:HD2	30:18:312:CLA:CGA	2.48	0.42
26:19:103:UNK:O	42:19:311:A86:O4	2.37	0.42
28:21:173:UNK:CB	42:21:310:A86:C14	2.96	0.42
3:C:53:ALA:HB1	32:C:518:BCR:H373	2.02	0.42
16:V:76:ILE:HD13	16:V:112:LEU:HD22	2.01	0.42
1:a:84:PRO:HA	1:a:112:TYR:CG	2.53	0.42
3:c:223:VAL:HA	3:c:287:TYR:CE1	2.54	0.42
30:15:309:CLA:H2A	30:15:309:CLA:HED2	2.00	0.42
25:18:182:VAL:HG11	42:18:315:A86:O	2.19	0.42
1:A:149:ALA:HB1	1:A:283:ILE:HB	2.01	0.42
2:B:477:ASP:OD1	2:B:477:ASP:N	2.51	0.42
30:C:507:CLA:H203	30:C:507:CLA:H162	1.85	0.42
4:D:47:TRP:NE1	4:D:172:PHE:O	2.32	0.42
32:F:101:BCR:H20C	32:F:101:BCR:H361	1.78	0.42
3:c:442:HIS:HE1	30:c:509:CLA:NA	2.12	0.42
36:m:102:LMG:O5	36:m:102:LMG:O4	2.27	0.42
17:y:33:ASN:HD21	19:z:27:PRO:HG3	1.84	0.42
25:14:112:ILE:HD11	30:14:305:CLA:H3A	2.01	0.42
25:16:46:PRO:HG2	42:16:311:A86:O5	2.19	0.42
25:17:174:ILE:HD13	25:17:174:ILE:HA	1.88	0.42
30:19:309:CLA:H2A	30:19:309:CLA:HED2	2.01	0.42
42:20:212:A86:C24	42:20:212:A86:C28	2.96	0.42
28:21:121:UNK:O	28:21:125:UNK:N	2.52	0.42
31:A:403:PHO:H102	31:A:403:PHO:H13	1.69	0.42
2:B:236:THR:HB	2:B:473:THR:HG21	2.02	0.42
30:C:505:CLA:H161	30:C:505:CLA:H141	1.77	0.42
2:b:463:PHE:CZ	30:b:608:CLA:HBB1	2.55	0.42
30:b:601:CLA:HBB2	32:h:101:BCR:H16C	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:388:ARG:NE	16:v:100:ILE:HG21	2.35	0.42
30:c:504:CLA:H102	30:c:504:CLA:H62	1.64	0.42
15:u:68:SER:OG	15:u:69:SER:N	2.51	0.42
16:v:76:ILE:HD13	16:v:112:LEU:HD22	2.01	0.42
25:14:183:LEU:HD21	42:14:315:A86:C21	2.50	0.42
25:18:183:LEU:HD21	42:18:315:A86:C21	2.49	0.42
27:20:125:UNK:CB	42:20:201:A86:C7	2.97	0.42
2:B:174:ILE:HD11	2:B:309:LEU:HB2	2.01	0.42
30:B:601:CLA:HBB1	30:B:601:CLA:H151	2.00	0.42
3:C:111:ALA:O	3:C:115:ILE:HG12	2.19	0.42
20:Q:86:TYR:HA	20:Q:94:PRO:HG3	2.01	0.42
1:a:149:ALA:HB1	1:a:283:ILE:HB	2.01	0.42
1:a:304:GLN:HG2	1:a:313:VAL:HG11	2.01	0.42
30:b:622:CLA:CAD	30:12:310:CLA:HAA1	2.50	0.42
13:o:56:VAL:HG11	13:o:65:LYS:HD3	2.02	0.42
13:o:160:ARG:NH1	13:o:189:ASN:OD1	2.51	0.42
30:11:315:CLA:H71	30:11:315:CLA:H112	1.82	0.42
30:13:302:CLA:H3A	30:13:302:CLA:HBA2	1.38	0.42
30:15:301:CLA:H3A	30:15:301:CLA:HBA2	1.57	0.42
30:15:307:CLA:H112	30:15:307:CLA:H151	1.83	0.42
30:15:308:CLA:HAB	42:15:315:A86:C2	2.49	0.42
25:16:117:LEU:HD23	25:16:120:ILE:HD12	2.01	0.42
25:18:37:VAL:HG13	25:18:42:GLY:HA2	2.02	0.42
42:21:313:A86:C35	42:21:313:A86:C39	2.97	0.42
30:B:608:CLA:HBB2	4:D:122:ILE:HG12	2.01	0.42
3:C:128:ILE:HD11	32:C:518:BCR:H21C	2.01	0.42
7:H:53:LEU:HD11	18:X:5:LEU:HA	2.00	0.42
32:H:101:BCR:H11C	32:H:101:BCR:H341	1.90	0.42
32:H:101:BCR:H15C	32:H:101:BCR:H351	1.86	0.42
30:b:601:CLA:CBB	32:h:101:BCR:H16C	2.49	0.42
32:c:515:BCR:H11C	32:c:515:BCR:H341	1.91	0.42
25:14:112:ILE:HD11	30:14:305:CLA:HAA2	2.01	0.42
30:17:301:CLA:H71	30:17:301:CLA:H112	1.88	0.42
2:B:463:PHE:CZ	30:B:608:CLA:HBB1	2.55	0.42
4:D:193:ASN:HD22	4:D:194:PRO:HD2	1.84	0.42
1:a:308:ASP:OD1	1:a:312:ARG:N	2.53	0.42
30:b:602:CLA:H102	30:b:609:CLA:H202	2.01	0.42
30:b:613:CLA:H111	30:b:613:CLA:H152	1.87	0.42
30:c:508:CLA:H142	30:c:508:CLA:H112	1.83	0.42
4:d:193:ASN:HD22	4:d:194:PRO:HD2	1.84	0.42
30:d:401:CLA:H152	30:d:401:CLA:H111	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:102:LHG:H312	12:m:18:PRO:HB3	2.01	0.42
30:12:303:CLA:H192	30:12:308:CLA:HAA2	2.01	0.42
30:14:305:CLA:HMB2	42:14:313:A86:O	2.20	0.42
25:18:117:LEU:HD23	25:18:120:ILE:HD12	2.02	0.42
30:20:209:CLA:H13	30:20:209:CLA:H171	1.78	0.42
1:A:272:HIS:CD2	4:D:213:HIS:NE2	2.88	0.42
1:a:98:GLU:HB3	21:w:21:GLU:HG2	2.01	0.42
30:w:102:CLA:H111	30:w:102:CLA:H152	1.70	0.42
25:17:120:ILE:HD13	42:17:315:A86:C7	2.49	0.42
25:18:45:ASP:OD1	25:18:45:ASP:N	2.53	0.42
2:b:236:THR:HB	2:b:473:THR:HG21	2.02	0.42
30:b:622:CLA:H11	32:b:623:BCR:H23C	2.02	0.42
30:d:406:CLA:H203	30:d:406:CLA:H162	1.92	0.42
40:d:408:PL9:H252	35:l:102:LHG:H142	2.02	0.42
21:w:67:ASP:OD1	21:w:67:ASP:N	2.47	0.42
25:12:112:ILE:HD11	30:12:307:CLA:H3A	2.01	0.42
42:13:315:A86:O5	25:14:146:PHE:CB	2.56	0.42
30:15:302:CLA:HMA3	42:15:313:A86:C26	2.50	0.42
25:16:83:ASN:ND2	42:17:302:A86:O1	2.45	0.42
30:19:303:CLA:C3B	42:19:311:A86:C41	2.98	0.42
30:21:303:CLA:C1	42:21:314:A86:C7	2.85	0.42
1:A:308:ASP:OD1	1:A:312:ARG:N	2.53	0.41
30:B:623:CLA:H143	30:B:623:CLA:H111	1.89	0.41
17:Y:6:VAL:HG11	24:2:19:UNK:CB	2.50	0.41
30:W:103:CLA:H112	30:W:103:CLA:H72	1.89	0.41
36:b:619:LMG:H412	36:b:619:LMG:H381	1.89	0.41
32:h:101:BCR:H11C	32:h:101:BCR:H341	1.90	0.41
30:14:302:CLA:H71	30:14:302:CLA:H112	1.83	0.41
25:18:81:HIS:HE1	30:18:305:CLA:NB	2.16	0.41
30:B:602:CLA:H102	30:B:609:CLA:H202	2.02	0.41
30:C:520:CLA:H93	30:C:520:CLA:H62	1.86	0.41
13:O:185:LEU:HD12	13:O:189:ASN:HD21	1.85	0.41
1:a:193:LEU:HD11	30:a:402:CLA:HMC2	2.01	0.41
20:q:86:TYR:HA	20:q:94:PRO:HG3	2.01	0.41
30:A:404:CLA:HBB2	8:I:15:PHE:CB	2.49	0.41
3:C:389:ARG:NH2	20:Q:147:TYR:OH	2.42	0.41
30:C:504:CLA:H193	30:C:504:CLA:H161	1.92	0.41
4:D:59:THR:OG1	4:D:60:HIS:N	2.53	0.41
16:V:99:ASP:N	16:V:99:ASP:OD1	2.54	0.41
20:Q:78:GLY:HA2	20:Q:81:GLN:HE22	1.85	0.41
2:b:419:LYS:O	2:b:423:LYS:NZ	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:90:ASP:OD1	15:u:90:ASP:N	2.49	0.41
36:12:301:LMG:H141	30:12:308:CLA:O1D	2.20	0.41
30:17:305:CLA:H71	42:17:315:A86:C9	2.50	0.41
1:A:219:VAL:HG21	4:D:267:HIS:CD2	2.56	0.41
2:B:82:GLY:HA3	13:o:57:GLY:O	2.20	0.41
32:C:518:BCR:H20C	32:C:518:BCR:H361	1.82	0.41
4:D:203:ILE:HD13	4:D:203:ILE:HA	1.90	0.41
30:D:401:CLA:H91	40:D:407:PL9:H402	2.02	0.41
13:O:130:ASN:OD1	13:O:130:ASN:N	2.53	0.41
13:O:226:THR:OG1	13:O:231:LYS:O	2.34	0.41
25:11:60:ARG:NH2	42:11:313:A86:O3	2.54	0.41
25:11:174:ILE:HD13	25:11:174:ILE:HA	1.90	0.41
25:12:184:THR:OG1	25:12:191:GLN:NE2	2.52	0.41
25:13:163:GLU:HB2	30:13:308:CLA:C1B	2.51	0.41
25:16:76:VAL:CG2	42:16:310:A86:C	2.98	0.41
25:17:154:GLU:HA	30:18:309:CLA:H193	2.03	0.41
30:20:202:CLA:H3A	30:20:202:CLA:HBA2	1.56	0.41
2:B:25:MET:HG2	32:B:616:BCR:H23C	2.02	0.41
15:U:90:ASP:OD1	15:U:90:ASP:N	2.50	0.41
2:b:174:ILE:HD11	2:b:309:LEU:HB2	2.01	0.41
25:12:131:TRP:HD1	30:12:303:CLA:NB	2.12	0.41
25:13:112:ILE:HD11	30:13:304:CLA:HAA2	2.01	0.41
25:17:50:LEU:HD21	30:17:303:CLA:HAA2	2.01	0.41
27:20:54:UNK:C	42:20:212:A86:C39	2.98	0.41
13:O:56:VAL:HG11	13:O:65:LYS:HD3	2.02	0.41
36:Q:301:LMG:H161	36:Q:301:LMG:H132	1.88	0.41
2:b:25:MET:HG2	32:m:103:BCR:H23C	2.02	0.41
8:i:6:ILE:HG23	21:w:37:VAL:HG21	2.03	0.41
8:i:7:LEU:O	8:i:10:THR:OG1	2.39	0.41
13:o:185:LEU:HD12	13:o:189:ASN:HD21	1.85	0.41
13:o:226:THR:OG1	13:o:231:LYS:O	2.34	0.41
30:16:302:CLA:H202	30:16:302:CLA:H162	1.83	0.41
25:17:157:ALA:O	25:17:161:ASN:N	2.41	0.41
3:c:128:ILE:HD11	32:c:521:BCR:H21C	2.02	0.41
3:c:128:ILE:HG22	19:z:24:LEU:HD12	2.02	0.41
3:c:280:MET:HG2	30:c:502:CLA:H72	2.03	0.41
3:c:355:ARG:NH2	38:c:501:OEX:O4	2.51	0.41
30:c:509:CLA:H193	30:c:509:CLA:H161	1.80	0.41
4:d:59:THR:OG1	4:d:60:HIS:N	2.53	0.41
6:f:42:GLN:NE2	20:q:70:SER:OG	2.51	0.41
25:11:163:GLU:HB2	30:11:307:CLA:C1B	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:15:90:TYR:OH	25:15:96:ASN:OD1	2.39	0.41
25:16:140:ASP:OD1	25:16:140:ASP:N	2.51	0.41
32:A:405:BCR:H24C	32:A:405:BCR:H371	1.75	0.41
2:B:475:PHE:HA	4:D:133:ARG:NH1	2.35	0.41
30:B:604:CLA:H111	30:B:604:CLA:H152	1.79	0.41
32:B:624:BCR:H11C	32:B:624:BCR:H341	1.85	0.41
40:d:408:PL9:HC2	40:d:408:PL9:HC8	1.77	0.41
30:z:101:CLA:H93	30:z:101:CLA:H111	1.91	0.41
20:q:78:GLY:HA2	20:q:81:GLN:HE22	1.85	0.41
25:11:184:THR:OG1	25:11:191:GLN:NE2	2.52	0.41
25:12:49:TRP:HH2	42:12:318:A86:C39	2.34	0.41
25:13:184:THR:OG1	25:13:191:GLN:NE2	2.52	0.41
30:15:307:CLA:H93	25:18:155:GLU:HG3	2.03	0.41
25:18:72:MET:HE2	42:18:313:A86:C2	2.51	0.41
1:A:150:PRO:HB2	30:A:402:CLA:H92	2.02	0.41
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.56	0.41
32:C:515:BCR:H24C	32:C:515:BCR:H371	1.92	0.41
30:D:405:CLA:H203	30:D:405:CLA:H162	1.92	0.41
8:I:7:LEU:O	8:I:10:THR:OG1	2.39	0.41
1:a:301:ASN:H	3:c:403:ASN:ND2	2.17	0.41
30:b:604:CLA:H111	30:b:604:CLA:H152	1.79	0.41
30:b:614:CLA:H2	30:b:615:CLA:HBB2	2.02	0.41
3:c:403:ASN:OD1	3:c:403:ASN:N	2.54	0.41
30:c:505:CLA:H141	30:c:505:CLA:H161	1.77	0.41
6:f:39:GLN:OE1	9:j:30:GLY:HA3	2.21	0.41
32:m:103:BCR:H15C	32:m:103:BCR:H351	1.87	0.41
25:12:61:ARG:NH2	30:12:305:CLA:O1D	2.40	0.41
25:12:163:GLU:HB2	30:12:311:CLA:C1B	2.51	0.41
25:14:163:GLU:HB2	30:14:309:CLA:C1B	2.51	0.41
25:15:114:THR:HA	25:15:117:LEU:HB2	2.03	0.41
25:18:57:PHE:O	25:18:61:ARG:N	2.51	0.41
25:18:156:LYS:HE3	30:18:309:CLA:H12	2.03	0.41
27:20:144:UNK:HA	30:20:207:CLA:HBD	2.03	0.41
2:B:298:GLU:OE2	2:B:302:TRP:NE1	2.46	0.41
13:O:17:THR:HG21	26:19:208:UNK:CB	2.50	0.41
1:a:277:LEU:HD11	35:a:407:LHG:H292	2.03	0.41
30:b:602:CLA:H111	30:b:602:CLA:H152	1.90	0.41
13:o:174:ALA:HA	13:o:177:LEU:HD23	2.03	0.41
16:v:81:THR:OG1	16:v:83:ASP:OD1	2.38	0.41
25:11:174:ILE:HG22	25:11:178:MET:HE2	2.03	0.41
42:16:310:A86:O2	30:17:306:CLA:OBD	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TRP:CD2	22:5:29:UNK:O	2.73	0.40
1:A:97:TRP:CD1	1:A:98:GLU:HG2	2.56	0.40
1:A:301:ASN:H	3:C:403:ASN:HD21	1.68	0.40
30:B:611:CLA:HAB	30:B:613:CLA:HMA3	2.03	0.40
3:C:280:MET:HG2	30:C:502:CLA:H72	2.03	0.40
30:D:405:CLA:H143	30:D:405:CLA:H161	1.95	0.40
9:J:14:LEU:HD11	17:Y:21:PRO:HB3	2.02	0.40
20:Q:78:GLY:HA2	20:Q:81:GLN:NE2	2.36	0.40
1:a:97:TRP:CD1	1:a:98:GLU:HG2	2.56	0.40
30:b:601:CLA:H93	30:b:601:CLA:H111	1.99	0.40
39:h:102:DGD:HB91	39:h:102:DGD:HB62	1.71	0.40
25:14:174:ILE:HG22	25:14:178:MET:HE2	2.03	0.40
25:15:166:ASN:HD21	30:15:308:CLA:C4D	2.34	0.40
30:16:307:CLA:HMB3	30:16:308:CLA:HAA1	2.03	0.40
30:20:202:CLA:C4	42:20:211:A86:C29	2.89	0.40
1:A:41:LEU:HA	1:A:41:LEU:HD23	1.87	0.40
1:A:118:HIS:HE1	30:A:404:CLA:C4D	2.33	0.40
30:B:602:CLA:H62	30:B:602:CLA:H41	1.66	0.40
30:B:605:CLA:H161	30:B:605:CLA:H141	1.87	0.40
11:L:23:LEU:HD22	35:L:101:LHG:H261	2.02	0.40
16:V:43:GLY:O	16:V:131:GLY:N	2.44	0.40
30:W:103:CLA:HMD2	42:11:313:A86:C35	2.52	0.40
2:b:6:TYR:HE1	35:l:102:LHG:HC41	1.86	0.40
30:b:603:CLA:H91	30:b:603:CLA:H112	1.86	0.40
3:c:74:VAL:HG12	3:c:76:GLU:H	1.86	0.40
30:c:508:CLA:H202	30:c:508:CLA:H161	1.85	0.40
35:d:409:LHG:H281	35:d:409:LHG:H132	2.04	0.40
39:j:101:DGD:HAF1	39:j:101:DGD:HAE2	1.85	0.40
30:A:404:CLA:H3A	36:W:101:LMG:H131	2.03	0.40
36:B:620:LMG:H381	36:B:620:LMG:H412	1.90	0.40
16:V:123:PRO:HG3	16:V:130:TRP:CD1	2.56	0.40
1:a:61:ASP:HB2	1:a:63:ILE:HG12	2.04	0.40
1:a:143:ILE:HG13	4:d:219:ASN:HD22	1.86	0.40
2:b:298:GLU:OE2	2:b:302:TRP:NE1	2.46	0.40
2:b:348:ASP:OD1	2:b:348:ASP:N	2.53	0.40
30:b:611:CLA:HAB	30:b:613:CLA:HMA3	2.03	0.40
15:u:88:SER:HA	15:u:89:PRO:HD3	1.87	0.40
20:q:78:GLY:HA2	20:q:81:GLN:NE2	2.36	0.40
25:12:67:HIS:HE1	30:12:306:CLA:ND	2.16	0.40
25:12:174:ILE:HD13	25:12:174:ILE:HA	1.90	0.40
30:A:404:CLA:H42	8:I:13:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:373:LEU:HB3	3:C:378:ILE:HD11	2.03	0.40
40:D:404:PL9:HC8	40:D:404:PL9:H121	1.74	0.40
40:D:407:PL9:H512	14:T:10:LEU:HD13	2.03	0.40
32:b:623:BCR:H11C	32:b:623:BCR:H341	1.86	0.40
3:c:215:PRO:HB3	36:w:101:LMG:H352	2.04	0.40
3:c:346:GLU:OE2	13:o:15:LYS:HA	2.21	0.40
3:c:373:LEU:HB3	3:c:378:ILE:HD11	2.03	0.40
15:u:28:ASN:OD1	15:u:28:ASN:N	2.54	0.40
16:v:123:PRO:HG3	16:v:130:TRP:CD1	2.56	0.40
4:D:161:LEU:HD13	39:H:102:DGD:HB92	2.04	0.40
16:V:81:THR:OG1	16:V:83:ASP:OD1	2.38	0.40
2:b:164:PRO:HG3	30:b:606:CLA:O1D	2.22	0.40
2:b:472:ARG:HA	2:b:479:PHE:CE2	2.56	0.40
4:d:297:PHE:HB3	11:l:38:ASN:O	2.21	0.40
30:11:315:CLA:HBC2	30:14:310:CLA:HBC1	2.02	0.40
25:12:130:ALA:HB1	30:12:303:CLA:C3B	2.52	0.40
25:13:67:HIS:HE1	30:13:303:CLA:ND	2.16	0.40
25:16:191:GLN:O	25:16:195:GLY:N	2.54	0.40
30:18:305:CLA:H161	30:18:305:CLA:H122	1.92	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	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
1	a	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
2	B	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	21	54
All	All	6884/7712 (89%)	6586 (96%)	297 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	18	142	GLY

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	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	385/405 (95%)	385 (100%)	0	100	100
2	b	385/405 (95%)	385 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	356/376 (95%)	354 (99%)	2 (1%)	78	79
3	c	356/376 (95%)	354 (99%)	2 (1%)	78	79
4	D	273/281 (97%)	273 (100%)	0	100	100
4	d	273/281 (97%)	273 (100%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	59	71
5	e	69/75 (92%)	68 (99%)	1 (1%)	59	71
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100
9	J	27/31 (87%)	27 (100%)	0	100	100
9	j	27/31 (87%)	27 (100%)	0	100	100
10	K	32/38 (84%)	32 (100%)	0	100	100
10	k	32/38 (84%)	32 (100%)	0	100	100
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	196 (100%)	0	100	100
13	o	196/201 (98%)	196 (100%)	0	100	100
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	77/77 (100%)	77 (100%)	0	100	100
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	110 (99%)	1 (1%)	70	76
20	q	111/124 (90%)	110 (99%)	1 (1%)	70	76
21	W	43/55 (78%)	42 (98%)	1 (2%)	44	64
21	w	43/55 (78%)	42 (98%)	1 (2%)	44	64
25	11	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	12	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	13	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	14	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	15	138/158 (87%)	138 (100%)	0	100	100
25	16	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	17	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	18	138/158 (87%)	138 (100%)	0	100	100
All	All	5628/6184 (91%)	5612 (100%)	16 (0%)	84	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	138	LEU
3	C	270	LEU
5	E	31	LEU
20	Q	142	LEU
21	W	45	ILE
3	c	138	LEU
3	c	270	LEU
5	e	31	LEU
20	q	142	LEU
21	w	45	ILE
25	11	91	LEU
25	12	91	LEU
25	13	91	LEU
25	14	91	LEU
25	16	128	GLU
25	17	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	92	HIS
1	A	303	ASN
2	B	87	ASN
2	B	179	GLN
2	B	457	ASN
3	C	311	GLN
3	C	325	ASN
3	C	371	ASN
3	C	416	ASN
4	D	82	ASN
4	D	193	ASN
4	D	229	ASN
4	D	291	ASN
4	D	349	ASN
11	L	9	GLN
13	O	7	ASN
13	O	109	GLN
13	O	197	GLN
13	O	208	ASN
13	O	222	GLN
15	U	29	ASN
16	V	68	ASN
17	Y	9	GLN
20	Q	105	ASN
20	Q	162	GLN
1	a	26	ASN
1	a	303	ASN
2	b	87	ASN
2	b	179	GLN
2	b	394	GLN
2	b	457	ASN
3	c	325	ASN
3	c	371	ASN
3	c	416	ASN
4	d	193	ASN
4	d	219	ASN
4	d	229	ASN
4	d	349	ASN
7	h	50	ASN
13	o	7	ASN

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Mol	Chain	Res	Type
13	o	109	GLN
13	o	197	GLN
13	o	208	ASN
13	o	222	GLN
15	u	29	ASN
16	v	68	ASN
17	y	9	GLN
17	y	33	ASN
20	q	105	ASN
20	q	162	GLN
25	11	82	ASN
25	11	161	ASN
25	12	82	ASN
25	12	161	ASN
25	13	82	ASN
25	13	83	ASN
25	13	161	ASN
25	14	82	ASN
25	14	161	ASN
25	15	82	ASN
25	15	83	ASN
25	15	96	ASN
25	15	161	ASN
25	16	82	ASN
25	16	83	ASN
25	16	161	ASN
25	16	177	ASN
25	17	82	ASN
25	17	161	ASN
25	18	82	ASN
25	18	96	ASN
25	18	161	ASN
25	18	186	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 323 ligands modelled in this entry, 2 are monoatomic - leaving 321 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	$\#\|Z\| > 2$
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	8 (13%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	8 (14%)
42	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
30	CLA	D	405	4	69,73,73	1.33	12 (17%)	83,113,113	1.47	11 (13%)
42	A86	21	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)
30	CLA	15	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	5 (8%)
30	CLA	14	310	25	49,53,73	1.50	10 (20%)	59,89,113	1.59	6 (10%)
30	CLA	c	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	12 (14%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	5 (8%)
30	CLA	14	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.37	6 (7%)
36	LMG	1	101	-	39,39,55	1.01	4 (10%)	47,47,63	1.18	4 (8%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	d	407	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
30	CLA	20	204	-	69,73,73	1.23	10 (14%)	83,113,113	1.43	9 (10%)
40	PL9	D	404	4	55,55,55	1.35	6 (10%)	68,69,69	1.49	15 (22%)
42	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
30	CLA	b	614	2	69,73,73	1.25	12 (17%)	83,113,113	1.48	8 (9%)
30	CLA	b	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.42	7 (8%)
42	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	c	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.46	12 (14%)
30	CLA	B	605	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
31	PHO	d	404	-	58,69,69	1.91	12 (20%)	56,99,99	1.77	8 (14%)
31	PHO	d	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.83	10 (17%)
30	CLA	11	304	25	49,53,73	1.51	10 (20%)	59,89,113	1.83	13 (22%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
42	A86	14	313	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
36	LMG	Q	301	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	b	613	2	69,73,73	1.34	10 (14%)	83,113,113	1.48	9 (10%)
42	A86	19	310	-	44,50,50	3.88	23 (52%)	51,76,76	7.70	16 (31%)
42	A86	13	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	C	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
42	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
30	CLA	18	310	25	69,73,73	1.27	9 (13%)	83,113,113	1.33	7 (8%)
37	LMU	12	302	25,30	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
30	CLA	20	209	30	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
30	CLA	17	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.53	8 (9%)
30	CLA	12	306	37,25	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)
30	CLA	17	308	25	69,73,73	1.33	8 (11%)	83,113,113	1.45	11 (13%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
30	CLA	12	307	25	69,73,73	1.25	11 (15%)	83,113,113	1.48	9 (10%)
30	CLA	21	301	28	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
30	CLA	b	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
30	CLA	13	309	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
30	CLA	18	312	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
30	CLA	15	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	6 (10%)
30	CLA	18	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
30	CLA	b	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
42	A86	13	301	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	14	304	25	49,53,73	1.45	11 (22%)	59,89,113	1.62	6 (10%)
42	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	17	309	25	49,53,73	1.50	11 (22%)	59,89,113	1.91	11 (18%)
30	CLA	17	301	25	69,73,73	1.29	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	13	304	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	16	301	25	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
40	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
35	LHG	b	621	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	13	303	25	49,53,73	1.45	11 (22%)	59,89,113	1.63	7 (11%)
30	CLA	19	301	-	69,73,73	1.31	11 (15%)	83,113,113	1.39	10 (12%)
30	CLA	15	303	25	69,73,73	1.22	9 (13%)	83,113,113	1.43	10 (12%)
42	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
42	A86	13	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
42	A86	17	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
41	HEM	F	102	5,6	50,50,50	1.35	4 (8%)	66,82,82	1.15	4 (6%)
42	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	b	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	15 (18%)
30	CLA	c	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	10 (12%)
41	HEM	V	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	9 (13%)
30	CLA	19	303	-	69,73,73	1.24	10 (14%)	83,113,113	1.46	8 (9%)
42	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
42	A86	19	312	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
36	LMG	w	101	-	51,51,55	0.89	4 (7%)	59,59,63	1.40	7 (11%)
30	CLA	B	613	2	69,73,73	1.33	10 (14%)	83,113,113	1.46	11 (13%)
30	CLA	17	305	25	69,73,73	1.24	11 (15%)	83,113,113	1.44	11 (13%)
30	CLA	b	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
30	CLA	b	603	2	69,73,73	1.27	11 (15%)	83,113,113	1.52	13 (15%)
30	CLA	11	308	25	49,53,73	1.48	11 (22%)	59,89,113	1.59	7 (11%)
30	CLA	19	309	-	49,53,73	1.45	9 (18%)	59,89,113	1.63	10 (16%)
42	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
42	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	B	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	B	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.42	9 (10%)
30	CLA	16	304	25	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
42	A86	14	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
39	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
30	CLA	b	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
42	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	14	308	25	49,53,73	1.45	8 (16%)	59,89,113	1.69	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	15	301	25	69,73,73	1.26	11 (15%)	83,113,113	1.52	10 (12%)
39	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
30	CLA	c	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.52	13 (15%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	C	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	11 (13%)
30	CLA	C	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.45	12 (14%)
30	CLA	W	103	-	69,73,73	1.26	7 (10%)	83,113,113	1.30	7 (8%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	C	504	3	69,73,73	1.29	11 (15%)	83,113,113	1.45	10 (12%)
30	CLA	12	310	25	49,53,73	1.47	9 (18%)	59,89,113	1.70	8 (13%)
32	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
32	BCR	Z	101	-	41,41,41	1.32	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	12	312	25	69,73,73	1.27	10 (14%)	83,113,113	1.39	6 (7%)
42	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	B	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.56	16 (19%)
38	OEX	c	501	1,3	0,14,14	-	-	-		
40	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
30	CLA	17	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.77	13 (22%)
30	CLA	21	302	-	49,53,73	1.49	9 (18%)	59,89,113	1.57	9 (15%)
30	CLA	18	306	25	49,53,73	1.47	8 (16%)	59,89,113	1.66	10 (16%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
30	CLA	16	305	25	49,53,73	1.46	9 (18%)	59,89,113	1.70	11 (18%)
30	CLA	18	307	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	7 (11%)
30	CLA	11	306	25	49,53,73	1.45	9 (18%)	59,89,113	1.71	7 (11%)
30	CLA	C	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
30	CLA	B	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
42	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
30	CLA	19	302	-	49,53,73	1.49	11 (22%)	59,89,113	1.65	10 (16%)
30	CLA	21	303	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	6 (7%)
42	A86	12	317	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	21	308	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
42	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.42	21 (41%)
36	LMG	B	620	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	c	513	3	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	16	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.62	6 (10%)
30	CLA	m	101	36,12,2	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
30	CLA	B	614	2	69,73,73	1.24	11 (15%)	83,113,113	1.46	8 (9%)
30	CLA	16	307	25	49,53,73	1.51	10 (20%)	59,89,113	1.75	9 (15%)
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
30	CLA	15	307	25	69,73,73	1.27	11 (15%)	83,113,113	1.52	12 (14%)
30	CLA	B	612	2	69,73,73	1.38	8 (11%)	83,113,113	1.67	11 (13%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
30	CLA	c	505	-	69,73,73	1.27	11 (15%)	83,113,113	1.57	10 (12%)
30	CLA	16	308	25	49,53,73	1.48	10 (20%)	59,89,113	1.57	10 (16%)
30	CLA	17	304	25	49,53,73	1.45	12 (24%)	59,89,113	1.64	9 (15%)
30	CLA	21	309	-	49,53,73	1.50	10 (20%)	59,89,113	1.54	9 (15%)
30	CLA	20	208	-	49,53,73	1.48	8 (16%)	59,89,113	1.56	8 (13%)
30	CLA	C	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.52	10 (12%)
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
30	CLA	19	304	26	49,53,73	1.47	9 (18%)	59,89,113	1.67	12 (20%)
30	CLA	14	306	25	49,53,73	1.50	10 (20%)	59,89,113	1.86	13 (22%)
42	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	d	401	-	69,73,73	1.33	9 (13%)	83,113,113	1.45	11 (13%)
32	BCR	c	520	-	41,41,41	1.27	3 (7%)	56,56,56	1.47	10 (17%)
30	CLA	z	101	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	7 (8%)
42	A86	14	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
30	CLA	c	512	3	69,73,73	1.32	11 (15%)	83,113,113	1.51	13 (15%)
30	CLA	21	307	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	6 (7%)
30	CLA	12	308	25	49,53,73	1.51	10 (20%)	59,89,113	1.85	13 (22%)
30	CLA	A	404	1	69,73,73	1.28	11 (15%)	83,113,113	1.50	9 (10%)
30	CLA	16	309	-	49,53,73	1.49	11 (22%)	59,89,113	1.48	8 (13%)
30	CLA	w	103	-	69,73,73	1.27	9 (13%)	83,113,113	1.30	7 (8%)
30	CLA	B	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
42	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.13	21 (41%)
30	CLA	13	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
42	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	15	302	25	49,53,73	1.45	8 (16%)	59,89,113	1.70	6 (10%)
30	CLA	b	607	-	69,73,73	1.27	10 (14%)	83,113,113	1.41	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	18	304	25	49,53,73	1.45	9 (18%)	59,89,113	1.65	6 (10%)
30	CLA	17	307	25	49,53,73	1.48	9 (18%)	59,89,113	1.65	13 (22%)
30	CLA	D	401	-	69,73,73	1.33	10 (14%)	83,113,113	1.45	11 (13%)
30	CLA	16	303	25	49,53,73	1.47	11 (22%)	59,89,113	1.78	10 (16%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
30	CLA	13	308	25	69,73,73	1.27	10 (14%)	83,113,113	1.45	12 (14%)
30	CLA	20	206	27	49,53,73	1.48	10 (20%)	59,89,113	1.64	7 (11%)
30	CLA	B	603	2	69,73,73	1.26	10 (14%)	83,113,113	1.52	13 (15%)
30	CLA	18	311	25	49,53,73	1.48	9 (18%)	59,89,113	1.65	9 (15%)
39	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
30	CLA	C	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.56	13 (15%)
30	CLA	13	310	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
42	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
32	BCR	B	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
31	PHO	A	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.83	10 (17%)
39	DGD	J	101	-	63,63,67	1.11	10 (15%)	77,77,81	1.56	15 (19%)
30	CLA	19	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.39	8 (9%)
30	CLA	b	605	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
30	CLA	B	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.42	9 (10%)
34	BCT	a	406	29,1	2,3,3	1.27	0	2,3,3	3.96	2 (100%)
30	CLA	20	203	30	49,53,73	1.48	9 (18%)	59,89,113	1.59	7 (11%)
30	CLA	B	601	-	69,73,73	1.25	10 (14%)	83,113,113	1.42	8 (9%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	14	305	25	69,73,73	1.22	11 (15%)	83,113,113	1.51	10 (12%)
30	CLA	C	514	3,30	69,73,73	1.26	10 (14%)	83,113,113	1.47	8 (9%)
42	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	12	305	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
30	CLA	13	305	25	49,53,73	1.51	10 (20%)	59,89,113	1.84	13 (22%)
30	CLA	12	313	25	49,53,73	1.49	11 (22%)	59,89,113	1.61	7 (11%)
30	CLA	B	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.50	13 (15%)
42	A86	11	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
36	LMG	c	519	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	13	307	25	49,53,73	1.46	9 (18%)	59,89,113	1.71	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	C	512	3	69,73,73	1.33	10 (14%)	83,113,113	1.52	11 (13%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.59	11 (17%)
30	CLA	C	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	11 (13%)
30	CLA	20	205	-	49,53,73	1.47	9 (18%)	59,89,113	1.66	12 (20%)
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
39	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.42	8 (10%)
30	CLA	21	304	-	49,53,73	1.44	9 (18%)	59,89,113	1.43	5 (8%)
30	CLA	13	306	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	15	308	25	49,53,73	1.47	10 (20%)	59,89,113	1.61	9 (15%)
30	CLA	C	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.53	11 (13%)
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	B	623	-	69,73,73	1.28	11 (15%)	83,113,113	1.50	13 (15%)
30	CLA	18	308	25	49,53,73	1.51	9 (18%)	59,89,113	1.57	6 (10%)
42	A86	14	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
42	A86	21	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	19	308	-	49,53,73	1.47	11 (22%)	59,89,113	1.59	8 (13%)
42	A86	17	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
30	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	10 (12%)
30	CLA	11	315	25	69,73,73	1.27	11 (15%)	83,113,113	1.38	6 (7%)
30	CLA	11	305	-	49,53,73	1.46	10 (20%)	59,89,113	1.54	7 (11%)
42	A86	15	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	14	307	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	7 (11%)
33	SQD	b	620	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
30	CLA	c	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
30	CLA	A	402	1	69,73,73	1.29	11 (15%)	83,113,113	1.47	9 (10%)
30	CLA	19	305	-	49,53,73	1.47	11 (22%)	59,89,113	1.54	5 (8%)
37	LMU	B	625	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
42	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	12	311	25	69,73,73	1.28	10 (14%)	83,113,113	1.44	11 (13%)
38	OEX	C	501	1,3	0,14,14	-	-	-		
42	A86	18	302	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	15	306	25	49,53,73	1.47	9 (18%)	59,89,113	1.60	6 (10%)
32	BCR	c	516	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	9 (16%)
42	A86	14	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	b	622	-	69,73,73	1.29	10 (14%)	83,113,113	1.51	13 (15%)
30	CLA	16	302	25	69,73,73	1.30	10 (14%)	83,113,113	1.79	17 (20%)
30	CLA	C	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.57	10 (12%)
30	CLA	C	519	-	69,73,73	1.28	11 (15%)	83,113,113	1.41	7 (8%)
36	LMG	m	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
42	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	19	306	-	49,53,73	1.48	11 (22%)	59,89,113	1.49	5 (8%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	w	102	21	69,73,73	1.24	11 (15%)	83,113,113	1.35	9 (10%)
30	CLA	11	307	25	69,73,73	1.28	10 (14%)	83,113,113	1.45	11 (13%)
30	CLA	18	301	25	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
42	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
42	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)
42	A86	20	212	-	44,50,50	4.17	23 (52%)	51,76,76	8.24	15 (29%)
30	CLA	18	305	25	69,73,73	1.22	10 (14%)	83,113,113	1.38	5 (6%)
42	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.34	19 (37%)
30	CLA	C	513	3	69,73,73	1.26	10 (14%)	83,113,113	1.38	7 (8%)
30	CLA	b	612	2	69,73,73	1.39	9 (13%)	83,113,113	1.66	11 (13%)
30	CLA	21	306	-	69,73,73	1.28	10 (14%)	83,113,113	1.36	7 (8%)
30	CLA	B	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.43	8 (9%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
30	CLA	Z	102	19,30	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
30	CLA	21	305	28	49,53,73	1.53	8 (16%)	59,89,113	1.62	10 (16%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
30	CLA	b	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.48	13 (15%)
30	CLA	D	402	-	69,73,73	1.27	10 (14%)	83,113,113	1.42	7 (8%)
31	PHO	D	403	-	58,69,69	1.91	12 (20%)	56,99,99	1.77	8 (14%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	b	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	10 (12%)
30	CLA	M	101	36,12,2	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
42	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	12	314	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	5 (8%)
30	CLA	18	309	25	69,73,73	1.32	10 (14%)	83,113,113	1.49	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	a	403	1	69,73,73	1.28	10 (14%)	83,113,113	1.50	8 (9%)
30	CLA	b	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
30	CLA	d	406	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	12 (14%)
30	CLA	11	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
30	CLA	11	301	25	69,73,73	1.28	11 (15%)	83,113,113	1.58	8 (9%)
30	CLA	11	302	25	49,53,73	1.45	11 (22%)	59,89,113	1.60	7 (11%)
42	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
42	A86	11	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	W	102	21	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
42	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
42	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
32	BCR	f	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
42	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	14	311	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
42	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	D	406	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
30	CLA	d	402	-	69,73,73	1.28	10 (14%)	83,113,113	1.42	7 (8%)
30	CLA	11	303	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	8 (9%)
36	LMG	b	618	-	51,51,55	0.88	4 (7%)	59,59,63	1.43	9 (15%)
42	A86	14	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
41	HEM	f	102	5,6	50,50,50	1.35	4 (8%)	66,82,82	1.16	4 (6%)
34	BCT	A	407	29,1	2,3,3	1.26	0	2,3,3	3.94	2 (100%)
39	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
36	LMG	d	410	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
30	CLA	14	309	25	69,73,73	1.30	11 (15%)	83,113,113	1.44	12 (14%)
30	CLA	15	304	25	49,53,73	1.48	8 (16%)	59,89,113	1.61	11 (18%)
30	CLA	C	520	-	69,73,73	1.25	10 (14%)	83,113,113	1.57	12 (14%)
42	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	B	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
30	CLA	c	504	3	69,73,73	1.28	11 (15%)	83,113,113	1.44	10 (12%)
41	HEM	v	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	7 (10%)
30	CLA	c	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.54	13 (15%)
42	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
42	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	14	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
42	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	12	309	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
39	DGD	C	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.60	15 (19%)
42	A86	17	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	20	207	-	49,53,73	1.49	11 (22%)	59,89,113	1.59	8 (13%)
40	PL9	d	408	-	55,55,55	2.32	14 (25%)	68,69,69	1.48	14 (20%)
30	CLA	20	202	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	9 (10%)
42	A86	16	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
39	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	c	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
30	CLA	12	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.38	6 (7%)
30	CLA	17	310	-	49,53,73	1.46	10 (20%)	59,89,113	1.48	5 (8%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	7 (12%)
30	CLA	c	514	3	69,73,73	1.27	11 (15%)	83,113,113	1.46	8 (9%)
30	CLA	a	402	1	69,73,73	1.30	11 (15%)	83,113,113	1.46	8 (9%)
42	A86	19	311	-	44,50,50	4.09	21 (47%)	51,76,76	7.17	19 (37%)
36	LMG	12	301	-	39,39,55	1.00	4 (10%)	47,47,63	1.21	5 (10%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.37	6 (10%)

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
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
42	A86	17	315	-	-	13/34/90/90	0/3/3/3
30	CLA	D	405	4	-	8/39/115/115	-
42	A86	21	312	-	-	7/34/90/90	0/3/3/3
30	CLA	15	305	-	-	10/15/91/115	-
30	CLA	14	310	25	-	8/15/91/115	-
30	CLA	c	507	3	-	19/39/115/115	-
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
30	CLA	14	302	25	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	1	101	-	-	14/34/54/70	0/1/1/1
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
35	LHG	d	409	-	-	29/53/53/53	-
30	CLA	d	407	4	-	6/39/115/115	-
30	CLA	20	204	-	-	15/39/115/115	-
40	PL9	D	404	4	-	17/53/73/73	0/1/1/1
42	A86	21	313	-	-	16/34/90/90	0/3/3/3
30	CLA	b	614	2	-	8/39/115/115	-
30	CLA	b	601	-	-	20/39/115/115	-
42	A86	12	318	-	-	10/34/90/90	0/3/3/3
30	CLA	c	511	3	-	12/39/115/115	-
30	CLA	B	605	2	-	19/39/115/115	-
42	A86	15	311	-	-	3/34/90/90	0/3/3/3
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
30	CLA	11	304	25	-	9/15/91/115	-
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1
42	A86	14	313	-	-	3/34/90/90	0/3/3/3
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
30	CLA	b	613	2	-	8/39/115/115	-
42	A86	19	310	-	-	11/34/90/90	0/3/3/3
42	A86	13	315	-	-	16/34/90/90	0/3/3/3
30	CLA	C	510	3	-	12/39/115/115	-
35	LHG	L	101	-	-	29/53/53/53	-
42	A86	11	313	-	-	10/34/90/90	0/3/3/3
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
30	CLA	18	310	25	-	12/39/115/115	-
37	LMU	12	302	25,30	-	7/18/58/61	0/2/2/2
30	CLA	20	209	30	-	13/39/115/115	-
30	CLA	17	303	25	-	15/39/115/115	-
30	CLA	12	306	37,25	-	4/15/91/115	-
30	CLA	17	308	25	-	19/39/115/115	-
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
30	CLA	12	307	25	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	21	301	28	-	16/39/115/115	-
30	CLA	b	610	-	-	16/39/115/115	-
30	CLA	13	309	25	-	8/15/91/115	-
30	CLA	18	312	-	-	6/15/91/115	-
30	CLA	15	309	-	-	6/15/91/115	-
30	CLA	18	303	25	-	16/39/115/115	-
30	CLA	b	615	2	-	13/39/115/115	-
42	A86	13	301	-	-	15/34/90/90	0/3/3/3
30	CLA	14	304	25	-	4/15/91/115	-
42	A86	13	312	-	-	3/34/90/90	0/3/3/3
30	CLA	17	309	25	-	4/15/91/115	-
30	CLA	17	301	25	-	16/39/115/115	-
30	CLA	13	304	25	-	15/39/115/115	-
30	CLA	16	301	25	-	12/39/115/115	-
40	PL9	D	407	-	-	13/53/73/73	0/1/1/1
35	LHG	b	621	-	-	20/53/53/53	-
30	CLA	13	303	25	-	5/15/91/115	-
30	CLA	19	301	-	-	14/39/115/115	-
30	CLA	15	303	25	-	17/39/115/115	-
42	A86	20	213	-	-	12/34/90/90	0/3/3/3
42	A86	13	313	-	-	9/34/90/90	0/3/3/3
42	A86	17	312	-	-	3/34/90/90	0/3/3/3
41	HEM	F	102	5,6	-	7/14/54/54	-
42	A86	15	313	-	-	10/34/90/90	0/3/3/3
30	CLA	b	604	2	-	14/39/115/115	-
30	CLA	c	509	3	-	12/39/115/115	-
41	HEM	V	201	16	-	1/14/54/54	-
30	CLA	19	303	-	-	17/39/115/115	-
42	A86	16	310	-	-	12/34/90/90	0/3/3/3
42	A86	19	312	-	-	8/34/90/90	0/3/3/3
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	B	613	2	-	8/39/115/115	-
30	CLA	17	305	25	-	21/39/115/115	-
30	CLA	b	611	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	603	2	-	12/39/115/115	-
30	CLA	11	308	25	-	8/15/91/115	-
30	CLA	19	309	-	-	10/15/91/115	-
42	A86	15	310	-	-	8/34/90/90	0/3/3/3
42	A86	12	316	-	-	3/34/90/90	0/3/3/3
30	CLA	B	608	2	-	9/39/115/115	-
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	CLA	B	607	-	-	12/39/115/115	-
30	CLA	16	304	25	-	17/39/115/115	-
42	A86	14	312	-	-	8/34/90/90	0/3/3/3
39	DGD	h	102	-	-	24/51/91/95	0/2/2/2
30	CLA	b	608	2	-	9/39/115/115	-
42	A86	11	312	-	-	8/34/90/90	0/3/3/3
30	CLA	14	308	25	-	10/15/91/115	-
30	CLA	15	301	25	-	12/39/115/115	-
39	DGD	C	517	-	-	22/51/91/95	0/2/2/2
30	CLA	c	502	3	-	14/39/115/115	-
35	LHG	B	622	-	-	20/53/53/53	-
30	CLA	C	506	3	-	18/39/115/115	-
30	CLA	C	511	3	-	12/39/115/115	-
30	CLA	W	103	-	-	21/39/115/115	-
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
30	CLA	C	504	3	-	19/39/115/115	-
30	CLA	12	310	25	-	10/15/91/115	-
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
30	CLA	12	312	25	-	13/39/115/115	-
42	A86	11	316	-	-	16/34/90/90	0/3/3/3
30	CLA	B	604	2	-	14/39/115/115	-
40	PL9	d	405	4	-	17/53/73/73	0/1/1/1
30	CLA	17	306	25	-	8/15/91/115	-
30	CLA	21	302	-	-	9/15/91/115	-
30	CLA	18	306	25	-	9/15/91/115	-
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	16	305	25	-	8/15/91/115	-
30	CLA	18	307	-	-	8/15/91/115	-
30	CLA	11	306	25	-	10/15/91/115	-
30	CLA	C	503	3	-	13/39/115/115	-
30	CLA	B	610	-	-	16/39/115/115	-
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
42	A86	20	201	-	-	12/34/90/90	0/3/3/3
30	CLA	19	302	-	-	4/15/91/115	-
30	CLA	21	303	-	-	19/39/115/115	-
42	A86	12	317	-	-	9/34/90/90	0/3/3/3
30	CLA	21	308	-	-	10/15/91/115	-
42	A86	21	310	-	-	9/34/90/90	0/3/3/3
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
30	CLA	c	513	3	-	18/39/115/115	-
30	CLA	16	306	25	-	9/15/91/115	-
30	CLA	m	101	36,12,2	-	21/39/115/115	-
30	CLA	B	614	2	-	8/39/115/115	-
30	CLA	16	307	25	-	9/15/91/115	-
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
30	CLA	15	307	25	-	13/39/115/115	-
30	CLA	B	612	2	-	13/39/115/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1
30	CLA	c	505	-	-	19/39/115/115	-
30	CLA	16	308	25	-	9/15/91/115	-
30	CLA	17	304	25	-	6/15/91/115	-
30	CLA	21	309	-	-	8/15/91/115	-
30	CLA	20	208	-	-	8/15/91/115	-
30	CLA	C	509	3	-	12/39/115/115	-
35	LHG	a	407	-	-	23/50/50/53	-
30	CLA	19	304	26	-	11/15/91/115	-
30	CLA	14	306	25	-	9/15/91/115	-
42	A86	12	319	-	-	7/34/90/90	0/3/3/3
30	CLA	d	401	-	-	14/39/115/115	-
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	z	101	-	-	23/39/115/115	-
42	A86	14	316	-	-	7/34/90/90	0/3/3/3
30	CLA	c	512	3	-	10/39/115/115	-
30	CLA	21	307	-	-	13/39/115/115	-
30	CLA	12	308	25	-	9/15/91/115	-
30	CLA	A	404	1	-	12/39/115/115	-
30	CLA	16	309	-	-	7/15/91/115	-
30	CLA	w	103	-	-	21/39/115/115	-
30	CLA	B	611	2	-	14/39/115/115	-
42	A86	17	302	-	-	16/34/90/90	1/3/3/3
30	CLA	13	302	25	-	14/39/115/115	-
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
42	A86	18	314	-	-	3/34/90/90	0/3/3/3
30	CLA	15	302	25	-	10/15/91/115	-
30	CLA	b	607	-	-	12/39/115/115	-
30	CLA	18	304	25	-	5/15/91/115	-
30	CLA	17	307	25	-	9/15/91/115	-
30	CLA	D	401	-	-	14/39/115/115	-
30	CLA	16	303	25	-	6/15/91/115	-
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
30	CLA	13	308	25	-	16/39/115/115	-
30	CLA	20	206	27	-	9/15/91/115	-
30	CLA	B	603	2	-	12/39/115/115	-
30	CLA	18	311	25	-	10/15/91/115	-
39	DGD	c	518	-	-	22/51/91/95	0/2/2/2
30	CLA	C	508	-	-	18/39/115/115	-
30	CLA	13	310	-	-	8/15/91/115	-
35	LHG	A	408	-	-	23/50/50/53	-
42	A86	15	315	-	-	15/34/90/90	0/3/3/3
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
39	DGD	J	101	-	-	15/51/91/95	0/2/2/2
30	CLA	19	307	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	605	2	-	19/39/115/115	-
30	CLA	B	602	2	-	15/39/115/115	-
30	CLA	20	203	30	-	7/15/91/115	-
30	CLA	B	601	-	-	20/39/115/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
30	CLA	14	305	25	-	15/39/115/115	-
30	CLA	C	514	3,30	-	13/39/115/115	-
42	A86	20	211	-	-	8/34/90/90	0/3/3/3
30	CLA	12	305	25	-	13/39/115/115	-
30	CLA	13	305	25	-	9/15/91/115	-
30	CLA	12	313	25	-	8/15/91/115	-
30	CLA	B	606	2	-	7/39/115/115	-
42	A86	11	314	-	-	7/34/90/90	0/3/3/3
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
30	CLA	13	307	25	-	10/15/91/115	-
30	CLA	C	512	3	-	10/39/115/115	-
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
30	CLA	C	507	3	-	19/39/115/115	-
30	CLA	20	205	-	-	11/15/91/115	-
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
39	DGD	H	102	-	-	24/51/91/95	0/2/2/2
30	CLA	21	304	-	-	8/15/91/115	-
30	CLA	13	306	-	-	10/15/91/115	-
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
30	CLA	15	308	25	-	8/15/91/115	-
30	CLA	C	502	3	-	14/39/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
30	CLA	B	623	-	-	17/39/115/115	-
30	CLA	18	308	25	-	10/15/91/115	-
42	A86	14	314	-	-	8/34/90/90	0/3/3/3
42	A86	21	311	-	-	8/34/90/90	0/3/3/3
30	CLA	19	308	-	-	3/15/91/115	-
42	A86	17	313	-	-	9/34/90/90	0/3/3/3
30	CLA	c	506	3	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	11	315	25	-	13/39/115/115	-
30	CLA	11	305	-	-	10/15/91/115	-
42	A86	15	312	-	-	8/34/90/90	0/3/3/3
30	CLA	14	307	-	-	10/15/91/115	-
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
30	CLA	c	510	3	-	12/39/115/115	-
30	CLA	A	402	1	-	7/39/115/115	-
30	CLA	19	305	-	-	9/15/91/115	-
37	LMU	B	625	-	-	7/18/58/61	0/2/2/2
42	A86	21	314	-	-	12/34/90/90	0/3/3/3
30	CLA	12	311	25	-	16/39/115/115	-
42	A86	18	302	-	-	15/34/90/90	0/3/3/3
30	CLA	15	306	25	-	10/15/91/115	-
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
42	A86	14	315	-	-	10/34/90/90	0/3/3/3
30	CLA	b	622	-	-	17/39/115/115	-
30	CLA	16	302	25	-	17/39/115/115	-
30	CLA	C	505	-	-	19/39/115/115	-
30	CLA	C	519	-	-	23/39/115/115	-
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
42	A86	18	315	-	-	10/34/90/90	0/3/3/3
30	CLA	19	306	-	-	10/15/91/115	-
35	LHG	L	102	-	-	22/53/53/53	-
30	CLA	w	102	21	-	16/39/115/115	-
30	CLA	11	307	25	-	16/39/115/115	-
30	CLA	18	301	25	-	13/39/115/115	-
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
42	A86	11	310	-	-	8/34/90/90	0/3/3/3
42	A86	12	304	-	-	16/34/90/90	0/3/3/3
42	A86	20	212	-	-	11/34/90/90	0/3/3/3
30	CLA	18	305	25	-	21/39/115/115	-
42	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	C	513	3	-	18/39/115/115	-
30	CLA	b	612	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	21	306	-	-	16/39/115/115	-
30	CLA	B	609	2	-	10/39/115/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
30	CLA	Z	102	19,30	-	17/39/115/115	-
30	CLA	21	305	28	-	11/15/91/115	-
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
30	CLA	b	606	2	-	7/39/115/115	-
30	CLA	D	402	-	-	15/39/115/115	-
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
35	LHG	l	102	-	-	22/53/53/53	-
30	CLA	b	602	2	-	15/39/115/115	-
30	CLA	M	101	36,12,2	-	21/39/115/115	-
42	A86	18	313	-	-	8/34/90/90	0/3/3/3
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
30	CLA	12	314	-	-	8/15/91/115	-
30	CLA	18	309	25	-	17/39/115/115	-
30	CLA	a	403	1	-	12/39/115/115	-
30	CLA	b	609	2	-	10/39/115/115	-
30	CLA	d	406	4	-	8/39/115/115	-
30	CLA	11	309	-	-	8/15/91/115	-
30	CLA	11	301	25	-	13/39/115/115	-
30	CLA	11	302	25	-	5/15/91/115	-
42	A86	15	316	-	-	16/34/90/90	0/3/3/3
42	A86	11	311	-	-	3/34/90/90	0/3/3/3
30	CLA	W	102	21	-	16/39/115/115	-
42	A86	13	314	-	-	10/34/90/90	0/3/3/3
42	A86	16	312	-	-	8/34/90/90	0/3/3/3
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
42	A86	20	210	-	-	14/34/90/90	0/3/3/3
30	CLA	14	311	-	-	8/15/91/115	-
42	A86	16	313	-	-	7/34/90/90	0/3/3/3
30	CLA	D	406	4	-	6/39/115/115	-
30	CLA	d	402	-	-	15/39/115/115	-
30	CLA	11	303	25	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
42	A86	14	301	-	-	7/34/90/90	0/3/3/3
41	HEM	f	102	5,6	-	7/14/54/54	-
39	DGD	c	517	-	-	19/51/91/95	0/2/2/2
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
30	CLA	14	309	25	-	16/39/115/115	-
30	CLA	15	304	25	-	7/15/91/115	-
30	CLA	C	520	-	-	16/39/115/115	-
42	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	B	615	2	-	13/39/115/115	-
30	CLA	c	504	3	-	19/39/115/115	-
41	HEM	v	201	16	-	1/14/54/54	-
30	CLA	c	508	-	-	18/39/115/115	-
42	A86	13	311	-	-	8/34/90/90	0/3/3/3
42	A86	12	315	-	-	8/34/90/90	0/3/3/3
30	CLA	14	303	25	-	14/39/115/115	-
42	A86	15	314	-	-	7/34/90/90	0/3/3/3
30	CLA	12	309	-	-	10/15/91/115	-
39	DGD	C	516	-	-	19/51/91/95	0/2/2/2
42	A86	17	314	-	-	10/34/90/90	0/3/3/3
30	CLA	20	207	-	-	9/15/91/115	-
40	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	20	202	-	-	19/39/115/115	-
42	A86	16	311	-	-	3/34/90/90	0/3/3/3
39	DGD	j	101	-	-	15/51/91/95	0/2/2/2
30	CLA	c	503	3	-	13/39/115/115	-
30	CLA	12	303	25	-	13/39/115/115	-
30	CLA	17	310	-	-	9/15/91/115	-
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
30	CLA	c	514	3	-	13/39/115/115	-
30	CLA	a	402	1	-	7/39/115/115	-
42	A86	19	311	-	-	17/34/90/90	0/3/3/3
36	LMG	12	301	-	-	17/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2

All (3538) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	311	A86	C14-C13	14.34	1.68	1.51
42	11	313	A86	C14-C13	14.10	1.68	1.51
42	12	318	A86	C14-C13	14.06	1.68	1.51
42	13	314	A86	C14-C13	14.04	1.68	1.51
42	18	315	A86	C14-C13	14.01	1.68	1.51
42	15	313	A86	C14-C13	14.01	1.68	1.51
42	17	314	A86	C14-C13	13.97	1.68	1.51
42	14	315	A86	C14-C13	13.96	1.68	1.51
42	16	312	A86	C14-C13	13.94	1.68	1.51
42	17	313	A86	C14-C13	13.94	1.68	1.51
42	13	313	A86	C14-C13	13.93	1.68	1.51
42	12	317	A86	C14-C13	13.92	1.68	1.51
42	15	312	A86	C14-C13	13.91	1.68	1.51
42	20	212	A86	C14-C13	13.90	1.68	1.51
42	14	314	A86	C14-C13	13.90	1.68	1.51
42	14	316	A86	C14-C13	13.86	1.68	1.51
42	17	316	A86	C14-C13	13.86	1.68	1.51
42	11	314	A86	C14-C13	13.85	1.68	1.51
42	15	314	A86	C14-C13	13.85	1.68	1.51
42	11	312	A86	C14-C13	13.85	1.68	1.51
42	16	313	A86	C14-C13	13.85	1.68	1.51
42	12	319	A86	C14-C13	13.84	1.68	1.51
42	14	301	A86	C14-C13	13.84	1.68	1.51
42	14	312	A86	C14-C13	13.81	1.67	1.51
42	11	310	A86	C14-C13	13.80	1.67	1.51
42	18	313	A86	C14-C13	13.80	1.67	1.51
42	13	311	A86	C14-C13	13.77	1.67	1.51
42	13	315	A86	C14-C13	13.76	1.67	1.51
42	15	310	A86	C14-C13	13.76	1.67	1.51
42	18	302	A86	C14-C13	13.75	1.67	1.51
42	15	315	A86	C14-C13	13.74	1.67	1.51
42	12	315	A86	C14-C13	13.73	1.67	1.51
42	18	314	A86	C14-C13	13.73	1.67	1.51
42	20	210	A86	C14-C13	13.71	1.67	1.51
42	12	304	A86	C14-C13	13.71	1.67	1.51
42	16	311	A86	C14-C13	13.70	1.67	1.51
42	12	316	A86	C14-C13	13.69	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	316	A86	C14-C13	13.67	1.67	1.51
42	17	312	A86	C14-C13	13.67	1.67	1.51
42	13	301	A86	C14-C13	13.66	1.67	1.51
42	15	316	A86	C14-C13	13.66	1.67	1.51
42	17	315	A86	C14-C13	13.64	1.67	1.51
42	14	313	A86	C14-C13	13.63	1.67	1.51
42	13	312	A86	C14-C13	13.62	1.67	1.51
42	15	311	A86	C14-C13	13.58	1.67	1.51
42	11	311	A86	C14-C13	13.56	1.67	1.51
42	20	213	A86	C14-C13	13.51	1.67	1.51
42	21	314	A86	C14-C13	13.51	1.67	1.51
42	16	310	A86	C14-C13	13.44	1.67	1.51
42	17	311	A86	C14-C13	13.33	1.67	1.51
42	19	312	A86	C14-C13	13.24	1.67	1.51
42	17	302	A86	C14-C13	13.12	1.67	1.51
42	21	311	A86	C14-C13	13.03	1.67	1.51
42	20	211	A86	C14-C13	12.94	1.66	1.51
42	21	313	A86	C14-C13	12.93	1.66	1.51
42	21	312	A86	C14-C13	12.92	1.66	1.51
42	19	310	A86	C14-C13	12.89	1.66	1.51
42	21	310	A86	C14-C13	12.74	1.66	1.51
42	20	201	A86	C14-C13	11.39	1.65	1.51
42	19	311	A86	C30-C29	9.23	1.47	1.32
42	20	212	A86	C30-C29	9.23	1.47	1.32
42	19	312	A86	C30-C29	8.92	1.46	1.32
42	15	315	A86	C30-C29	8.91	1.46	1.32
42	11	316	A86	C30-C29	8.89	1.46	1.32
42	13	301	A86	C30-C29	8.87	1.46	1.32
42	12	304	A86	C30-C29	8.86	1.46	1.32
42	13	315	A86	C30-C29	8.86	1.46	1.32
42	15	316	A86	C30-C29	8.85	1.46	1.32
42	18	302	A86	C30-C29	8.82	1.46	1.32
42	17	315	A86	C30-C29	8.80	1.46	1.32
42	21	310	A86	C30-C29	8.80	1.46	1.32
42	20	201	A86	C30-C29	8.79	1.46	1.32
42	17	311	A86	C30-C29	8.77	1.46	1.32
42	20	210	A86	C30-C29	8.75	1.46	1.32
42	17	312	A86	C30-C29	8.73	1.46	1.32
42	14	314	A86	C30-C29	8.71	1.46	1.32
42	13	312	A86	C30-C29	8.71	1.46	1.32
42	21	313	A86	C30-C29	8.70	1.46	1.32
42	16	312	A86	C30-C29	8.69	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	12	317	A86	C30-C29	8.69	1.46	1.32
42	20	213	A86	C30-C29	8.68	1.46	1.32
42	15	312	A86	C30-C29	8.67	1.46	1.32
42	11	312	A86	C30-C29	8.67	1.46	1.32
42	18	314	A86	C30-C29	8.67	1.46	1.32
42	17	313	A86	C30-C29	8.66	1.46	1.32
42	15	311	A86	C30-C29	8.66	1.46	1.32
42	21	314	A86	C30-C29	8.66	1.46	1.32
42	11	311	A86	C30-C29	8.66	1.46	1.32
42	17	302	A86	C30-C29	8.65	1.46	1.32
42	12	316	A86	C30-C29	8.64	1.46	1.32
42	20	211	A86	C30-C29	8.63	1.46	1.32
42	13	313	A86	C30-C29	8.62	1.46	1.32
42	14	313	A86	C30-C29	8.62	1.46	1.32
42	21	311	A86	C30-C29	8.60	1.46	1.32
42	15	313	A86	C30-C29	8.59	1.46	1.32
42	18	315	A86	C30-C29	8.58	1.46	1.32
42	12	318	A86	C30-C29	8.57	1.46	1.32
42	17	314	A86	C30-C29	8.57	1.46	1.32
42	16	311	A86	C30-C29	8.57	1.46	1.32
42	16	310	A86	C30-C29	8.57	1.46	1.32
42	14	315	A86	C30-C29	8.54	1.46	1.32
42	13	314	A86	C30-C29	8.53	1.46	1.32
42	14	312	A86	C30-C29	8.52	1.46	1.32
42	18	313	A86	C30-C29	8.52	1.46	1.32
42	11	313	A86	C30-C29	8.52	1.46	1.32
42	19	310	A86	C30-C29	8.52	1.46	1.32
42	12	315	A86	C30-C29	8.49	1.46	1.32
42	11	310	A86	C30-C29	8.48	1.46	1.32
42	13	311	A86	C30-C29	8.45	1.46	1.32
42	15	310	A86	C30-C29	8.44	1.46	1.32
31	d	404	PHO	C1B-C2B	8.38	1.48	1.39
42	17	316	A86	C30-C29	8.37	1.45	1.32
42	14	301	A86	C30-C29	8.35	1.45	1.32
42	14	316	A86	C30-C29	8.32	1.45	1.32
31	d	403	PHO	C1B-C2B	8.32	1.48	1.39
31	D	403	PHO	C1B-C2B	8.32	1.48	1.39
42	16	313	A86	C30-C29	8.30	1.45	1.32
42	15	314	A86	C30-C29	8.30	1.45	1.32
42	12	319	A86	C30-C29	8.30	1.45	1.32
42	21	312	A86	C30-C29	8.29	1.45	1.32
31	A	403	PHO	C1B-C2B	8.29	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	314	A86	C30-C29	8.29	1.45	1.32
40	D	407	PL9	C7-C3	-7.79	1.43	1.51
42	20	201	A86	C4-C5	7.72	1.67	1.43
42	20	201	A86	C8-C6	7.62	1.62	1.45
40	d	408	PL9	C7-C3	-7.59	1.43	1.51
42	20	212	A86	C4-C5	7.57	1.66	1.43
42	19	311	A86	C4-C5	7.55	1.66	1.43
42	20	210	A86	C4-C5	7.53	1.66	1.43
42	20	212	A86	C8-C6	7.52	1.62	1.45
42	17	315	A86	C4-C5	7.51	1.66	1.43
42	13	315	A86	C4-C5	7.50	1.66	1.43
42	15	315	A86	C4-C5	7.49	1.66	1.43
42	12	304	A86	C4-C5	7.49	1.66	1.43
42	13	301	A86	C4-C5	7.49	1.66	1.43
42	15	316	A86	C4-C5	7.48	1.66	1.43
42	19	312	A86	C4-C5	7.48	1.66	1.43
42	11	316	A86	C4-C5	7.47	1.66	1.43
42	12	304	A86	C8-C6	7.46	1.62	1.45
42	18	302	A86	C4-C5	7.46	1.66	1.43
42	11	316	A86	C8-C6	7.43	1.61	1.45
42	15	315	A86	C8-C6	7.43	1.61	1.45
42	13	315	A86	C8-C6	7.42	1.61	1.45
42	17	302	A86	C4-C5	7.42	1.66	1.43
42	16	312	A86	C4-C5	7.42	1.66	1.43
42	15	316	A86	C8-C6	7.41	1.61	1.45
42	13	313	A86	C4-C5	7.41	1.66	1.43
42	14	314	A86	C4-C5	7.40	1.66	1.43
42	20	213	A86	C4-C5	7.40	1.66	1.43
42	21	314	A86	C4-C5	7.40	1.66	1.43
42	17	313	A86	C4-C5	7.39	1.66	1.43
42	18	302	A86	C8-C6	7.39	1.61	1.45
42	13	301	A86	C8-C6	7.39	1.61	1.45
42	12	317	A86	C4-C5	7.39	1.66	1.43
42	19	312	A86	C8-C6	7.38	1.61	1.45
42	15	312	A86	C4-C5	7.38	1.66	1.43
42	17	311	A86	C4-C5	7.38	1.66	1.43
42	11	312	A86	C4-C5	7.38	1.66	1.43
42	16	310	A86	C4-C5	7.36	1.66	1.43
42	20	211	A86	C4-C5	7.36	1.66	1.43
42	21	310	A86	C4-C5	7.35	1.66	1.43
42	11	314	A86	C4-C5	7.33	1.66	1.43
42	21	311	A86	C4-C5	7.32	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	301	A86	C4-C5	7.32	1.66	1.43
42	18	314	A86	C4-C5	7.32	1.66	1.43
42	16	311	A86	C4-C5	7.32	1.66	1.43
42	18	315	A86	C4-C5	7.31	1.66	1.43
42	17	314	A86	C4-C5	7.31	1.66	1.43
42	17	315	A86	C8-C6	7.31	1.61	1.45
42	16	313	A86	C4-C5	7.31	1.66	1.43
42	13	312	A86	C4-C5	7.31	1.66	1.43
42	15	311	A86	C4-C5	7.31	1.66	1.43
42	11	313	A86	C4-C5	7.30	1.66	1.43
42	14	315	A86	C4-C5	7.30	1.66	1.43
42	13	314	A86	C4-C5	7.29	1.66	1.43
42	19	310	A86	C4-C5	7.29	1.66	1.43
42	11	311	A86	C4-C5	7.29	1.66	1.43
42	15	313	A86	C4-C5	7.29	1.66	1.43
42	15	314	A86	C4-C5	7.29	1.66	1.43
42	12	319	A86	C4-C5	7.29	1.66	1.43
42	12	318	A86	C4-C5	7.29	1.66	1.43
42	17	312	A86	C4-C5	7.29	1.66	1.43
42	14	316	A86	C4-C5	7.28	1.66	1.43
42	18	313	A86	C4-C5	7.28	1.66	1.43
42	14	313	A86	C4-C5	7.28	1.66	1.43
42	17	313	A86	C8-C6	7.28	1.61	1.45
42	17	315	A86	C19-C20	7.28	1.62	1.52
42	12	316	A86	C4-C5	7.28	1.66	1.43
42	17	302	A86	C8-C6	7.28	1.61	1.45
42	17	316	A86	C4-C5	7.27	1.66	1.43
42	17	311	A86	C8-C6	7.27	1.61	1.45
42	21	313	A86	C4-C5	7.26	1.65	1.43
42	13	313	A86	C8-C6	7.26	1.61	1.45
42	14	314	A86	C8-C6	7.26	1.61	1.45
42	15	312	A86	C8-C6	7.26	1.61	1.45
42	14	312	A86	C4-C5	7.25	1.65	1.43
42	16	312	A86	C8-C6	7.25	1.61	1.45
42	15	310	A86	C4-C5	7.25	1.65	1.43
42	12	315	A86	C4-C5	7.24	1.65	1.43
42	12	317	A86	C8-C6	7.24	1.61	1.45
42	11	310	A86	C4-C5	7.24	1.65	1.43
42	19	311	A86	C8-C6	7.23	1.61	1.45
42	20	210	A86	C8-C6	7.23	1.61	1.45
42	11	312	A86	C8-C6	7.23	1.61	1.45
42	13	311	A86	C4-C5	7.23	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	21	312	A86	C4-C5	7.22	1.65	1.43
42	21	314	A86	C8-C6	7.17	1.61	1.45
42	14	315	A86	C8-C6	7.16	1.61	1.45
42	20	213	A86	C8-C6	7.15	1.61	1.45
42	18	315	A86	C8-C6	7.15	1.61	1.45
42	20	210	A86	C19-C20	7.14	1.62	1.52
42	15	313	A86	C8-C6	7.14	1.61	1.45
42	18	315	A86	C19-C20	7.13	1.62	1.52
42	15	313	A86	C19-C20	7.13	1.62	1.52
42	20	212	A86	C19-C20	7.12	1.62	1.52
42	14	315	A86	C19-C20	7.11	1.62	1.52
42	13	314	A86	C19-C20	7.11	1.62	1.52
42	11	313	A86	C8-C6	7.10	1.61	1.45
42	11	313	A86	C19-C20	7.10	1.62	1.52
42	21	312	A86	C8-C6	7.09	1.61	1.45
42	12	318	A86	C19-C20	7.09	1.62	1.52
42	17	314	A86	C8-C6	7.09	1.61	1.45
42	13	314	A86	C8-C6	7.08	1.61	1.45
42	17	314	A86	C19-C20	7.08	1.62	1.52
42	16	311	A86	C8-C6	7.08	1.61	1.45
42	12	318	A86	C8-C6	7.07	1.61	1.45
42	17	311	A86	C19-C20	7.07	1.62	1.52
42	11	311	A86	C8-C6	7.06	1.61	1.45
42	21	313	A86	C8-C6	7.05	1.61	1.45
42	17	312	A86	C8-C6	7.05	1.61	1.45
42	12	316	A86	C8-C6	7.04	1.61	1.45
42	13	312	A86	C8-C6	7.04	1.61	1.45
40	d	408	PL9	C3-C4	-7.04	1.37	1.49
42	15	311	A86	C8-C6	7.02	1.61	1.45
42	16	310	A86	C8-C6	7.02	1.61	1.45
42	21	310	A86	C8-C6	7.01	1.61	1.45
42	14	316	A86	C8-C6	7.01	1.61	1.45
42	14	313	A86	C8-C6	7.00	1.61	1.45
42	16	313	A86	C8-C6	7.00	1.61	1.45
42	15	314	A86	C8-C6	7.00	1.61	1.45
42	11	314	A86	C8-C6	6.97	1.60	1.45
42	20	211	A86	C8-C6	6.96	1.60	1.45
42	14	301	A86	C8-C6	6.96	1.60	1.45
42	17	316	A86	C8-C6	6.96	1.60	1.45
42	12	319	A86	C8-C6	6.95	1.60	1.45
40	D	407	PL9	C3-C4	-6.95	1.38	1.49
42	15	310	A86	C8-C6	6.94	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	18	314	A86	C8-C6	6.94	1.60	1.45
42	13	311	A86	C8-C6	6.94	1.60	1.45
42	21	311	A86	C8-C6	6.93	1.60	1.45
42	11	310	A86	C8-C6	6.92	1.60	1.45
42	19	310	A86	C8-C6	6.91	1.60	1.45
42	18	313	A86	C19-C20	6.91	1.61	1.52
42	20	201	A86	C19-C20	6.91	1.61	1.52
42	15	311	A86	C19-C20	6.90	1.61	1.52
42	20	212	A86	C25-C26	6.89	1.64	1.43
42	12	315	A86	C8-C6	6.88	1.60	1.45
42	20	201	A86	C25-C26	6.88	1.64	1.43
42	15	310	A86	C19-C20	6.87	1.61	1.52
42	14	312	A86	C8-C6	6.87	1.60	1.45
42	12	316	A86	C19-C20	6.86	1.61	1.52
42	18	313	A86	C8-C6	6.85	1.60	1.45
42	11	311	A86	C19-C20	6.85	1.61	1.52
42	16	310	A86	C19-C20	6.84	1.61	1.52
42	17	312	A86	C25-C26	6.83	1.64	1.43
42	14	312	A86	C19-C20	6.82	1.61	1.52
42	12	315	A86	C19-C20	6.82	1.61	1.52
42	13	312	A86	C25-C26	6.82	1.64	1.43
42	13	311	A86	C19-C20	6.82	1.61	1.52
42	11	311	A86	C25-C26	6.81	1.64	1.43
42	17	312	A86	C19-C20	6.81	1.61	1.52
42	16	311	A86	C19-C20	6.81	1.61	1.52
42	16	311	A86	C25-C26	6.80	1.64	1.43
42	11	310	A86	C19-C20	6.80	1.61	1.52
42	14	313	A86	C25-C26	6.80	1.64	1.43
42	13	312	A86	C19-C20	6.79	1.61	1.52
42	12	316	A86	C25-C26	6.79	1.64	1.43
42	21	310	A86	C25-C26	6.79	1.64	1.43
42	18	314	A86	C25-C26	6.79	1.64	1.43
42	15	311	A86	C25-C26	6.78	1.64	1.43
42	19	312	A86	C25-C26	6.77	1.64	1.43
42	19	311	A86	C19-C20	6.77	1.61	1.52
42	17	313	A86	C25-C26	6.76	1.64	1.43
42	17	311	A86	C25-C26	6.76	1.64	1.43
42	13	313	A86	C25-C26	6.76	1.64	1.43
42	15	316	A86	C25-C26	6.76	1.64	1.43
42	20	213	A86	C19-C20	6.75	1.61	1.52
42	15	315	A86	C25-C26	6.75	1.64	1.43
42	21	314	A86	C19-C20	6.75	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	20	210	A86	C25-C26	6.75	1.64	1.43
42	19	312	A86	C19-C20	6.75	1.61	1.52
42	14	314	A86	C25-C26	6.74	1.64	1.43
42	12	317	A86	C25-C26	6.74	1.64	1.43
42	12	304	A86	C25-C26	6.74	1.64	1.43
42	11	316	A86	C25-C26	6.74	1.64	1.43
42	11	312	A86	C25-C26	6.73	1.64	1.43
42	16	312	A86	C25-C26	6.73	1.64	1.43
42	18	302	A86	C25-C26	6.73	1.64	1.43
42	13	315	A86	C25-C26	6.73	1.64	1.43
42	19	311	A86	C25-C26	6.72	1.64	1.43
42	18	314	A86	C19-C20	6.72	1.61	1.52
42	14	313	A86	C19-C20	6.72	1.61	1.52
42	15	312	A86	C25-C26	6.72	1.64	1.43
42	13	301	A86	C25-C26	6.71	1.64	1.43
42	21	311	A86	C25-C26	6.70	1.64	1.43
42	20	211	A86	C25-C26	6.69	1.64	1.43
42	17	315	A86	C25-C26	6.66	1.64	1.43
42	19	310	A86	C25-C26	6.66	1.64	1.43
31	A	403	PHO	C3B-C4B	6.64	1.49	1.41
42	16	310	A86	C25-C26	6.64	1.64	1.43
42	20	213	A86	C25-C26	6.64	1.64	1.43
42	17	302	A86	C19-C20	6.64	1.61	1.52
31	d	403	PHO	C3B-C4B	6.63	1.49	1.41
42	17	302	A86	C25-C26	6.63	1.64	1.43
42	21	314	A86	C25-C26	6.62	1.64	1.43
42	17	316	A86	C25-C26	6.61	1.63	1.43
42	21	312	A86	C25-C26	6.60	1.63	1.43
42	16	313	A86	C25-C26	6.60	1.63	1.43
42	21	313	A86	C25-C26	6.60	1.63	1.43
42	14	301	A86	C25-C26	6.60	1.63	1.43
42	14	316	A86	C25-C26	6.59	1.63	1.43
42	11	314	A86	C25-C26	6.59	1.63	1.43
42	12	319	A86	C25-C26	6.59	1.63	1.43
42	15	314	A86	C25-C26	6.59	1.63	1.43
42	15	312	A86	C19-C20	6.59	1.61	1.52
42	11	313	A86	C25-C26	6.59	1.63	1.43
42	11	310	A86	C25-C26	6.58	1.63	1.43
42	15	313	A86	C25-C26	6.58	1.63	1.43
42	16	312	A86	C19-C20	6.57	1.61	1.52
42	17	314	A86	C25-C26	6.57	1.63	1.43
42	12	318	A86	C25-C26	6.56	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	15	310	A86	C25-C26	6.56	1.63	1.43
42	13	313	A86	C19-C20	6.56	1.61	1.52
42	17	313	A86	C19-C20	6.56	1.61	1.52
42	21	313	A86	C19-C20	6.56	1.61	1.52
42	18	315	A86	C25-C26	6.55	1.63	1.43
42	12	315	A86	C25-C26	6.55	1.63	1.43
42	14	314	A86	C19-C20	6.55	1.61	1.52
42	11	312	A86	C19-C20	6.55	1.61	1.52
42	18	313	A86	C25-C26	6.54	1.63	1.43
42	14	312	A86	C25-C26	6.54	1.63	1.43
42	12	317	A86	C19-C20	6.53	1.61	1.52
42	14	315	A86	C25-C26	6.53	1.63	1.43
42	13	314	A86	C25-C26	6.53	1.63	1.43
42	13	311	A86	C25-C26	6.53	1.63	1.43
40	d	408	PL9	C6-C1	-6.52	1.36	1.48
40	D	407	PL9	C6-C1	-6.48	1.37	1.48
31	D	403	PHO	C3B-C4B	6.42	1.48	1.41
31	d	404	PHO	C3B-C4B	6.41	1.48	1.41
42	16	313	A86	C19-C20	6.41	1.61	1.52
42	12	319	A86	C19-C20	6.39	1.61	1.52
42	17	316	A86	C19-C20	6.39	1.61	1.52
42	19	310	A86	C19-C20	6.39	1.61	1.52
42	14	316	A86	C19-C20	6.37	1.61	1.52
42	20	211	A86	C19-C20	6.37	1.61	1.52
42	15	314	A86	C19-C20	6.30	1.61	1.52
42	14	301	A86	C19-C20	6.29	1.61	1.52
42	11	314	A86	C19-C20	6.28	1.61	1.52
42	21	311	A86	C19-C20	6.28	1.61	1.52
42	21	310	A86	C19-C20	6.18	1.60	1.52
42	13	315	A86	C19-C20	6.11	1.60	1.52
42	13	301	A86	C19-C20	6.06	1.60	1.52
42	15	315	A86	C19-C20	6.05	1.60	1.52
42	12	304	A86	C19-C20	6.05	1.60	1.52
42	18	302	A86	C19-C20	6.04	1.60	1.52
42	15	316	A86	C19-C20	5.99	1.60	1.52
42	11	316	A86	C19-C20	5.97	1.60	1.52
42	21	312	A86	C19-C20	5.84	1.60	1.52
40	d	405	PL9	C7-C3	-5.75	1.45	1.51
40	D	404	PL9	C7-C3	-5.73	1.45	1.51
42	20	201	A86	C9-C8	5.19	1.47	1.34
42	12	317	A86	C9-C8	4.99	1.47	1.34
42	19	311	A86	C9-C8	4.97	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	20	212	A86	C9-C8	4.96	1.47	1.34
42	16	312	A86	C9-C8	4.95	1.47	1.34
42	13	313	A86	C9-C8	4.95	1.47	1.34
42	11	312	A86	C9-C8	4.94	1.47	1.34
42	17	313	A86	C9-C8	4.94	1.47	1.34
42	17	311	A86	C9-C8	4.93	1.47	1.34
42	14	314	A86	C9-C8	4.93	1.47	1.34
42	13	301	A86	C9-C8	4.91	1.47	1.34
42	15	312	A86	C9-C8	4.91	1.47	1.34
42	20	212	A86	C26-C27	4.89	1.42	1.35
42	17	315	A86	C9-C8	4.89	1.47	1.34
42	13	315	A86	C9-C8	4.88	1.47	1.34
42	18	302	A86	C9-C8	4.87	1.47	1.34
42	15	315	A86	C9-C8	4.86	1.47	1.34
42	11	316	A86	C9-C8	4.86	1.47	1.34
42	12	304	A86	C9-C8	4.84	1.47	1.34
42	15	316	A86	C9-C8	4.84	1.47	1.34
42	20	210	A86	C9-C8	4.82	1.47	1.34
42	19	312	A86	C9-C8	4.80	1.46	1.34
42	19	311	A86	C26-C27	4.78	1.42	1.35
42	18	314	A86	C9-C8	4.77	1.46	1.34
42	20	213	A86	C9-C8	4.77	1.46	1.34
42	21	314	A86	C9-C8	4.76	1.46	1.34
42	17	312	A86	C9-C8	4.74	1.46	1.34
42	21	312	A86	C9-C8	4.74	1.46	1.34
42	11	311	A86	C9-C8	4.73	1.46	1.34
42	17	302	A86	C9-C8	4.73	1.46	1.34
42	15	311	A86	C9-C8	4.72	1.46	1.34
42	13	312	A86	C9-C8	4.72	1.46	1.34
30	c	510	CLA	C4D-ND	-4.72	1.31	1.37
42	14	301	A86	C9-C8	4.72	1.46	1.34
42	17	313	A86	C26-C27	4.71	1.42	1.35
42	14	313	A86	C9-C8	4.71	1.46	1.34
30	C	510	CLA	C4D-ND	-4.70	1.31	1.37
42	18	313	A86	C9-C8	4.69	1.46	1.34
42	12	316	A86	C9-C8	4.69	1.46	1.34
42	15	310	A86	C9-C8	4.69	1.46	1.34
42	17	311	A86	C26-C27	4.68	1.42	1.35
42	19	310	A86	C17-C18	-4.68	1.45	1.52
42	16	311	A86	C9-C8	4.68	1.46	1.34
42	14	314	A86	C26-C27	4.68	1.42	1.35
42	12	318	A86	C9-C8	4.67	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	15	314	A86	C9-C8	4.67	1.46	1.34
42	12	315	A86	C9-C8	4.67	1.46	1.34
42	12	319	A86	C9-C8	4.67	1.46	1.34
42	21	314	A86	C17-C18	-4.66	1.45	1.52
42	13	313	A86	C26-C27	4.66	1.42	1.35
42	16	313	A86	C9-C8	4.66	1.46	1.34
42	11	310	A86	C9-C8	4.66	1.46	1.34
42	21	310	A86	C17-C18	-4.66	1.45	1.52
42	15	313	A86	C9-C8	4.65	1.46	1.34
42	14	312	A86	C9-C8	4.65	1.46	1.34
42	16	312	A86	C26-C27	4.64	1.41	1.35
42	21	311	A86	C9-C8	4.64	1.46	1.34
42	12	317	A86	C26-C27	4.64	1.41	1.35
42	11	313	A86	C9-C8	4.64	1.46	1.34
42	17	313	A86	O4-C38	4.64	1.45	1.35
42	13	311	A86	C9-C8	4.64	1.46	1.34
42	21	313	A86	C9-C8	4.64	1.46	1.34
42	11	314	A86	C9-C8	4.64	1.46	1.34
42	19	312	A86	C26-C27	4.64	1.41	1.35
42	17	316	A86	C9-C8	4.62	1.46	1.34
42	20	213	A86	C17-C18	-4.62	1.45	1.52
42	13	314	A86	C9-C8	4.62	1.46	1.34
42	14	315	A86	C9-C8	4.62	1.46	1.34
30	B	612	CLA	C4D-ND	-4.62	1.31	1.37
42	14	316	A86	C9-C8	4.62	1.46	1.34
42	18	315	A86	C9-C8	4.62	1.46	1.34
42	16	310	A86	C9-C8	4.61	1.46	1.34
42	20	211	A86	C9-C8	4.61	1.46	1.34
30	b	612	CLA	C4D-ND	-4.61	1.31	1.37
42	17	314	A86	C9-C8	4.61	1.46	1.34
42	14	314	A86	O4-C38	4.60	1.45	1.35
42	21	310	A86	C9-C8	4.59	1.46	1.34
42	16	312	A86	O4-C38	4.59	1.45	1.35
42	15	312	A86	C26-C27	4.59	1.41	1.35
42	11	312	A86	C26-C27	4.58	1.41	1.35
42	13	313	A86	O4-C38	4.57	1.45	1.35
42	15	312	A86	O4-C38	4.57	1.45	1.35
42	20	212	A86	C2-C1	4.57	1.41	1.35
42	20	210	A86	C26-C27	4.56	1.41	1.35
42	11	312	A86	O4-C38	4.55	1.45	1.35
42	16	310	A86	C2-C1	4.55	1.41	1.35
42	12	317	A86	O4-C38	4.55	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	312	A86	C17-C18	-4.54	1.45	1.52
42	21	310	A86	C26-C27	4.54	1.41	1.35
42	19	310	A86	C9-C8	4.54	1.46	1.34
42	19	311	A86	O4-C38	4.54	1.45	1.35
42	19	312	A86	O4-C38	4.54	1.45	1.35
42	21	311	A86	C17-C18	-4.53	1.45	1.52
42	19	311	A86	C19-C18	4.53	1.58	1.52
42	20	211	A86	C17-C18	-4.52	1.45	1.52
42	20	213	A86	C26-C27	4.51	1.41	1.35
42	21	314	A86	C26-C27	4.49	1.41	1.35
42	17	311	A86	C17-C18	-4.48	1.45	1.52
42	18	314	A86	C17-C18	-4.48	1.45	1.52
42	17	315	A86	C26-C27	4.48	1.41	1.35
42	13	312	A86	C17-C18	-4.47	1.45	1.52
42	12	316	A86	C17-C18	-4.46	1.45	1.52
42	20	212	A86	O4-C38	4.45	1.45	1.35
42	11	311	A86	C17-C18	-4.44	1.45	1.52
42	19	310	A86	C26-C27	4.44	1.41	1.35
42	16	311	A86	C17-C18	-4.43	1.45	1.52
42	16	313	A86	C26-C27	4.43	1.41	1.35
42	15	311	A86	C17-C18	-4.43	1.46	1.52
42	12	304	A86	C26-C27	4.42	1.41	1.35
42	20	210	A86	C2-C1	4.42	1.41	1.35
42	17	313	A86	C17-C18	-4.41	1.46	1.52
42	11	316	A86	C26-C27	4.41	1.41	1.35
42	20	201	A86	C26-C27	4.41	1.41	1.35
42	21	313	A86	C17-C18	-4.41	1.46	1.52
42	21	314	A86	C2-C1	4.40	1.41	1.35
42	14	313	A86	C17-C18	-4.40	1.46	1.52
42	17	312	A86	C17-C18	-4.40	1.46	1.52
42	18	314	A86	C26-C27	4.40	1.41	1.35
42	15	311	A86	C26-C27	4.39	1.41	1.35
42	16	310	A86	C17-C18	-4.39	1.46	1.52
42	14	313	A86	C26-C27	4.39	1.41	1.35
30	d	401	CLA	C4D-ND	-4.38	1.31	1.37
42	20	201	A86	C2-C1	4.38	1.41	1.35
42	12	316	A86	C26-C27	4.38	1.41	1.35
42	11	311	A86	C26-C27	4.37	1.41	1.35
42	13	312	A86	C26-C27	4.37	1.41	1.35
42	13	313	A86	C17-C18	-4.37	1.46	1.52
42	20	213	A86	C2-C1	4.37	1.41	1.35
42	15	316	A86	C26-C27	4.37	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	13	301	A86	C26-C27	4.36	1.41	1.35
42	15	315	A86	C26-C27	4.36	1.41	1.35
42	18	302	A86	C26-C27	4.36	1.41	1.35
42	12	317	A86	C2-C1	4.35	1.41	1.35
42	18	315	A86	C26-C27	4.35	1.41	1.35
42	15	312	A86	C17-C18	-4.35	1.46	1.52
42	15	314	A86	C26-C27	4.34	1.41	1.35
42	21	312	A86	C17-C18	-4.33	1.46	1.52
42	15	312	A86	C2-C1	4.33	1.41	1.35
42	21	311	A86	C26-C27	4.33	1.41	1.35
42	11	312	A86	C17-C18	-4.33	1.46	1.52
42	16	312	A86	C2-C1	4.32	1.41	1.35
42	17	302	A86	C26-C27	4.32	1.41	1.35
42	14	314	A86	C2-C1	4.32	1.41	1.35
42	14	301	A86	C26-C27	4.31	1.41	1.35
42	16	312	A86	C17-C18	-4.31	1.46	1.52
42	11	314	A86	C26-C27	4.31	1.41	1.35
42	17	302	A86	C17-C18	-4.31	1.46	1.52
42	14	316	A86	C26-C27	4.31	1.41	1.35
42	14	314	A86	C17-C18	-4.30	1.46	1.52
30	C	509	CLA	C4D-ND	-4.30	1.31	1.37
42	13	315	A86	C26-C27	4.30	1.41	1.35
42	11	312	A86	C2-C1	4.30	1.41	1.35
42	16	311	A86	C26-C27	4.30	1.41	1.35
42	12	319	A86	C26-C27	4.30	1.41	1.35
42	20	201	A86	C19-C18	4.29	1.58	1.52
42	12	317	A86	C17-C18	-4.29	1.46	1.52
42	14	315	A86	C26-C27	4.29	1.41	1.35
42	20	212	A86	C7-C6	4.29	1.59	1.50
42	17	312	A86	C26-C27	4.29	1.41	1.35
42	18	302	A86	C17-C18	-4.29	1.46	1.52
42	16	313	A86	C17-C18	-4.28	1.46	1.52
42	17	311	A86	O4-C38	4.28	1.44	1.35
42	20	211	A86	C26-C27	4.28	1.41	1.35
30	d	406	CLA	C4D-ND	-4.27	1.31	1.37
42	12	319	A86	C17-C18	-4.27	1.46	1.52
42	20	201	A86	C10-C11	4.27	1.46	1.34
42	13	315	A86	C17-C18	-4.27	1.46	1.52
30	b	613	CLA	C4D-ND	-4.27	1.31	1.37
42	16	310	A86	C26-C27	4.26	1.41	1.35
42	17	314	A86	O4-C38	4.26	1.44	1.35
42	15	313	A86	C26-C27	4.26	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	313	A86	C26-C27	4.26	1.41	1.35
30	D	401	CLA	C4D-ND	-4.26	1.31	1.37
42	13	301	A86	O4-C38	4.26	1.44	1.35
42	21	311	A86	C2-C1	4.26	1.41	1.35
42	17	316	A86	C26-C27	4.26	1.41	1.35
42	13	315	A86	C2-C1	4.25	1.41	1.35
30	B	611	CLA	C4D-ND	-4.25	1.31	1.37
42	14	316	A86	C17-C18	-4.25	1.46	1.52
42	12	304	A86	O4-C38	4.25	1.44	1.35
42	15	315	A86	C2-C1	4.25	1.41	1.35
42	12	318	A86	C26-C27	4.25	1.41	1.35
42	13	315	A86	O4-C38	4.24	1.44	1.35
42	17	313	A86	C2-C1	4.24	1.41	1.35
42	12	318	A86	C7-C6	4.24	1.59	1.50
42	20	210	A86	C7-C6	4.24	1.59	1.50
42	12	318	A86	O4-C38	4.24	1.44	1.35
42	17	314	A86	C26-C27	4.24	1.41	1.35
42	17	316	A86	C17-C18	-4.24	1.46	1.52
30	13	302	CLA	C4D-ND	-4.24	1.31	1.37
42	12	304	A86	C7-C6	4.23	1.59	1.50
42	15	313	A86	O4-C38	4.23	1.44	1.35
42	19	310	A86	O4-C38	4.23	1.44	1.35
42	13	301	A86	C17-C18	-4.23	1.46	1.52
30	B	613	CLA	C4D-ND	-4.22	1.31	1.37
42	11	316	A86	C7-C6	4.22	1.59	1.50
42	15	315	A86	C7-C6	4.22	1.59	1.50
42	11	316	A86	O4-C38	4.22	1.44	1.35
42	13	313	A86	C2-C1	4.22	1.41	1.35
42	13	314	A86	O4-C38	4.22	1.44	1.35
42	20	212	A86	C17-C18	-4.22	1.46	1.52
42	15	313	A86	C7-C6	4.22	1.59	1.50
42	11	314	A86	C17-C18	-4.22	1.46	1.52
42	11	316	A86	C17-C18	-4.21	1.46	1.52
42	17	315	A86	C17-C18	-4.21	1.46	1.52
42	15	316	A86	O4-C38	4.21	1.44	1.35
42	21	312	A86	O4-C38	4.21	1.44	1.35
30	c	502	CLA	C4D-ND	-4.21	1.31	1.37
42	20	210	A86	O4-C38	4.21	1.44	1.35
42	13	315	A86	C7-C6	4.20	1.59	1.50
42	13	301	A86	C7-C6	4.20	1.59	1.50
42	11	313	A86	C7-C6	4.20	1.59	1.50
42	18	302	A86	O4-C38	4.20	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	313	A86	O4-C38	4.20	1.44	1.35
42	18	315	A86	O4-C38	4.20	1.44	1.35
42	12	304	A86	C2-C1	4.20	1.41	1.35
30	C	502	CLA	C4D-ND	-4.20	1.31	1.37
30	a	402	CLA	C4D-ND	-4.20	1.31	1.37
42	20	213	A86	O4-C38	4.20	1.44	1.35
42	18	302	A86	C7-C6	4.20	1.59	1.50
42	21	313	A86	O4-C38	4.20	1.44	1.35
42	15	315	A86	O4-C38	4.20	1.44	1.35
42	15	316	A86	C7-C6	4.19	1.59	1.50
42	15	315	A86	C17-C18	-4.19	1.46	1.52
42	18	315	A86	C7-C6	4.19	1.59	1.50
42	17	314	A86	C2-C1	4.19	1.41	1.35
42	13	314	A86	C7-C6	4.19	1.59	1.50
30	D	405	CLA	C4D-ND	-4.19	1.31	1.37
42	15	316	A86	C17-C18	-4.19	1.46	1.52
42	14	315	A86	O4-C38	4.19	1.44	1.35
42	17	312	A86	O4-C38	4.19	1.44	1.35
42	17	315	A86	C2-C1	4.19	1.41	1.35
42	15	316	A86	C2-C1	4.18	1.41	1.35
42	13	314	A86	C26-C27	4.18	1.41	1.35
42	21	313	A86	C26-C27	4.18	1.41	1.35
42	12	304	A86	C17-C18	-4.18	1.46	1.52
42	16	310	A86	O4-C38	4.18	1.44	1.35
42	17	314	A86	C7-C6	4.18	1.59	1.50
42	19	312	A86	C2-C1	4.17	1.41	1.35
42	14	315	A86	C7-C6	4.17	1.59	1.50
30	c	509	CLA	C4D-ND	-4.17	1.32	1.37
42	14	301	A86	C21-C20	4.17	1.58	1.51
42	17	316	A86	C7-C6	4.17	1.59	1.50
42	18	302	A86	C2-C1	4.17	1.41	1.35
30	12	305	CLA	C4D-ND	-4.16	1.32	1.37
42	11	312	A86	C7-C6	4.16	1.59	1.50
42	17	315	A86	O4-C38	4.16	1.44	1.35
42	20	211	A86	C2-C1	4.16	1.41	1.35
42	14	301	A86	C17-C18	-4.16	1.46	1.52
42	15	314	A86	C17-C18	-4.16	1.46	1.52
42	20	201	A86	C7-C6	4.16	1.59	1.50
42	17	302	A86	C2-C1	4.16	1.41	1.35
42	21	314	A86	O4-C38	4.16	1.44	1.35
42	18	314	A86	O4-C38	4.16	1.44	1.35
42	19	311	A86	C7-C6	4.15	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	17	314	A86	C17-C18	-4.15	1.46	1.52
42	12	318	A86	C17-C18	-4.15	1.46	1.52
42	13	312	A86	O4-C38	4.15	1.44	1.35
42	13	301	A86	C2-C1	4.15	1.41	1.35
30	b	611	CLA	C4D-ND	-4.15	1.32	1.37
42	11	311	A86	O4-C38	4.15	1.44	1.35
42	11	316	A86	C2-C1	4.15	1.41	1.35
42	15	312	A86	C7-C6	4.15	1.59	1.50
30	B	604	CLA	C4D-ND	-4.14	1.32	1.37
42	15	313	A86	C17-C18	-4.14	1.46	1.52
42	21	311	A86	O4-C38	4.14	1.44	1.35
42	14	316	A86	C7-C6	4.14	1.59	1.50
30	A	402	CLA	C4D-ND	-4.14	1.32	1.37
42	14	301	A86	C7-C6	4.14	1.59	1.50
42	11	313	A86	C17-C18	-4.14	1.46	1.52
42	18	315	A86	C17-C18	-4.14	1.46	1.52
42	20	213	A86	C7-C6	4.13	1.59	1.50
42	15	311	A86	O4-C38	4.13	1.44	1.35
42	21	313	A86	C7-C6	4.13	1.59	1.50
42	21	314	A86	C7-C6	4.13	1.59	1.50
42	17	302	A86	C7-C6	4.13	1.59	1.50
42	17	302	A86	O4-C38	4.13	1.44	1.35
42	12	319	A86	C7-C6	4.13	1.59	1.50
42	18	313	A86	C17-C18	-4.13	1.46	1.52
42	21	313	A86	C2-C1	4.13	1.41	1.35
42	11	314	A86	C7-C6	4.13	1.59	1.50
42	17	311	A86	C7-C6	4.12	1.59	1.50
30	14	303	CLA	C4D-ND	-4.12	1.32	1.37
42	16	311	A86	O4-C38	4.12	1.44	1.35
42	20	211	A86	O4-C38	4.12	1.44	1.35
30	A	404	CLA	C4D-ND	-4.12	1.32	1.37
42	21	312	A86	C26-C27	4.12	1.41	1.35
42	16	313	A86	C7-C6	4.12	1.59	1.50
30	b	604	CLA	C4D-ND	-4.11	1.32	1.37
42	12	316	A86	O4-C38	4.11	1.44	1.35
42	14	316	A86	C21-C20	4.11	1.58	1.51
42	13	313	A86	C7-C6	4.11	1.59	1.50
42	15	314	A86	C21-C20	4.11	1.58	1.51
42	12	315	A86	C17-C18	-4.11	1.46	1.52
42	14	314	A86	C7-C6	4.11	1.59	1.50
30	a	403	CLA	C4D-ND	-4.11	1.32	1.37
30	11	301	CLA	C4D-ND	-4.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	16	312	A86	C7-C6	4.10	1.59	1.50
30	d	402	CLA	C4D-ND	-4.10	1.32	1.37
42	14	313	A86	O4-C38	4.10	1.44	1.35
42	14	313	A86	C7-C6	4.10	1.59	1.50
42	20	201	A86	O4-C38	4.10	1.44	1.35
42	14	312	A86	C17-C18	-4.09	1.46	1.52
42	21	310	A86	C2-C1	4.09	1.41	1.35
42	11	314	A86	C21-C20	4.09	1.58	1.51
30	B	610	CLA	C4D-ND	-4.09	1.32	1.37
42	13	314	A86	C17-C18	-4.09	1.46	1.52
42	18	314	A86	C7-C6	4.08	1.59	1.50
42	17	311	A86	C2-C1	4.08	1.41	1.35
42	17	313	A86	C7-C6	4.08	1.59	1.50
42	14	315	A86	C17-C18	-4.08	1.46	1.52
42	12	319	A86	O4-C38	4.08	1.44	1.35
30	B	623	CLA	C4D-ND	-4.08	1.32	1.37
42	15	314	A86	C7-C6	4.08	1.59	1.50
42	16	313	A86	C2-C1	4.08	1.41	1.35
42	16	313	A86	O4-C38	4.08	1.44	1.35
30	19	301	CLA	C4D-ND	-4.07	1.32	1.37
42	16	311	A86	C7-C6	4.07	1.59	1.50
42	11	316	A86	C21-C20	4.07	1.58	1.51
42	12	317	A86	C7-C6	4.07	1.59	1.50
42	16	310	A86	C7-C6	4.07	1.59	1.50
42	11	313	A86	C21-C20	4.07	1.58	1.51
30	c	514	CLA	C4D-ND	-4.07	1.32	1.37
42	12	318	A86	C21-C20	4.06	1.58	1.51
42	17	316	A86	C21-C20	4.06	1.58	1.51
30	D	402	CLA	C4D-ND	-4.06	1.32	1.37
42	17	316	A86	O4-C38	4.06	1.44	1.35
30	c	508	CLA	C4D-ND	-4.06	1.32	1.37
42	21	311	A86	C7-C6	4.06	1.59	1.50
42	14	316	A86	O4-C38	4.06	1.44	1.35
42	15	314	A86	O4-C38	4.06	1.44	1.35
42	12	319	A86	C2-C1	4.06	1.41	1.35
42	20	211	A86	C7-C6	4.06	1.59	1.50
42	12	319	A86	C21-C20	4.06	1.58	1.51
42	21	310	A86	C7-C6	4.06	1.59	1.50
42	14	301	A86	O4-C38	4.05	1.44	1.35
42	19	312	A86	C7-C6	4.05	1.59	1.50
42	17	316	A86	C2-C1	4.05	1.41	1.35
42	15	311	A86	C7-C6	4.05	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	310	A86	C7-C6	4.04	1.59	1.50
42	12	316	A86	C7-C6	4.04	1.59	1.50
30	C	508	CLA	C4D-ND	-4.04	1.32	1.37
42	15	313	A86	C21-C20	4.04	1.58	1.51
42	13	314	A86	C2-C1	4.04	1.41	1.35
42	12	315	A86	C7-C6	4.04	1.59	1.50
30	b	622	CLA	C4D-ND	-4.04	1.32	1.37
42	16	313	A86	C21-C20	4.04	1.58	1.51
42	15	314	A86	C2-C1	4.04	1.41	1.35
42	11	310	A86	C17-C18	-4.04	1.46	1.52
40	d	408	PL9	C7-C8	-4.04	1.44	1.50
42	13	311	A86	C26-C27	4.04	1.41	1.35
30	c	503	CLA	C4D-ND	-4.03	1.32	1.37
42	11	311	A86	C7-C6	4.03	1.59	1.50
30	C	514	CLA	C4D-ND	-4.03	1.32	1.37
42	11	313	A86	C2-C1	4.03	1.41	1.35
42	13	315	A86	C21-C20	4.03	1.58	1.51
30	b	610	CLA	C4D-ND	-4.03	1.32	1.37
42	13	311	A86	C17-C18	-4.03	1.46	1.52
42	11	314	A86	C2-C1	4.03	1.41	1.35
42	15	316	A86	C21-C20	4.03	1.58	1.51
42	14	312	A86	C7-C6	4.02	1.59	1.50
30	c	513	CLA	C4D-ND	-4.02	1.32	1.37
42	11	310	A86	C7-C6	4.01	1.59	1.50
42	18	313	A86	C7-C6	4.01	1.59	1.50
42	17	312	A86	C7-C6	4.01	1.59	1.50
42	14	313	A86	C2-C1	4.01	1.41	1.35
42	15	310	A86	C7-C6	4.01	1.59	1.50
42	11	310	A86	C21-C20	4.01	1.58	1.51
42	12	315	A86	C21-C20	4.01	1.58	1.51
42	20	210	A86	C21-C20	4.01	1.58	1.51
30	c	505	CLA	C4D-ND	-4.01	1.32	1.37
30	C	503	CLA	C4D-ND	-4.00	1.32	1.37
42	17	315	A86	C7-C6	4.00	1.59	1.50
42	11	314	A86	O4-C38	4.00	1.44	1.35
30	b	607	CLA	C4D-ND	-4.00	1.32	1.37
42	15	315	A86	C21-C20	4.00	1.58	1.51
42	13	312	A86	C7-C6	4.00	1.59	1.50
42	13	301	A86	C21-C20	4.00	1.58	1.51
42	12	318	A86	C2-C1	3.99	1.41	1.35
42	17	311	A86	C21-C20	3.99	1.58	1.51
42	21	310	A86	O4-C38	3.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	17	315	A86	C9-C10	3.99	1.55	1.43
42	14	315	A86	C21-C20	3.99	1.58	1.51
42	12	304	A86	C21-C20	3.99	1.58	1.51
42	18	315	A86	C2-C1	3.99	1.41	1.35
42	18	315	A86	C21-C20	3.99	1.58	1.51
42	18	313	A86	C26-C27	3.98	1.41	1.35
30	B	607	CLA	C4D-ND	-3.98	1.32	1.37
42	14	312	A86	C21-C20	3.98	1.58	1.51
42	15	313	A86	C2-C1	3.98	1.41	1.35
42	17	312	A86	C2-C1	3.98	1.41	1.35
42	18	314	A86	C2-C1	3.98	1.41	1.35
42	20	210	A86	C17-C18	-3.98	1.46	1.52
30	16	307	CLA	C4D-ND	-3.97	1.32	1.37
42	15	310	A86	C17-C18	-3.97	1.46	1.52
42	14	301	A86	C2-C1	3.97	1.41	1.35
42	21	312	A86	C7-C6	3.97	1.59	1.50
42	18	313	A86	C21-C20	3.97	1.58	1.51
42	17	315	A86	C10-C11	3.97	1.46	1.34
42	15	311	A86	C2-C1	3.97	1.41	1.35
42	19	310	A86	C2-C1	3.97	1.41	1.35
30	c	511	CLA	C4D-ND	-3.97	1.32	1.37
42	11	310	A86	O4-C38	3.96	1.44	1.35
42	18	302	A86	C21-C20	3.96	1.58	1.51
42	13	311	A86	O4-C38	3.96	1.44	1.35
42	16	311	A86	C2-C1	3.96	1.41	1.35
42	18	313	A86	O4-C38	3.95	1.44	1.35
42	14	316	A86	C2-C1	3.95	1.41	1.35
42	13	312	A86	C2-C1	3.95	1.41	1.35
42	13	311	A86	C7-C6	3.95	1.59	1.50
42	15	310	A86	C21-C20	3.95	1.58	1.51
42	13	311	A86	C21-C20	3.95	1.58	1.51
42	20	212	A86	C5-C6	3.95	1.41	1.35
42	21	312	A86	C2-C1	3.95	1.41	1.35
42	13	314	A86	C21-C20	3.95	1.58	1.51
42	14	312	A86	C26-C27	3.94	1.41	1.35
30	B	606	CLA	C4D-ND	-3.94	1.32	1.37
42	14	315	A86	C2-C1	3.94	1.41	1.35
30	17	301	CLA	C4D-ND	-3.94	1.32	1.37
30	C	513	CLA	C4D-ND	-3.94	1.32	1.37
42	20	201	A86	C9-C10	3.94	1.55	1.43
42	11	310	A86	C2-C1	3.94	1.41	1.35
30	16	302	CLA	C4D-ND	-3.94	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	15	310	A86	C2-C1	3.94	1.41	1.35
42	15	310	A86	O4-C38	3.94	1.44	1.35
30	C	512	CLA	C4D-ND	-3.93	1.32	1.37
40	D	407	PL9	C7-C8	-3.93	1.45	1.50
30	d	407	CLA	C4D-ND	-3.93	1.32	1.37
42	12	316	A86	C2-C1	3.92	1.41	1.35
30	b	606	CLA	C4D-ND	-3.92	1.32	1.37
42	12	315	A86	O4-C38	3.92	1.44	1.35
30	15	304	CLA	C1D-ND	3.92	1.42	1.37
42	14	312	A86	O4-C38	3.92	1.44	1.35
42	20	210	A86	C19-C18	3.92	1.58	1.52
42	20	212	A86	C10-C11	3.91	1.45	1.34
30	c	512	CLA	C4D-ND	-3.90	1.32	1.37
42	15	310	A86	C26-C27	3.90	1.41	1.35
42	11	311	A86	C2-C1	3.90	1.41	1.35
42	20	212	A86	C21-C20	3.90	1.57	1.51
42	13	311	A86	C2-C1	3.90	1.41	1.35
42	20	212	A86	C9-C10	3.90	1.55	1.43
30	16	306	CLA	C1D-ND	3.89	1.42	1.37
30	D	406	CLA	C4D-ND	-3.89	1.32	1.37
42	17	314	A86	C21-C20	3.89	1.57	1.51
42	12	315	A86	C26-C27	3.88	1.40	1.35
30	C	505	CLA	C4D-ND	-3.88	1.32	1.37
42	16	311	A86	C21-C20	3.88	1.57	1.51
42	11	310	A86	C26-C27	3.87	1.40	1.35
42	20	210	A86	C10-C11	3.87	1.45	1.34
30	C	504	CLA	C4D-ND	-3.87	1.32	1.37
30	W	103	CLA	C1D-ND	3.86	1.42	1.37
42	12	316	A86	C21-C20	3.86	1.57	1.51
30	w	103	CLA	C1D-ND	3.86	1.42	1.37
42	14	312	A86	C2-C1	3.86	1.40	1.35
30	17	303	CLA	C4D-ND	-3.85	1.32	1.37
30	b	603	CLA	C4D-ND	-3.85	1.32	1.37
42	14	314	A86	C9-C10	3.85	1.55	1.43
42	17	313	A86	C9-C10	3.85	1.55	1.43
42	19	312	A86	C9-C10	3.85	1.55	1.43
42	17	311	A86	C9-C10	3.84	1.55	1.43
42	15	312	A86	C9-C10	3.84	1.55	1.43
42	17	312	A86	C21-C20	3.84	1.57	1.51
30	c	507	CLA	C4D-ND	-3.84	1.32	1.37
42	19	311	A86	C2-C1	3.83	1.40	1.35
30	C	511	CLA	C4D-ND	-3.83	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	507	CLA	C4D-ND	-3.83	1.32	1.37
42	13	313	A86	C9-C10	3.83	1.55	1.43
42	11	312	A86	C9-C10	3.83	1.55	1.43
30	18	309	CLA	C4D-ND	-3.83	1.32	1.37
30	19	308	CLA	C4D-ND	-3.83	1.32	1.37
42	21	314	A86	C9-C10	3.83	1.55	1.43
42	20	213	A86	C9-C10	3.83	1.55	1.43
42	17	311	A86	C19-C18	3.82	1.57	1.52
42	16	312	A86	C9-C10	3.82	1.55	1.43
42	11	316	A86	C9-C10	3.82	1.55	1.43
42	12	304	A86	C9-C10	3.81	1.55	1.43
42	13	301	A86	C9-C10	3.81	1.55	1.43
40	D	407	PL9	C52-C5	-3.81	1.42	1.50
42	15	315	A86	C9-C10	3.81	1.55	1.43
42	13	315	A86	C9-C10	3.81	1.55	1.43
42	12	315	A86	C2-C1	3.81	1.40	1.35
40	d	408	PL9	C52-C5	-3.81	1.42	1.50
42	19	311	A86	C10-C11	3.81	1.45	1.34
42	19	311	A86	C9-C10	3.80	1.55	1.43
42	14	314	A86	C10-C11	3.80	1.45	1.34
42	15	312	A86	C10-C11	3.80	1.45	1.34
42	12	317	A86	C9-C10	3.80	1.55	1.43
42	18	313	A86	C2-C1	3.80	1.40	1.35
42	12	317	A86	C10-C11	3.80	1.45	1.34
42	20	210	A86	C9-C10	3.80	1.55	1.43
42	15	316	A86	C9-C10	3.79	1.55	1.43
42	20	212	A86	C19-C18	3.79	1.57	1.52
35	d	409	LHG	O7-C5	-3.79	1.37	1.46
42	19	312	A86	C21-C20	3.78	1.57	1.51
42	16	312	A86	C10-C11	3.78	1.45	1.34
42	11	312	A86	C10-C11	3.78	1.45	1.34
32	B	616	BCR	C30-C25	-3.78	1.48	1.53
30	21	305	CLA	C1D-ND	3.78	1.42	1.37
30	B	603	CLA	C4D-ND	-3.78	1.32	1.37
42	17	311	A86	C10-C11	3.78	1.45	1.34
30	z	101	CLA	C4D-ND	-3.78	1.32	1.37
42	20	201	A86	C21-C20	3.77	1.57	1.51
35	L	101	LHG	O7-C5	-3.77	1.37	1.46
30	21	309	CLA	C1D-ND	3.77	1.42	1.37
42	16	313	A86	C9-C10	3.77	1.55	1.43
42	17	313	A86	C10-C11	3.77	1.45	1.34
32	H	101	BCR	C1-C6	-3.77	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	20	213	A86	C10-C11	3.77	1.45	1.34
30	19	302	CLA	C4D-ND	-3.77	1.32	1.37
30	17	305	CLA	C4D-ND	-3.77	1.32	1.37
42	20	210	A86	C5-C6	3.77	1.40	1.35
42	17	315	A86	C21-C20	3.76	1.57	1.51
42	13	312	A86	C21-C20	3.76	1.57	1.51
42	18	302	A86	C9-C10	3.76	1.55	1.43
42	13	313	A86	C10-C11	3.76	1.45	1.34
42	14	313	A86	C21-C20	3.76	1.57	1.51
32	m	103	BCR	C30-C25	-3.76	1.48	1.53
30	C	519	CLA	C4D-ND	-3.75	1.32	1.37
30	c	504	CLA	C4D-ND	-3.75	1.32	1.37
42	21	314	A86	C10-C11	3.75	1.45	1.34
30	15	307	CLA	C4D-ND	-3.75	1.32	1.37
32	h	101	BCR	C1-C6	-3.74	1.48	1.53
42	12	317	A86	C5-C6	3.74	1.40	1.35
42	11	311	A86	C21-C20	3.74	1.57	1.51
30	16	304	CLA	C4D-ND	-3.74	1.32	1.37
42	14	316	A86	C9-C10	3.74	1.55	1.43
42	12	319	A86	C9-C10	3.74	1.55	1.43
42	14	313	A86	C9-C10	3.73	1.55	1.43
42	11	314	A86	C9-C10	3.73	1.55	1.43
42	15	311	A86	C21-C20	3.73	1.57	1.51
42	20	211	A86	C9-C10	3.73	1.55	1.43
42	18	314	A86	C9-C10	3.73	1.55	1.43
42	17	302	A86	C9-C10	3.73	1.55	1.43
42	17	316	A86	C9-C10	3.73	1.55	1.43
30	b	602	CLA	C4D-ND	-3.73	1.32	1.37
42	16	310	A86	C9-C10	3.73	1.55	1.43
42	13	314	A86	C9-C10	3.72	1.55	1.43
30	Z	102	CLA	C1D-ND	3.72	1.42	1.37
42	17	312	A86	C9-C10	3.72	1.55	1.43
42	15	314	A86	C9-C10	3.72	1.55	1.43
42	12	316	A86	C9-C10	3.71	1.54	1.43
30	18	303	CLA	C4D-ND	-3.71	1.32	1.37
42	17	314	A86	C9-C10	3.71	1.54	1.43
42	14	301	A86	C9-C10	3.71	1.54	1.43
42	17	302	A86	C10-C11	3.71	1.45	1.34
42	21	310	A86	C21-C20	3.71	1.57	1.51
42	14	315	A86	C9-C10	3.71	1.54	1.43
42	13	312	A86	C10-C11	3.71	1.45	1.34
30	14	309	CLA	C4D-ND	-3.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	13	312	A86	C9-C10	3.70	1.54	1.43
42	14	314	A86	C5-C6	3.70	1.40	1.35
42	11	313	A86	C9-C10	3.70	1.54	1.43
30	15	306	CLA	C1D-ND	3.70	1.42	1.37
30	21	305	CLA	C3B-C4B	3.70	1.51	1.42
32	C	518	BCR	C30-C25	-3.70	1.48	1.53
42	15	313	A86	C9-C10	3.70	1.54	1.43
42	11	312	A86	C21-C20	3.70	1.57	1.51
30	B	601	CLA	C4D-ND	-3.70	1.32	1.37
42	11	311	A86	C9-C10	3.69	1.54	1.43
42	18	314	A86	C21-C20	3.69	1.57	1.51
42	15	311	A86	C9-C10	3.69	1.54	1.43
30	B	602	CLA	C4D-ND	-3.69	1.32	1.37
30	17	308	CLA	C4D-ND	-3.69	1.32	1.37
42	21	313	A86	C9-C10	3.69	1.54	1.43
42	12	318	A86	C9-C10	3.69	1.54	1.43
30	21	301	CLA	C1D-ND	3.69	1.42	1.37
30	M	101	CLA	C4D-ND	-3.68	1.32	1.37
42	16	312	A86	C5-C6	3.68	1.40	1.35
42	16	311	A86	C9-C10	3.68	1.54	1.43
42	15	311	A86	C10-C11	3.68	1.45	1.34
42	21	311	A86	C9-C10	3.68	1.54	1.43
42	21	312	A86	C9-C10	3.67	1.54	1.43
42	14	314	A86	C21-C20	3.67	1.57	1.51
42	19	310	A86	C9-C10	3.67	1.54	1.43
42	13	313	A86	C21-C20	3.67	1.57	1.51
42	12	316	A86	C10-C11	3.67	1.45	1.34
42	18	314	A86	C10-C11	3.67	1.45	1.34
42	13	313	A86	C5-C6	3.67	1.40	1.35
42	19	312	A86	C10-C11	3.67	1.45	1.34
42	15	312	A86	C5-C6	3.67	1.40	1.35
30	m	101	CLA	C4D-ND	-3.66	1.32	1.37
42	21	314	A86	C5-C6	3.66	1.40	1.35
42	17	302	A86	C21-C20	3.66	1.57	1.51
42	21	313	A86	C21-C20	3.66	1.57	1.51
30	b	601	CLA	C4D-ND	-3.66	1.32	1.37
42	11	311	A86	C10-C11	3.66	1.45	1.34
42	14	313	A86	C10-C11	3.66	1.45	1.34
42	17	313	A86	C5-C6	3.66	1.40	1.35
42	20	213	A86	C5-C6	3.66	1.40	1.35
42	17	312	A86	C10-C11	3.65	1.45	1.34
42	14	315	A86	C19-C18	3.65	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	312	A86	C9-C10	3.65	1.54	1.43
30	B	608	CLA	C4D-ND	-3.65	1.32	1.37
42	16	312	A86	C21-C20	3.65	1.57	1.51
42	15	314	A86	C10-C11	3.65	1.45	1.34
42	11	312	A86	C5-C6	3.65	1.40	1.35
30	18	306	CLA	C1D-ND	3.65	1.42	1.37
42	17	313	A86	C21-C20	3.65	1.57	1.51
30	20	204	CLA	C4D-ND	-3.65	1.32	1.37
30	12	307	CLA	C4D-ND	-3.65	1.32	1.37
30	c	506	CLA	C4D-ND	-3.64	1.32	1.37
30	13	308	CLA	C4D-ND	-3.64	1.32	1.37
30	W	102	CLA	C4D-ND	-3.64	1.32	1.37
42	18	315	A86	C9-C10	3.64	1.54	1.43
30	21	306	CLA	C1D-ND	3.64	1.42	1.37
42	15	312	A86	C21-C20	3.64	1.57	1.51
30	12	311	CLA	C4D-ND	-3.64	1.32	1.37
42	21	310	A86	C9-C10	3.64	1.54	1.43
42	20	201	A86	C5-C6	3.64	1.40	1.35
42	11	316	A86	C10-C11	3.63	1.45	1.34
42	19	311	A86	C5-C6	3.63	1.40	1.35
42	21	314	A86	C21-C20	3.63	1.57	1.51
42	12	318	A86	C19-C18	3.63	1.57	1.52
30	b	608	CLA	C4D-ND	-3.63	1.32	1.37
30	b	615	CLA	C4D-ND	-3.63	1.32	1.37
30	11	307	CLA	C4D-ND	-3.63	1.32	1.37
42	16	313	A86	C10-C11	3.63	1.45	1.34
42	13	311	A86	C9-C10	3.63	1.54	1.43
42	16	311	A86	C10-C11	3.63	1.45	1.34
42	14	316	A86	C10-C11	3.63	1.45	1.34
42	12	319	A86	C10-C11	3.63	1.45	1.34
30	b	614	CLA	C4D-ND	-3.63	1.32	1.37
30	20	208	CLA	C1D-ND	3.63	1.42	1.37
42	15	316	A86	C10-C11	3.63	1.45	1.34
32	c	515	BCR	C30-C25	-3.62	1.48	1.53
30	18	305	CLA	C4D-ND	-3.62	1.32	1.37
42	17	316	A86	C10-C11	3.62	1.45	1.34
42	12	315	A86	C9-C10	3.62	1.54	1.43
42	11	314	A86	C10-C11	3.62	1.45	1.34
42	13	315	A86	C10-C11	3.62	1.45	1.34
30	B	605	CLA	C4D-ND	-3.62	1.32	1.37
42	18	302	A86	C5-C6	3.62	1.40	1.35
30	15	301	CLA	C4D-ND	-3.62	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	301	A86	C10-C11	3.62	1.45	1.34
42	16	310	A86	C21-C20	3.61	1.57	1.51
42	18	313	A86	C9-C10	3.61	1.54	1.43
42	18	315	A86	C10-C11	3.61	1.45	1.34
42	12	317	A86	C21-C20	3.61	1.57	1.51
42	11	310	A86	C9-C10	3.61	1.54	1.43
42	16	310	A86	C19-C18	3.61	1.57	1.52
42	20	213	A86	C21-C20	3.61	1.57	1.51
42	12	315	A86	C10-C11	3.61	1.45	1.34
42	13	311	A86	C10-C11	3.61	1.45	1.34
37	B	625	LMU	O5B-C1B	3.61	1.51	1.41
42	15	310	A86	C9-C10	3.61	1.54	1.43
42	18	302	A86	C10-C11	3.61	1.45	1.34
37	12	302	LMU	O5B-C1B	3.61	1.51	1.41
42	15	310	A86	C10-C11	3.61	1.45	1.34
42	19	310	A86	C10-C11	3.61	1.45	1.34
42	13	314	A86	C19-C18	3.61	1.57	1.52
42	17	315	A86	C19-C18	3.61	1.57	1.52
42	15	315	A86	C10-C11	3.61	1.45	1.34
42	13	301	A86	C10-C11	3.61	1.45	1.34
42	19	310	A86	C21-C20	3.60	1.57	1.51
32	c	521	BCR	C30-C25	-3.60	1.48	1.53
30	B	615	CLA	C4D-ND	-3.60	1.32	1.37
30	19	309	CLA	C4D-ND	-3.60	1.32	1.37
30	16	309	CLA	C4D-ND	-3.60	1.32	1.37
42	15	315	A86	C5-C6	3.60	1.40	1.35
42	11	310	A86	C10-C11	3.60	1.45	1.34
30	13	304	CLA	C4D-ND	-3.60	1.32	1.37
30	19	306	CLA	C4D-ND	-3.60	1.32	1.37
42	18	313	A86	C10-C11	3.60	1.45	1.34
42	14	312	A86	C10-C11	3.59	1.45	1.34
42	21	310	A86	C10-C11	3.59	1.45	1.34
30	w	102	CLA	C4D-ND	-3.59	1.32	1.37
42	13	301	A86	C5-C6	3.59	1.40	1.35
31	d	403	PHO	C4D-ND	-3.59	1.33	1.38
32	Z	101	BCR	C30-C25	-3.59	1.48	1.53
42	12	304	A86	C10-C11	3.59	1.45	1.34
42	21	311	A86	C10-C11	3.58	1.45	1.34
42	11	313	A86	C10-C11	3.58	1.45	1.34
30	15	305	CLA	C1D-ND	3.58	1.42	1.37
42	11	316	A86	C5-C6	3.58	1.40	1.35
42	17	314	A86	C19-C18	3.58	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	12	304	A86	C5-C6	3.58	1.40	1.35
42	18	315	A86	C19-C18	3.58	1.57	1.52
30	19	307	CLA	C4D-ND	-3.58	1.32	1.37
32	B	616	BCR	C1-C6	-3.57	1.48	1.53
42	13	315	A86	C5-C6	3.57	1.40	1.35
30	21	308	CLA	C1D-ND	3.56	1.42	1.37
30	14	307	CLA	C1D-ND	3.56	1.42	1.37
30	18	308	CLA	C1D-ND	3.56	1.42	1.37
42	20	211	A86	C10-C11	3.56	1.44	1.34
30	20	205	CLA	C1D-ND	3.56	1.42	1.37
31	A	403	PHO	C4D-ND	-3.56	1.33	1.38
42	12	318	A86	C10-C11	3.56	1.44	1.34
42	14	315	A86	C10-C11	3.56	1.44	1.34
30	11	303	CLA	C4D-ND	-3.56	1.32	1.37
42	11	313	A86	C19-C18	3.55	1.57	1.52
42	17	314	A86	C10-C11	3.55	1.44	1.34
42	15	313	A86	C10-C11	3.55	1.44	1.34
30	18	310	CLA	C1D-ND	3.55	1.42	1.37
42	15	316	A86	C5-C6	3.55	1.40	1.35
42	15	313	A86	C19-C18	3.55	1.57	1.52
30	11	305	CLA	C1D-ND	3.55	1.42	1.37
40	d	405	PL9	C3-C4	-3.55	1.43	1.49
42	16	310	A86	C5-C6	3.54	1.40	1.35
42	21	312	A86	C10-C11	3.54	1.44	1.34
32	m	103	BCR	C1-C6	-3.54	1.48	1.53
30	B	614	CLA	C4D-ND	-3.54	1.32	1.37
30	C	506	CLA	C4D-ND	-3.54	1.32	1.37
42	21	311	A86	C21-C20	3.54	1.57	1.51
30	21	302	CLA	C1D-ND	3.53	1.42	1.37
42	16	310	A86	C10-C11	3.53	1.44	1.34
42	13	314	A86	C10-C11	3.53	1.44	1.34
30	20	202	CLA	C1D-ND	3.52	1.42	1.37
30	C	520	CLA	C4D-ND	-3.52	1.32	1.37
32	c	520	BCR	C1-C6	-3.52	1.48	1.53
30	18	307	CLA	C1D-ND	3.51	1.42	1.37
32	Y	101	BCR	C1-C6	-3.51	1.48	1.53
30	b	612	CLA	CMD-C2D	-3.51	1.43	1.50
30	14	305	CLA	C4D-ND	-3.51	1.32	1.37
30	12	312	CLA	C4D-ND	-3.51	1.32	1.37
42	20	211	A86	C21-C20	3.51	1.57	1.51
42	14	315	A86	C5-C6	3.50	1.40	1.35
42	17	315	A86	C5-C6	3.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	21	313	A86	C10-C11	3.50	1.44	1.34
30	20	206	CLA	C1D-ND	3.50	1.42	1.37
30	C	507	CLA	CMB-C2B	-3.50	1.43	1.50
30	b	605	CLA	C4D-ND	-3.50	1.32	1.37
42	17	311	A86	C5-C6	3.49	1.40	1.35
30	21	309	CLA	C4B-NB	3.48	1.42	1.37
30	11	315	CLA	C4D-ND	-3.47	1.32	1.37
30	19	305	CLA	C4D-ND	-3.47	1.32	1.37
42	15	314	A86	C5-C6	3.47	1.40	1.35
32	a	404	BCR	C1-C6	-3.47	1.49	1.53
42	14	316	A86	C5-C6	3.47	1.40	1.35
30	14	310	CLA	C4D-ND	-3.47	1.32	1.37
30	B	609	CLA	C4D-ND	-3.46	1.32	1.37
30	b	609	CLA	C4D-ND	-3.46	1.32	1.37
30	c	507	CLA	CMB-C2B	-3.46	1.43	1.50
30	21	302	CLA	C4D-ND	-3.46	1.32	1.37
30	16	305	CLA	C1D-ND	3.46	1.42	1.37
30	B	612	CLA	CMD-C2D	-3.46	1.43	1.50
30	20	207	CLA	C4D-ND	-3.45	1.32	1.37
30	b	611	CLA	CMB-C2B	-3.45	1.43	1.50
40	D	404	PL9	C3-C4	-3.44	1.43	1.49
42	11	314	A86	C5-C6	3.44	1.40	1.35
42	20	213	A86	C19-C18	3.44	1.57	1.52
30	21	304	CLA	C1D-ND	3.44	1.42	1.37
32	c	515	BCR	C1-C6	-3.43	1.49	1.53
30	12	303	CLA	C4D-ND	-3.43	1.33	1.37
30	18	311	CLA	C4B-NB	3.42	1.42	1.37
30	b	602	CLA	C1D-ND	3.42	1.42	1.37
42	18	314	A86	C5-C6	3.42	1.40	1.35
30	B	611	CLA	CMB-C2B	-3.42	1.43	1.50
32	c	516	BCR	C1-C6	-3.42	1.49	1.53
30	c	509	CLA	CMB-C2B	-3.42	1.43	1.50
32	C	515	BCR	C1-C6	-3.41	1.49	1.53
42	21	314	A86	C19-C18	3.41	1.57	1.52
30	B	602	CLA	C1D-ND	3.41	1.42	1.37
30	20	209	CLA	C4D-ND	-3.41	1.33	1.37
42	18	315	A86	C5-C6	3.41	1.40	1.35
30	21	307	CLA	C1D-ND	3.40	1.42	1.37
30	17	310	CLA	C4D-ND	-3.40	1.33	1.37
42	20	201	A86	C17-C18	-3.40	1.47	1.52
42	11	313	A86	C5-C6	3.40	1.40	1.35
30	15	309	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	301	A86	C5-C6	3.40	1.40	1.35
42	17	316	A86	C5-C6	3.40	1.40	1.35
30	14	302	CLA	C4D-ND	-3.40	1.33	1.37
30	11	309	CLA	C1D-ND	3.40	1.42	1.37
32	Z	101	BCR	C1-C6	-3.39	1.49	1.53
30	18	312	CLA	C1D-ND	3.39	1.42	1.37
30	11	308	CLA	C4D-ND	-3.39	1.33	1.37
30	12	313	CLA	C4D-ND	-3.39	1.33	1.37
30	15	302	CLA	C1D-ND	3.38	1.41	1.37
30	20	208	CLA	C4D-ND	-3.38	1.33	1.37
30	15	304	CLA	C4B-NB	3.38	1.41	1.37
30	16	308	CLA	C4D-ND	-3.38	1.33	1.37
42	21	312	A86	C21-C20	3.38	1.57	1.51
30	17	308	CLA	MG-NB	-3.38	1.99	2.05
42	12	315	A86	C19-C18	3.38	1.57	1.52
32	A	405	BCR	C1-C6	-3.38	1.49	1.53
30	13	306	CLA	C1D-ND	3.37	1.41	1.37
30	C	511	CLA	MG-NB	-3.37	1.99	2.05
42	14	312	A86	C19-C18	3.37	1.57	1.52
42	13	311	A86	C19-C18	3.37	1.57	1.52
42	12	319	A86	C5-C6	3.37	1.40	1.35
30	20	203	CLA	C1D-ND	3.37	1.41	1.37
42	13	314	A86	C5-C6	3.37	1.40	1.35
30	17	309	CLA	C1D-ND	3.37	1.41	1.37
30	C	509	CLA	CMB-C2B	-3.37	1.43	1.50
42	15	313	A86	C5-C6	3.37	1.40	1.35
42	18	313	A86	C19-C18	3.36	1.57	1.52
30	11	309	CLA	C4D-ND	-3.36	1.33	1.37
30	17	306	CLA	C1D-ND	3.36	1.41	1.37
30	21	303	CLA	C1D-ND	3.36	1.41	1.37
30	c	511	CLA	MG-NB	-3.36	1.99	2.05
30	17	310	CLA	C1D-ND	3.36	1.41	1.37
30	17	307	CLA	C4D-ND	-3.36	1.33	1.37
30	12	306	CLA	C4D-ND	-3.35	1.33	1.37
42	21	311	A86	C5-C6	3.35	1.40	1.35
42	20	211	A86	C5-C6	3.35	1.40	1.35
30	15	303	CLA	C4D-ND	-3.35	1.33	1.37
30	12	309	CLA	C1D-ND	3.35	1.41	1.37
30	13	310	CLA	C1D-ND	3.35	1.41	1.37
30	11	302	CLA	C4D-ND	-3.35	1.33	1.37
30	14	311	CLA	C1D-ND	3.34	1.41	1.37
30	z	101	CLA	C1D-ND	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	18	301	CLA	C4D-ND	-3.34	1.33	1.37
30	19	304	CLA	C1D-ND	3.34	1.41	1.37
30	13	303	CLA	C4D-ND	-3.34	1.33	1.37
30	B	612	CLA	MG-ND	-3.34	1.99	2.05
30	16	301	CLA	C1D-ND	3.34	1.41	1.37
42	17	314	A86	C5-C6	3.34	1.40	1.35
30	11	305	CLA	C4D-ND	-3.33	1.33	1.37
30	18	307	CLA	C4D-ND	-3.33	1.33	1.37
40	D	407	PL9	C53-C6	-3.33	1.43	1.50
32	b	623	BCR	C1-C6	-3.33	1.49	1.53
30	19	303	CLA	C4D-ND	-3.33	1.33	1.37
30	16	302	CLA	C1D-ND	3.33	1.41	1.37
30	Z	102	CLA	C4D-ND	-3.33	1.33	1.37
30	21	303	CLA	C4D-ND	-3.33	1.33	1.37
30	16	303	CLA	C1D-ND	3.33	1.41	1.37
30	14	311	CLA	C4D-ND	-3.33	1.33	1.37
42	16	313	A86	C5-C6	3.33	1.40	1.35
42	17	302	A86	C5-C6	3.32	1.40	1.35
42	21	313	A86	C5-C6	3.32	1.40	1.35
30	C	519	CLA	C1D-ND	3.32	1.41	1.37
30	12	309	CLA	C4D-ND	-3.32	1.33	1.37
30	16	303	CLA	C4D-ND	-3.32	1.33	1.37
30	20	209	CLA	C1D-ND	3.32	1.41	1.37
30	20	206	CLA	C4D-ND	-3.32	1.33	1.37
30	b	612	CLA	MG-ND	-3.31	1.99	2.05
42	12	318	A86	C5-C6	3.31	1.40	1.35
30	11	307	CLA	C1D-ND	3.31	1.41	1.37
42	11	310	A86	C19-C18	3.31	1.57	1.52
30	C	520	CLA	C1D-ND	3.31	1.41	1.37
30	11	301	CLA	C1D-ND	3.31	1.41	1.37
30	19	303	CLA	C1D-ND	3.31	1.41	1.37
30	13	306	CLA	C4D-ND	-3.31	1.33	1.37
30	13	309	CLA	C4D-ND	-3.31	1.33	1.37
30	18	304	CLA	C1D-ND	3.31	1.41	1.37
42	21	310	A86	C5-C6	3.31	1.40	1.35
42	17	302	A86	C19-C18	3.31	1.57	1.52
30	b	615	CLA	C1D-ND	3.31	1.41	1.37
30	18	309	CLA	C1D-ND	3.31	1.41	1.37
30	15	307	CLA	C1D-ND	3.31	1.41	1.37
30	12	312	CLA	C1D-ND	3.30	1.41	1.37
30	13	305	CLA	C1D-ND	3.30	1.41	1.37
30	17	304	CLA	C1D-ND	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	503	CLA	C1D-ND	3.30	1.41	1.37
30	20	207	CLA	C1D-ND	3.30	1.41	1.37
30	11	304	CLA	C1D-ND	3.30	1.41	1.37
42	19	312	A86	C5-C6	3.30	1.40	1.35
30	B	615	CLA	C1D-ND	3.30	1.41	1.37
31	D	403	PHO	C4D-ND	-3.30	1.34	1.38
30	12	314	CLA	C1D-ND	3.30	1.41	1.37
30	14	303	CLA	C1D-ND	3.30	1.41	1.37
30	14	307	CLA	C4D-ND	-3.29	1.33	1.37
42	15	310	A86	C19-C18	3.29	1.57	1.52
30	16	301	CLA	C4D-ND	-3.29	1.33	1.37
30	13	308	CLA	C1D-ND	3.29	1.41	1.37
30	20	203	CLA	C4D-ND	-3.29	1.33	1.37
30	16	308	CLA	C1D-ND	3.28	1.41	1.37
30	20	202	CLA	C4D-ND	-3.28	1.33	1.37
40	d	408	PL9	C53-C6	-3.28	1.43	1.50
30	c	511	CLA	CMD-C2D	-3.28	1.43	1.50
30	C	512	CLA	C1D-ND	3.28	1.41	1.37
30	19	309	CLA	C1D-ND	3.28	1.41	1.37
32	F	101	BCR	C1-C6	-3.28	1.49	1.53
30	12	308	CLA	C4D-ND	-3.27	1.33	1.37
30	12	305	CLA	C1D-ND	3.27	1.41	1.37
30	14	309	CLA	C1D-ND	3.27	1.41	1.37
30	w	103	CLA	C4B-NB	3.27	1.41	1.37
42	19	310	A86	C5-C6	3.27	1.40	1.35
30	C	503	CLA	C1D-ND	3.27	1.41	1.37
30	12	311	CLA	C1D-ND	3.27	1.41	1.37
30	18	308	CLA	C4D-ND	-3.27	1.33	1.37
30	16	306	CLA	C4D-ND	-3.27	1.33	1.37
30	C	511	CLA	CMD-C2D	-3.26	1.43	1.50
30	15	306	CLA	C4D-ND	-3.26	1.33	1.37
30	c	512	CLA	C1D-ND	3.26	1.41	1.37
42	21	312	A86	C5-C6	3.26	1.40	1.35
42	14	313	A86	C5-C6	3.25	1.40	1.35
30	12	303	CLA	C1D-ND	3.25	1.41	1.37
42	17	312	A86	C5-C6	3.25	1.40	1.35
30	15	303	CLA	C1D-ND	3.25	1.41	1.37
30	19	302	CLA	C1D-ND	3.25	1.41	1.37
30	17	307	CLA	C4B-NB	3.25	1.41	1.37
30	21	305	CLA	C4D-ND	-3.25	1.33	1.37
30	b	604	CLA	C1D-ND	3.25	1.41	1.37
42	13	312	A86	C5-C6	3.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	310	CLA	C1D-ND	3.24	1.41	1.37
30	13	302	CLA	C1D-ND	3.24	1.41	1.37
42	14	313	A86	C19-C18	3.24	1.57	1.52
31	d	404	PHO	C4D-ND	-3.24	1.34	1.38
30	12	310	CLA	C4B-NB	3.24	1.41	1.37
30	19	301	CLA	C1D-ND	3.23	1.41	1.37
42	19	312	A86	C19-C18	3.23	1.57	1.52
30	17	308	CLA	C1D-ND	3.23	1.41	1.37
42	18	314	A86	C19-C18	3.23	1.57	1.52
30	17	309	CLA	C3B-C4B	3.22	1.50	1.42
30	15	308	CLA	C4D-ND	-3.22	1.33	1.37
30	15	309	CLA	C4D-ND	-3.22	1.33	1.37
30	11	315	CLA	C1D-ND	3.22	1.41	1.37
30	14	304	CLA	C4D-ND	-3.22	1.33	1.37
32	B	624	BCR	C1-C6	-3.22	1.49	1.53
30	14	302	CLA	C1D-ND	3.22	1.41	1.37
30	b	612	CLA	MG-NB	-3.22	1.99	2.05
42	11	311	A86	C19-C18	3.22	1.57	1.52
42	19	310	A86	C19-C18	3.21	1.57	1.52
30	18	311	CLA	C1D-ND	3.21	1.41	1.37
30	w	103	CLA	C4D-ND	-3.21	1.33	1.37
30	11	304	CLA	C4D-ND	-3.21	1.33	1.37
30	13	309	CLA	C1D-ND	3.21	1.41	1.37
30	17	304	CLA	C4D-ND	-3.20	1.33	1.37
32	f	101	BCR	C1-C6	-3.20	1.49	1.53
42	19	311	A86	C25-C24	3.20	1.42	1.34
30	13	310	CLA	C4D-ND	-3.20	1.33	1.37
42	12	316	A86	C5-C6	3.20	1.40	1.35
30	14	306	CLA	C4D-ND	-3.20	1.33	1.37
30	14	306	CLA	C1D-ND	3.20	1.41	1.37
30	13	305	CLA	C4D-ND	-3.20	1.33	1.37
42	15	311	A86	C19-C18	3.20	1.56	1.52
30	18	311	CLA	C4D-ND	-3.19	1.33	1.37
30	12	310	CLA	C1D-ND	3.19	1.41	1.37
30	12	314	CLA	C4D-ND	-3.19	1.33	1.37
42	15	311	A86	C5-C6	3.19	1.40	1.35
30	18	312	CLA	C4D-ND	-3.19	1.33	1.37
30	B	604	CLA	C1D-ND	3.19	1.41	1.37
30	14	308	CLA	C4B-NB	3.19	1.41	1.37
30	B	612	CLA	MG-NB	-3.19	1.99	2.05
30	11	308	CLA	C1D-ND	3.19	1.41	1.37
30	C	503	CLA	MG-NB	-3.19	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	15	311	A86	C25-C24	3.19	1.42	1.34
42	21	313	A86	C19-C18	3.19	1.56	1.52
42	16	311	A86	C25-C24	3.18	1.42	1.34
42	11	311	A86	C25-C24	3.18	1.42	1.34
30	11	306	CLA	C4B-NB	3.18	1.41	1.37
30	17	306	CLA	C4D-ND	-3.18	1.33	1.37
42	13	312	A86	C19-C18	3.18	1.56	1.52
30	21	309	CLA	C4D-ND	-3.18	1.33	1.37
42	11	311	A86	C5-C6	3.18	1.40	1.35
42	12	316	A86	C25-C24	3.17	1.42	1.34
30	17	307	CLA	C1D-ND	3.17	1.41	1.37
30	C	509	CLA	MG-NB	-3.17	1.99	2.05
30	18	303	CLA	C1D-ND	3.17	1.41	1.37
30	12	308	CLA	C1D-ND	3.17	1.41	1.37
42	12	316	A86	C19-C18	3.17	1.56	1.52
30	W	103	CLA	C4B-NB	3.17	1.41	1.37
30	20	205	CLA	C4D-ND	-3.16	1.33	1.37
30	13	307	CLA	C4B-NB	3.16	1.41	1.37
30	21	308	CLA	C4D-ND	-3.16	1.33	1.37
42	17	312	A86	C25-C24	3.16	1.42	1.34
32	b	616	BCR	C1-C6	-3.16	1.49	1.53
30	12	307	CLA	C1D-ND	3.16	1.41	1.37
32	c	521	BCR	C1-C6	-3.16	1.49	1.53
42	13	312	A86	C25-C24	3.16	1.42	1.34
30	15	306	CLA	C4B-NB	3.16	1.41	1.37
30	14	308	CLA	C4D-ND	-3.16	1.33	1.37
30	D	401	CLA	MG-NB	-3.16	1.99	2.05
42	13	311	A86	C5-C6	3.15	1.40	1.35
30	21	305	CLA	C4B-NB	3.15	1.41	1.37
42	16	311	A86	C5-C6	3.15	1.40	1.35
30	c	509	CLA	MG-NB	-3.15	1.99	2.05
30	15	305	CLA	C4B-NB	3.15	1.41	1.37
30	13	303	CLA	C1D-ND	3.15	1.41	1.37
32	B	617	BCR	C1-C6	-3.15	1.49	1.53
42	17	312	A86	C19-C18	3.15	1.56	1.52
30	17	309	CLA	C4D-ND	-3.15	1.33	1.37
39	c	518	DGD	O2G-C2G	-3.15	1.38	1.46
30	21	301	CLA	C4B-NB	3.14	1.41	1.37
42	20	211	A86	C19-C18	3.14	1.56	1.52
30	20	204	CLA	C1D-ND	3.14	1.41	1.37
30	d	401	CLA	MG-NB	-3.14	1.99	2.05
39	C	517	DGD	O2G-C2G	-3.14	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	313	A86	C25-C24	3.14	1.42	1.34
42	16	311	A86	C19-C18	3.14	1.56	1.52
30	21	304	CLA	C4D-ND	-3.14	1.33	1.37
30	W	103	CLA	C4D-ND	-3.13	1.33	1.37
30	21	307	CLA	C4D-ND	-3.13	1.33	1.37
30	B	605	CLA	C1D-ND	3.13	1.41	1.37
30	17	301	CLA	C1D-ND	3.13	1.41	1.37
30	18	308	CLA	C4B-NB	3.13	1.41	1.37
42	20	210	A86	C25-C24	3.12	1.42	1.34
30	12	313	CLA	C1D-ND	3.12	1.41	1.37
30	13	307	CLA	C4D-ND	-3.12	1.33	1.37
30	18	304	CLA	C4D-ND	-3.12	1.33	1.37
30	18	301	CLA	C1D-ND	3.12	1.41	1.37
30	B	604	CLA	MG-NB	-3.12	1.99	2.05
30	14	304	CLA	C1D-ND	3.12	1.41	1.37
30	B	606	CLA	C4B-NB	3.12	1.41	1.37
42	20	201	A86	C25-C24	3.11	1.42	1.34
42	19	312	A86	C25-C24	3.11	1.42	1.34
30	14	308	CLA	C1D-ND	3.11	1.41	1.37
37	B	625	LMU	O5'-C1'	3.11	1.49	1.41
30	c	503	CLA	MG-NB	-3.11	1.99	2.05
30	21	301	CLA	C4D-ND	-3.11	1.33	1.37
30	c	511	CLA	C1B-NB	-3.11	1.34	1.37
30	21	307	CLA	C4B-NB	3.11	1.41	1.37
35	L	102	LHG	O7-C5	-3.11	1.38	1.46
42	14	312	A86	C5-C6	3.11	1.39	1.35
32	b	617	BCR	C1-C6	-3.10	1.49	1.53
42	18	313	A86	C5-C6	3.10	1.39	1.35
42	21	311	A86	C19-C18	3.10	1.56	1.52
32	C	518	BCR	C1-C6	-3.10	1.49	1.53
30	15	308	CLA	C1D-ND	3.10	1.41	1.37
37	12	302	LMU	O5'-C1'	3.10	1.49	1.41
42	20	212	A86	C25-C24	3.10	1.42	1.34
42	11	312	A86	C25-C24	3.10	1.42	1.34
30	15	301	CLA	C1D-ND	3.10	1.41	1.37
30	11	302	CLA	C1D-ND	3.09	1.41	1.37
30	15	305	CLA	C4D-ND	-3.09	1.33	1.37
40	D	407	PL9	C36-C34	-3.09	1.44	1.51
42	15	312	A86	C25-C24	3.09	1.42	1.34
42	17	313	A86	C25-C24	3.09	1.42	1.34
36	b	619	LMG	O8-C9	-3.09	1.38	1.45
30	b	601	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	314	A86	C25-C24	3.09	1.42	1.34
32	B	618	BCR	C30-C25	-3.09	1.49	1.53
30	13	307	CLA	C1D-ND	3.08	1.41	1.37
31	d	403	PHO	CMC-C2C	-3.08	1.45	1.50
30	18	305	CLA	C1D-ND	3.08	1.41	1.37
30	c	508	CLA	MG-NB	-3.08	1.99	2.05
32	B	618	BCR	C1-C6	-3.08	1.49	1.53
32	A	405	BCR	C30-C25	-3.08	1.49	1.53
31	A	403	PHO	CMC-C2C	-3.08	1.45	1.50
42	18	314	A86	C25-C24	3.08	1.42	1.34
42	17	311	A86	C25-C24	3.07	1.42	1.34
42	13	313	A86	C25-C24	3.07	1.42	1.34
32	a	404	BCR	C30-C25	-3.07	1.49	1.53
30	16	305	CLA	C4D-ND	-3.07	1.33	1.37
30	12	306	CLA	C1D-ND	3.07	1.41	1.37
40	d	408	PL9	C36-C34	-3.07	1.44	1.51
30	11	306	CLA	C4D-ND	-3.06	1.33	1.37
36	c	519	LMG	O7-C8	-3.06	1.38	1.46
30	18	310	CLA	C4D-ND	-3.06	1.33	1.37
30	C	511	CLA	C1B-NB	-3.06	1.34	1.37
30	12	310	CLA	C4D-ND	-3.06	1.33	1.37
42	21	311	A86	C25-C24	3.06	1.42	1.34
30	20	203	CLA	C4B-NB	3.06	1.41	1.37
30	b	613	CLA	C1B-NB	-3.06	1.34	1.37
30	b	605	CLA	C1D-ND	3.06	1.41	1.37
31	d	403	PHO	CAC-C3C	-3.06	1.46	1.51
42	21	313	A86	C25-C24	3.06	1.42	1.34
31	A	403	PHO	CAC-C3C	-3.06	1.46	1.51
30	18	309	CLA	C4B-NB	3.05	1.41	1.37
30	b	606	CLA	C4B-NB	3.05	1.41	1.37
30	17	303	CLA	C1D-ND	3.05	1.41	1.37
30	15	304	CLA	C4D-ND	-3.05	1.33	1.37
30	c	510	CLA	MG-NB	-3.05	1.99	2.05
30	18	306	CLA	C4B-NB	3.05	1.41	1.37
35	l	102	LHG	O7-C5	-3.05	1.39	1.46
36	Q	301	LMG	O7-C8	-3.05	1.39	1.46
30	b	604	CLA	MG-NB	-3.04	1.99	2.05
42	19	311	A86	C17-C18	-3.04	1.47	1.52
42	12	317	A86	C25-C24	3.04	1.42	1.34
36	B	620	LMG	O8-C9	-3.04	1.38	1.45
42	16	312	A86	C25-C24	3.04	1.42	1.34
42	20	211	A86	C25-C24	3.04	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	103	SQD	O47-C7	3.04	1.42	1.34
31	A	403	PHO	CMD-C2D	-3.04	1.45	1.51
39	J	101	DGD	O2G-C2G	-3.04	1.39	1.46
30	21	306	CLA	C4D-ND	-3.03	1.33	1.37
30	d	407	CLA	MG-NB	-3.03	1.99	2.05
42	12	315	A86	C5-C6	3.03	1.39	1.35
30	18	307	CLA	C4B-NB	3.03	1.41	1.37
39	j	101	DGD	O2G-C2G	-3.03	1.39	1.46
30	15	301	CLA	C4B-NB	3.03	1.41	1.37
42	11	310	A86	C5-C6	3.02	1.39	1.35
30	C	510	CLA	MG-NB	-3.02	1.99	2.05
30	19	304	CLA	C4D-ND	-3.02	1.33	1.37
30	C	508	CLA	MG-NB	-3.02	1.99	2.05
42	12	317	A86	C19-C18	3.02	1.56	1.52
42	11	312	A86	C19-C18	3.02	1.56	1.52
30	c	507	CLA	MG-NB	-3.02	1.99	2.05
30	17	310	CLA	C4B-NB	3.01	1.41	1.37
30	b	606	CLA	C1D-ND	3.01	1.41	1.37
39	c	517	DGD	O1G-C1G	-3.01	1.38	1.45
42	19	311	A86	C21-C20	3.01	1.56	1.51
42	13	314	A86	C25-C24	3.01	1.42	1.34
42	12	304	A86	C19-C18	3.01	1.56	1.52
30	b	613	CLA	MG-NB	-3.01	1.99	2.05
33	l	101	SQD	O47-C7	3.01	1.42	1.34
30	B	610	CLA	MG-NB	-3.01	1.99	2.05
30	B	613	CLA	MG-NB	-3.01	1.99	2.05
30	b	610	CLA	MG-NB	-3.00	1.99	2.05
30	13	310	CLA	C4B-NB	3.00	1.41	1.37
42	15	312	A86	C19-C18	3.00	1.56	1.52
30	B	601	CLA	C1D-ND	3.00	1.41	1.37
30	14	305	CLA	C1D-ND	3.00	1.41	1.37
30	19	306	CLA	C1D-ND	3.00	1.41	1.37
30	21	308	CLA	C4B-NB	3.00	1.41	1.37
31	d	403	PHO	CMD-C2D	-3.00	1.45	1.51
42	15	310	A86	C5-C6	3.00	1.39	1.35
42	13	315	A86	C25-C24	2.99	1.42	1.34
42	18	315	A86	C25-C24	2.99	1.42	1.34
30	11	306	CLA	C1D-ND	2.99	1.41	1.37
30	17	309	CLA	C4B-NB	2.99	1.41	1.37
30	b	611	CLA	MG-NB	-2.99	1.99	2.05
30	b	622	CLA	CMD-C2D	-2.99	1.44	1.50
42	17	302	A86	C25-C24	2.99	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	403	PHO	CMC-C2C	-2.98	1.45	1.50
42	11	313	A86	C25-C24	2.98	1.42	1.34
42	16	310	A86	C25-C24	2.98	1.42	1.34
42	21	312	A86	C25-C24	2.98	1.42	1.34
30	W	102	CLA	C1D-ND	2.98	1.41	1.37
36	D	408	LMG	O7-C8	-2.98	1.39	1.46
30	D	406	CLA	MG-NB	-2.98	1.99	2.05
36	c	519	LMG	O1-C7	-2.98	1.38	1.43
30	19	307	CLA	C1D-ND	2.98	1.41	1.37
42	14	315	A86	C25-C24	2.98	1.42	1.34
42	14	314	A86	C19-C18	2.98	1.56	1.52
30	17	301	CLA	MG-NB	-2.98	1.99	2.05
42	20	213	A86	C25-C24	2.97	1.42	1.34
30	D	402	CLA	C1D-ND	2.97	1.41	1.37
30	16	308	CLA	C4B-NB	2.97	1.41	1.37
30	b	622	CLA	MG-NB	-2.97	1.99	2.05
30	B	623	CLA	CMD-C2D	-2.97	1.44	1.50
42	21	314	A86	C25-C24	2.97	1.42	1.34
42	17	314	A86	C25-C24	2.97	1.42	1.34
30	d	402	CLA	C1D-ND	2.97	1.41	1.37
36	Q	301	LMG	O1-C7	-2.97	1.38	1.43
42	15	315	A86	C19-C18	2.97	1.56	1.52
30	11	303	CLA	C1D-ND	2.97	1.41	1.37
36	d	410	LMG	O7-C8	-2.97	1.39	1.46
42	21	312	A86	C19-C18	2.97	1.56	1.52
30	B	611	CLA	MG-NB	-2.97	1.99	2.05
39	C	516	DGD	O1G-C1G	-2.97	1.38	1.45
30	13	304	CLA	C1D-ND	2.97	1.41	1.37
42	16	312	A86	C19-C18	2.97	1.56	1.52
32	b	617	BCR	C30-C25	-2.97	1.49	1.53
32	c	520	BCR	C30-C25	-2.96	1.49	1.53
42	12	318	A86	C25-C24	2.96	1.42	1.34
30	17	306	CLA	MG-NB	-2.96	1.99	2.05
42	17	313	A86	C19-C18	2.96	1.56	1.52
42	15	313	A86	C25-C24	2.96	1.42	1.34
30	B	613	CLA	C1B-NB	-2.96	1.34	1.37
42	17	315	A86	C25-C24	2.96	1.42	1.34
42	13	301	A86	C25-C24	2.96	1.42	1.34
30	C	506	CLA	C1D-ND	2.96	1.41	1.37
30	15	302	CLA	C4D-ND	-2.96	1.33	1.37
30	Z	102	CLA	C4B-NB	2.96	1.41	1.37
30	B	623	CLA	MG-NB	-2.95	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	12	304	A86	C25-C24	2.95	1.42	1.34
31	d	404	PHO	C4D-CHA	2.95	1.44	1.39
30	18	306	CLA	C4D-ND	-2.95	1.33	1.37
42	13	301	A86	C19-C18	2.95	1.56	1.52
30	c	510	CLA	CMB-C2B	-2.95	1.44	1.50
30	b	608	CLA	C4B-NB	2.95	1.41	1.37
30	15	302	CLA	C4B-NB	2.95	1.41	1.37
32	b	616	BCR	C30-C25	-2.95	1.49	1.53
42	13	313	A86	C19-C18	2.94	1.56	1.52
33	B	621	SQD	O48-C23	2.94	1.41	1.33
30	B	606	CLA	C1D-ND	2.94	1.41	1.37
30	c	506	CLA	C1D-ND	2.94	1.41	1.37
32	H	101	BCR	C30-C25	-2.94	1.49	1.53
30	19	305	CLA	C1D-ND	2.94	1.41	1.37
30	11	309	CLA	C4B-NB	2.93	1.41	1.37
30	19	308	CLA	C1D-ND	2.93	1.41	1.37
30	B	608	CLA	C4B-NB	2.93	1.41	1.37
42	18	302	A86	C25-C24	2.93	1.42	1.34
42	15	315	A86	C25-C24	2.93	1.42	1.34
31	D	403	PHO	C4D-CHA	2.93	1.44	1.39
32	a	408	BCR	C1-C6	-2.93	1.49	1.53
30	C	510	CLA	CMB-C2B	-2.93	1.44	1.50
42	15	316	A86	C19-C18	2.93	1.56	1.52
30	w	102	CLA	C1D-ND	2.93	1.41	1.37
30	12	308	CLA	MG-NB	-2.93	2.00	2.05
30	16	304	CLA	C1D-ND	2.92	1.41	1.37
42	11	316	A86	C25-C24	2.92	1.42	1.34
30	21	302	CLA	C4B-NB	2.92	1.41	1.37
30	c	504	CLA	C1D-ND	2.92	1.41	1.37
30	18	304	CLA	C4B-NB	2.92	1.41	1.37
33	b	620	SQD	O48-C23	2.92	1.41	1.33
30	12	314	CLA	C4B-NB	2.92	1.41	1.37
31	A	403	PHO	C1D-C2D	2.92	1.42	1.39
42	21	310	A86	O-C13	-2.92	1.17	1.23
30	16	302	CLA	MG-NB	-2.92	2.00	2.05
42	11	316	A86	C19-C18	2.91	1.56	1.52
30	15	308	CLA	C4B-NB	2.91	1.41	1.37
42	19	310	A86	C25-C24	2.91	1.42	1.34
42	13	315	A86	C19-C18	2.91	1.56	1.52
42	18	302	A86	C19-C18	2.91	1.56	1.52
31	d	404	PHO	CMC-C2C	-2.91	1.45	1.50
30	b	609	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	18	309	CLA	MG-NB	-2.91	2.00	2.05
35	b	621	LHG	O7-C5	-2.90	1.39	1.46
30	18	305	CLA	C4B-NB	2.90	1.41	1.37
30	a	403	CLA	MG-NB	-2.90	2.00	2.05
30	C	511	CLA	MG-ND	-2.90	2.00	2.05
30	C	503	CLA	MG-ND	-2.90	2.00	2.05
30	19	301	CLA	MG-NB	-2.90	2.00	2.05
40	d	408	PL9	C26-C24	-2.90	1.45	1.51
31	d	403	PHO	C1D-C2D	2.90	1.42	1.39
30	c	503	CLA	CMC-C2C	-2.90	1.44	1.50
30	A	404	CLA	MG-NB	-2.90	2.00	2.05
32	Y	101	BCR	C30-C25	-2.89	1.49	1.53
30	C	519	CLA	MG-NB	-2.89	2.00	2.05
30	C	504	CLA	C1D-ND	2.89	1.41	1.37
42	15	316	A86	C25-C24	2.89	1.42	1.34
30	13	305	CLA	MG-NB	-2.89	2.00	2.05
30	14	306	CLA	MG-NB	-2.89	2.00	2.05
30	B	608	CLA	C3B-C4B	2.89	1.49	1.42
30	C	509	CLA	C1B-NB	-2.89	1.34	1.37
30	C	508	CLA	MG-ND	-2.88	2.00	2.05
30	15	309	CLA	C4B-NB	2.88	1.41	1.37
30	b	614	CLA	C1D-ND	2.88	1.41	1.37
30	21	306	CLA	C4B-NB	2.88	1.41	1.37
42	20	201	A86	C24-C1	2.88	1.52	1.45
30	b	607	CLA	MG-NB	-2.88	2.00	2.05
30	18	301	CLA	C4B-NB	2.88	1.41	1.37
30	14	311	CLA	C4B-NB	2.88	1.41	1.37
30	15	305	CLA	C3B-C4B	2.88	1.49	1.42
30	11	307	CLA	MG-NB	-2.88	2.00	2.05
35	B	622	LHG	O7-C5	-2.88	1.39	1.46
30	D	405	CLA	CMD-C2D	-2.88	1.44	1.50
30	21	309	CLA	C3B-C4B	2.88	1.49	1.42
32	B	617	BCR	C30-C25	-2.87	1.49	1.53
30	20	209	CLA	C4B-NB	2.87	1.41	1.37
30	20	202	CLA	C4B-NB	2.87	1.41	1.37
30	c	508	CLA	C1D-ND	2.87	1.41	1.37
30	17	305	CLA	C1D-ND	2.87	1.41	1.37
30	19	303	CLA	C4B-NB	2.87	1.41	1.37
30	C	507	CLA	MG-NB	-2.87	2.00	2.05
30	c	513	CLA	C1D-ND	2.87	1.41	1.37
30	C	514	CLA	C1D-ND	2.87	1.41	1.37
30	c	509	CLA	C1B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	307	CLA	C1D-ND	2.86	1.41	1.37
42	13	311	A86	C25-C24	2.86	1.42	1.34
30	B	609	CLA	C1D-ND	2.86	1.41	1.37
30	c	511	CLA	MG-ND	-2.86	2.00	2.05
40	d	408	PL9	C11-C9	-2.86	1.45	1.51
30	11	304	CLA	MG-NB	-2.86	2.00	2.05
30	C	513	CLA	C1D-ND	2.86	1.41	1.37
30	c	503	CLA	MG-ND	-2.85	2.00	2.05
30	B	607	CLA	MG-NB	-2.85	2.00	2.05
42	18	313	A86	C25-C24	2.85	1.41	1.34
30	B	611	CLA	CMC-C2C	-2.85	1.44	1.50
30	b	603	CLA	MG-NB	-2.85	2.00	2.05
30	b	611	CLA	CMC-C2C	-2.85	1.44	1.50
32	A	409	BCR	C1-C6	-2.85	1.49	1.53
30	16	307	CLA	C3B-C4B	2.84	1.49	1.42
30	C	503	CLA	CMC-C2C	-2.84	1.44	1.50
30	15	303	CLA	C4B-NB	2.84	1.41	1.37
42	17	316	A86	C19-C18	2.84	1.56	1.52
30	c	508	CLA	MG-ND	-2.84	2.00	2.05
40	D	407	PL9	C11-C9	-2.84	1.45	1.51
30	B	601	CLA	MG-NB	-2.84	2.00	2.05
30	c	506	CLA	CMD-C2D	-2.84	1.44	1.50
30	C	508	CLA	C1D-ND	2.84	1.41	1.37
30	C	506	CLA	CMD-C2D	-2.84	1.44	1.50
30	16	307	CLA	MG-NB	-2.84	2.00	2.05
30	18	312	CLA	C4B-NB	2.84	1.41	1.37
30	B	607	CLA	C1D-ND	2.83	1.41	1.37
31	A	403	PHO	CBD-CGD	-2.83	1.48	1.52
30	b	606	CLA	CMD-C2D	-2.83	1.44	1.50
30	z	101	CLA	MG-NB	-2.83	2.00	2.05
31	d	403	PHO	CBD-CGD	-2.83	1.48	1.52
30	d	406	CLA	CMD-C2D	-2.83	1.44	1.50
42	15	314	A86	C25-C24	2.83	1.41	1.34
42	21	310	A86	C25-C24	2.83	1.41	1.34
30	c	514	CLA	C1D-ND	2.83	1.41	1.37
30	B	615	CLA	C3B-C4B	2.83	1.49	1.42
42	14	316	A86	C25-C24	2.82	1.41	1.34
30	B	603	CLA	MG-NB	-2.82	2.00	2.05
30	d	402	CLA	MG-NB	-2.82	2.00	2.05
30	b	604	CLA	MG-ND	-2.82	2.00	2.05
32	c	516	BCR	C30-C25	-2.82	1.49	1.53
42	14	301	A86	C25-C24	2.82	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	401	CLA	CMB-C2B	-2.82	1.44	1.50
30	15	302	CLA	C3B-C4B	2.82	1.49	1.42
30	b	608	CLA	C3B-C4B	2.82	1.49	1.42
33	A	406	SQD	O48-C23	2.82	1.41	1.33
40	D	407	PL9	C26-C24	-2.82	1.45	1.51
31	d	403	PHO	CMB-C2B	-2.82	1.45	1.51
30	a	402	CLA	C1D-ND	2.82	1.41	1.37
42	16	313	A86	C25-C24	2.82	1.41	1.34
30	19	302	CLA	MG-NB	-2.82	2.00	2.05
32	A	409	BCR	C30-C25	-2.81	1.49	1.53
30	D	402	CLA	MG-NB	-2.81	2.00	2.05
30	D	401	CLA	CMB-C2B	-2.81	1.44	1.50
30	19	307	CLA	MG-NB	-2.81	2.00	2.05
30	D	401	CLA	CMD-C2D	-2.81	1.44	1.50
30	w	102	CLA	C3B-C4B	2.81	1.49	1.42
30	C	504	CLA	CMD-C2D	-2.81	1.44	1.50
42	11	314	A86	C25-C24	2.81	1.41	1.34
30	c	504	CLA	CMD-C2D	-2.81	1.44	1.50
31	A	403	PHO	CMB-C2B	-2.81	1.45	1.51
42	17	316	A86	C25-C24	2.81	1.41	1.34
30	13	308	CLA	MG-NB	-2.81	2.00	2.05
30	C	510	CLA	C1B-NB	-2.80	1.34	1.37
30	B	614	CLA	C1D-ND	2.80	1.41	1.37
30	16	309	CLA	C1D-ND	2.80	1.41	1.37
30	d	406	CLA	MG-NB	-2.80	2.00	2.05
30	C	502	CLA	MG-NB	-2.80	2.00	2.05
30	B	606	CLA	CMD-C2D	-2.80	1.44	1.50
33	a	405	SQD	O48-C23	2.80	1.41	1.33
30	16	301	CLA	C4B-NB	2.80	1.41	1.37
30	B	615	CLA	C1B-NB	-2.80	1.34	1.37
30	12	312	CLA	C3B-C4B	2.80	1.49	1.42
30	b	615	CLA	C1B-NB	-2.80	1.34	1.37
32	a	408	BCR	C30-C25	-2.80	1.49	1.53
30	19	306	CLA	MG-NB	-2.80	2.00	2.05
42	11	310	A86	C25-C24	2.80	1.41	1.34
42	14	312	A86	C25-C24	2.80	1.41	1.34
30	b	606	CLA	C3B-C4B	2.79	1.49	1.42
42	15	310	A86	C25-C24	2.79	1.41	1.34
42	12	319	A86	C25-C24	2.79	1.41	1.34
30	b	615	CLA	C3B-C4B	2.79	1.49	1.42
42	19	310	A86	O-C13	-2.79	1.17	1.23
30	20	208	CLA	C4B-NB	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	w	103	CLA	C3B-C4B	2.79	1.49	1.42
30	A	402	CLA	C1D-ND	2.79	1.41	1.37
30	20	202	CLA	C3B-C4B	2.79	1.49	1.42
30	19	304	CLA	C3B-C4B	2.79	1.49	1.42
30	14	309	CLA	MG-NB	-2.78	2.00	2.05
30	12	303	CLA	C3B-C4B	2.78	1.49	1.42
30	B	606	CLA	C3B-C4B	2.78	1.49	1.42
30	18	310	CLA	C4B-NB	2.78	1.41	1.37
30	19	304	CLA	C4B-NB	2.78	1.41	1.37
42	17	302	A86	O-C13	-2.78	1.17	1.23
30	11	315	CLA	C3B-C4B	2.78	1.49	1.42
40	d	405	PL9	C53-C6	-2.78	1.44	1.50
30	12	311	CLA	MG-NB	-2.78	2.00	2.05
30	20	205	CLA	MG-NB	-2.78	2.00	2.05
40	d	408	PL9	C41-C39	-2.78	1.45	1.51
30	15	301	CLA	C3B-C4B	2.78	1.49	1.42
30	c	510	CLA	C1B-NB	-2.78	1.34	1.37
40	D	407	PL9	C41-C39	-2.78	1.45	1.51
40	D	404	PL9	C6-C1	-2.78	1.43	1.48
40	d	405	PL9	C6-C1	-2.78	1.43	1.48
42	11	314	A86	C19-C18	2.78	1.56	1.52
42	14	316	A86	C19-C18	2.78	1.56	1.52
30	19	304	CLA	MG-NB	-2.77	2.00	2.05
39	J	101	DGD	O5D-C6D	-2.77	1.38	1.43
42	16	310	A86	O-C13	-2.77	1.17	1.23
30	B	604	CLA	MG-ND	-2.77	2.00	2.05
30	a	403	CLA	CMD-C2D	-2.77	1.44	1.50
30	16	309	CLA	MG-NB	-2.77	2.00	2.05
30	c	507	CLA	C4B-NB	2.77	1.41	1.37
30	W	103	CLA	C3B-C4B	2.77	1.49	1.42
39	c	518	DGD	O6D-C5D	-2.77	1.37	1.44
30	18	303	CLA	C4B-NB	2.76	1.41	1.37
30	B	612	CLA	CMC-C2C	-2.76	1.44	1.50
30	m	101	CLA	MG-NB	-2.76	2.00	2.05
32	h	101	BCR	C30-C25	-2.76	1.50	1.53
30	b	610	CLA	C1B-NB	-2.76	1.34	1.37
30	15	307	CLA	C4B-NB	2.76	1.41	1.37
41	F	102	HEM	CAB-C3B	2.76	1.54	1.47
30	b	601	CLA	MG-NB	-2.76	2.00	2.05
30	14	302	CLA	C3B-C4B	2.76	1.49	1.42
30	c	505	CLA	MG-NB	-2.76	2.00	2.05
42	20	213	A86	O-C13	-2.76	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	V	201	HEM	CAB-C3B	2.76	1.54	1.47
42	21	314	A86	O-C13	-2.76	1.17	1.23
41	v	201	HEM	CAB-C3B	2.76	1.54	1.47
30	b	612	CLA	C1B-NB	-2.75	1.34	1.37
30	14	307	CLA	C4B-NB	2.75	1.41	1.37
30	17	303	CLA	C4B-NB	2.75	1.41	1.37
30	b	612	CLA	CMC-C2C	-2.75	1.45	1.50
30	14	302	CLA	C4B-NB	2.75	1.41	1.37
30	D	405	CLA	MG-NB	-2.75	2.00	2.05
30	C	514	CLA	C1B-NB	-2.75	1.34	1.37
42	12	315	A86	C25-C24	2.75	1.41	1.34
30	W	102	CLA	C3B-C4B	2.75	1.49	1.42
41	f	102	HEM	CAB-C3B	2.75	1.54	1.47
42	21	310	A86	C19-C18	2.75	1.56	1.52
30	M	101	CLA	MG-NB	-2.75	2.00	2.05
42	17	315	A86	C14-C15	2.75	1.58	1.52
30	15	307	CLA	MG-NB	-2.75	2.00	2.05
42	12	319	A86	C19-C18	2.75	1.56	1.52
30	B	606	CLA	C1B-NB	-2.75	1.34	1.37
30	17	308	CLA	CMB-C2B	-2.75	1.45	1.50
30	M	101	CLA	C1D-ND	2.74	1.41	1.37
42	11	312	A86	C-C1	2.74	1.56	1.50
40	D	407	PL9	C46-C44	-2.74	1.45	1.51
42	18	315	A86	O-C13	-2.74	1.17	1.23
30	d	401	CLA	CMD-C2D	-2.74	1.45	1.50
30	C	507	CLA	MG-ND	-2.74	2.00	2.05
42	13	314	A86	O-C13	-2.74	1.17	1.23
41	F	102	HEM	CAC-C3C	2.74	1.54	1.47
30	b	607	CLA	C1D-ND	2.74	1.41	1.37
30	21	301	CLA	C3B-C4B	2.74	1.49	1.42
42	18	313	A86	O-C13	-2.74	1.17	1.23
40	d	408	PL9	C46-C44	-2.74	1.45	1.51
30	18	311	CLA	C3B-C4B	2.74	1.49	1.42
30	B	613	CLA	MG-ND	-2.74	2.00	2.05
30	B	609	CLA	MG-NB	-2.74	2.00	2.05
30	C	509	CLA	MG-ND	-2.73	2.00	2.05
30	20	209	CLA	C3B-C4B	2.73	1.49	1.42
30	b	604	CLA	CMD-C2D	-2.73	1.45	1.50
31	D	403	PHO	CMD-C2D	-2.73	1.46	1.51
42	17	314	A86	O-C13	-2.73	1.17	1.23
30	b	603	CLA	C1D-ND	2.73	1.41	1.37
30	11	305	CLA	C4B-NB	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	20	205	CLA	C4B-NB	2.73	1.41	1.37
30	C	505	CLA	C1D-ND	2.73	1.41	1.37
30	A	404	CLA	CMD-C2D	-2.73	1.45	1.50
30	C	503	CLA	CMB-C2B	-2.73	1.45	1.50
30	B	610	CLA	C1B-NB	-2.73	1.34	1.37
30	12	312	CLA	C4B-NB	2.73	1.41	1.37
30	18	308	CLA	C3B-C4B	2.73	1.49	1.42
30	21	307	CLA	C3B-C4B	2.73	1.49	1.42
30	c	509	CLA	MG-ND	-2.73	2.00	2.05
42	11	310	A86	O-C13	-2.73	1.17	1.23
32	C	515	BCR	C30-C25	-2.72	1.50	1.53
31	d	404	PHO	CMD-C2D	-2.72	1.46	1.51
30	12	308	CLA	C3B-C4B	2.72	1.49	1.42
30	c	509	CLA	CMC-C2C	-2.72	1.45	1.50
31	d	404	PHO	CMB-C2B	-2.72	1.46	1.51
42	21	311	A86	O-C13	-2.72	1.17	1.23
30	11	301	CLA	MG-NB	-2.72	2.00	2.05
33	L	103	SQD	O48-C23	2.72	1.41	1.33
30	17	303	CLA	MG-NB	-2.72	2.00	2.05
30	B	604	CLA	CMD-C2D	-2.72	1.45	1.50
30	b	611	CLA	C1D-ND	2.72	1.41	1.37
30	14	306	CLA	C3B-C4B	2.72	1.49	1.42
30	W	103	CLA	CMD-C2D	-2.72	1.45	1.50
30	b	615	CLA	CMC-C2C	-2.72	1.45	1.50
30	11	304	CLA	C3B-C4B	2.71	1.49	1.42
30	18	306	CLA	C3B-C4B	2.71	1.49	1.42
30	13	302	CLA	MG-NB	-2.71	2.00	2.05
30	C	508	CLA	C1B-NB	-2.71	1.34	1.37
30	C	505	CLA	CMB-C2B	-2.71	1.45	1.50
42	12	315	A86	O-C13	-2.71	1.17	1.23
42	11	313	A86	O-C13	-2.71	1.17	1.23
30	16	307	CLA	CMC-C2C	-2.71	1.45	1.50
30	20	208	CLA	C3B-C4B	2.71	1.49	1.42
30	B	615	CLA	CMD-C2D	-2.71	1.45	1.50
30	14	303	CLA	MG-NB	-2.71	2.00	2.05
30	15	304	CLA	C3B-C4B	2.71	1.49	1.42
30	19	308	CLA	MG-NB	-2.71	2.00	2.05
30	b	602	CLA	CMC-C2C	-2.71	1.45	1.50
39	c	518	DGD	O5D-C6D	-2.71	1.38	1.43
30	b	615	CLA	CMD-C2D	-2.71	1.45	1.50
30	20	207	CLA	C4B-NB	2.71	1.41	1.37
30	c	502	CLA	MG-NB	-2.71	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	517	DGD	O4D-C4D	-2.71	1.36	1.43
30	C	505	CLA	C1B-NB	-2.71	1.34	1.37
40	D	404	PL9	C53-C6	-2.71	1.45	1.50
36	12	301	LMG	O1-C1	2.71	1.44	1.40
33	l	101	SQD	O48-C23	2.71	1.41	1.33
31	D	403	PHO	CBD-CGD	-2.71	1.48	1.52
30	21	308	CLA	C3B-C4B	2.70	1.49	1.42
30	C	509	CLA	CMC-C2C	-2.70	1.45	1.50
42	12	318	A86	O-C13	-2.70	1.17	1.23
30	12	305	CLA	MG-NB	-2.70	2.00	2.05
30	B	609	CLA	C4B-NB	2.70	1.41	1.37
30	12	314	CLA	C3B-C4B	2.70	1.49	1.42
30	18	307	CLA	C3B-C4B	2.70	1.49	1.42
42	14	314	A86	C14-C15	2.70	1.58	1.52
42	20	212	A86	C24-C1	2.70	1.51	1.45
30	C	505	CLA	MG-NB	-2.70	2.00	2.05
30	13	306	CLA	C4B-NB	2.70	1.41	1.37
30	18	303	CLA	MG-NB	-2.70	2.00	2.05
30	15	303	CLA	C3B-C4B	2.70	1.49	1.42
30	c	507	CLA	MG-ND	-2.70	2.00	2.05
30	b	609	CLA	MG-NB	-2.70	2.00	2.05
42	15	313	A86	C-C1	2.70	1.56	1.50
30	B	615	CLA	CMC-C2C	-2.70	1.45	1.50
30	b	608	CLA	CMB-C2B	-2.70	1.45	1.50
42	14	312	A86	O-C13	-2.70	1.17	1.23
30	12	309	CLA	C4B-NB	2.70	1.41	1.37
30	b	604	CLA	CMB-C2B	-2.70	1.45	1.50
42	13	313	A86	C14-C15	2.69	1.58	1.52
42	15	314	A86	C19-C18	2.69	1.56	1.52
42	20	212	A86	C-C1	2.69	1.56	1.50
30	B	613	CLA	C1D-ND	2.69	1.41	1.37
42	14	315	A86	O-C13	-2.69	1.17	1.23
40	D	407	PL9	C5-C4	-2.69	1.37	1.47
39	C	517	DGD	O6D-C5D	-2.69	1.37	1.44
42	16	312	A86	C-C1	2.69	1.56	1.50
30	B	604	CLA	CMB-C2B	-2.69	1.45	1.50
30	w	103	CLA	CMD-C2D	-2.69	1.45	1.50
42	12	319	A86	C-C1	2.69	1.56	1.50
30	C	519	CLA	C4B-NB	2.69	1.41	1.37
42	20	211	A86	O-C13	-2.69	1.17	1.23
42	13	311	A86	O-C13	-2.69	1.17	1.23
30	C	502	CLA	CMD-C2D	-2.69	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	16	313	A86	C19-C18	2.68	1.56	1.52
30	11	315	CLA	C4B-NB	2.68	1.41	1.37
30	b	613	CLA	MG-ND	-2.68	2.00	2.05
42	15	313	A86	O-C13	-2.68	1.17	1.23
30	21	302	CLA	C3B-C4B	2.68	1.49	1.42
41	f	102	HEM	CAC-C3C	2.68	1.54	1.47
30	B	603	CLA	CMB-C2B	-2.68	1.45	1.50
30	C	520	CLA	MG-NB	-2.68	2.00	2.05
30	17	306	CLA	CMD-C2D	-2.68	1.45	1.50
30	C	512	CLA	MG-NB	-2.68	2.00	2.05
30	14	311	CLA	C3B-C4B	2.68	1.49	1.42
42	15	310	A86	O-C13	-2.68	1.17	1.23
42	17	313	A86	C14-C15	2.68	1.57	1.52
30	15	309	CLA	C3B-C4B	2.68	1.49	1.42
30	m	101	CLA	CMD-C2D	-2.68	1.45	1.50
30	13	310	CLA	C3B-C4B	2.67	1.49	1.42
30	B	608	CLA	CMB-C2B	-2.67	1.45	1.50
30	12	303	CLA	C4B-NB	2.67	1.41	1.37
39	j	101	DGD	O5D-C6D	-2.67	1.38	1.43
31	d	404	PHO	CBD-CGD	-2.67	1.48	1.52
39	C	517	DGD	O5D-C6D	-2.67	1.38	1.43
30	c	505	CLA	C1B-NB	-2.67	1.34	1.37
42	20	210	A86	C24-C1	2.67	1.51	1.45
30	b	606	CLA	C1B-NB	-2.67	1.34	1.37
41	V	201	HEM	C3C-C2C	-2.67	1.31	1.37
30	c	514	CLA	C1B-NB	-2.67	1.34	1.37
42	11	313	A86	C-C1	2.67	1.56	1.50
30	C	502	CLA	C1D-ND	2.67	1.41	1.37
30	c	503	CLA	CMB-C2B	-2.67	1.45	1.50
30	13	305	CLA	C3B-C4B	2.67	1.49	1.42
42	13	313	A86	C-C1	2.67	1.56	1.50
30	16	301	CLA	MG-NB	-2.67	2.00	2.05
42	14	316	A86	C-C1	2.67	1.56	1.50
30	14	305	CLA	MG-NB	-2.67	2.00	2.05
30	c	505	CLA	C1D-ND	2.67	1.41	1.37
30	c	502	CLA	CMD-C2D	-2.66	1.45	1.50
36	w	101	LMG	O7-C8	-2.66	1.39	1.46
42	20	210	A86	C-C1	2.66	1.56	1.50
30	14	307	CLA	C3B-C4B	2.66	1.49	1.42
30	21	304	CLA	C3B-C4B	2.66	1.49	1.42
30	B	602	CLA	CMC-C2C	-2.66	1.45	1.50
30	15	307	CLA	C3B-C4B	2.66	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	101	CLA	CMD-C2D	-2.66	1.45	1.50
30	C	510	CLA	MG-ND	-2.66	2.00	2.05
30	c	512	CLA	MG-NB	-2.66	2.00	2.05
30	18	309	CLA	C3B-C4B	2.66	1.49	1.42
42	16	312	A86	C14-C15	2.66	1.57	1.52
42	12	318	A86	C-C1	2.66	1.56	1.50
31	D	403	PHO	CMB-C2B	-2.66	1.46	1.51
33	A	406	SQD	O47-C7	2.65	1.41	1.34
30	c	502	CLA	C1D-ND	2.65	1.41	1.37
30	16	305	CLA	MG-NB	-2.65	2.00	2.05
30	B	610	CLA	CMC-C2C	-2.65	1.45	1.50
30	11	304	CLA	CMD-C2D	-2.65	1.45	1.50
40	d	408	PL9	C5-C4	-2.65	1.37	1.47
30	18	310	CLA	C1B-C2B	2.65	1.49	1.43
30	d	401	CLA	C1D-ND	2.65	1.41	1.37
42	15	314	A86	C-C1	2.65	1.56	1.50
42	21	313	A86	C-C1	2.65	1.56	1.50
36	W	101	LMG	O7-C8	-2.65	1.40	1.46
30	11	309	CLA	C3B-C4B	2.65	1.49	1.42
31	D	403	PHO	CAC-C3C	-2.65	1.46	1.51
42	13	313	A86	O-C13	-2.65	1.17	1.23
42	19	311	A86	O-C13	-2.65	1.17	1.23
42	21	314	A86	C-C1	2.65	1.56	1.50
42	17	316	A86	C-C1	2.65	1.56	1.50
30	c	505	CLA	CMB-C2B	-2.65	1.45	1.50
30	B	603	CLA	CMD-C2D	-2.65	1.45	1.50
30	B	611	CLA	C1D-ND	2.65	1.41	1.37
30	B	612	CLA	C1B-NB	-2.65	1.34	1.37
30	21	303	CLA	C3B-C4B	2.65	1.49	1.42
30	b	603	CLA	CMB-C2B	-2.65	1.45	1.50
30	12	307	CLA	MG-NB	-2.65	2.00	2.05
42	14	314	A86	C-C1	2.64	1.56	1.50
30	18	312	CLA	C3B-C4B	2.64	1.48	1.42
30	13	304	CLA	MG-NB	-2.64	2.00	2.05
42	19	311	A86	C24-C1	2.64	1.51	1.45
42	12	318	A86	C14-C15	2.64	1.57	1.52
42	12	317	A86	C-C1	2.64	1.56	1.50
42	14	315	A86	C-C1	2.64	1.56	1.50
42	15	312	A86	C-C1	2.64	1.56	1.50
42	21	312	A86	O-C13	-2.64	1.17	1.23
30	B	611	CLA	C1B-NB	-2.64	1.34	1.37
30	21	303	CLA	C4B-NB	2.64	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	17	314	A86	C14-C15	2.64	1.57	1.52
42	17	313	A86	C-C1	2.64	1.56	1.50
42	14	301	A86	C-C1	2.64	1.56	1.50
39	c	518	DGD	O4E-C4E	-2.64	1.36	1.43
30	b	603	CLA	CMD-C2D	-2.64	1.45	1.50
42	20	213	A86	C-C1	2.64	1.56	1.50
30	17	305	CLA	MG-NB	-2.64	2.00	2.05
30	b	610	CLA	CMC-C2C	-2.64	1.45	1.50
30	C	513	CLA	MG-NB	-2.64	2.00	2.05
30	c	510	CLA	MG-ND	-2.64	2.00	2.05
30	21	306	CLA	C3B-C4B	2.64	1.48	1.42
30	B	615	CLA	MG-NB	-2.64	2.00	2.05
42	15	313	A86	C14-C15	2.64	1.57	1.52
30	m	101	CLA	C1D-ND	2.64	1.41	1.37
42	11	314	A86	C-C1	2.64	1.56	1.50
42	11	312	A86	C14-C15	2.64	1.57	1.52
39	c	518	DGD	O4D-C4D	-2.64	1.36	1.43
31	d	403	PHO	C3B-C2B	-2.64	1.36	1.40
30	a	402	CLA	MG-NB	-2.63	2.00	2.05
30	13	305	CLA	CMD-C2D	-2.63	1.45	1.50
30	b	613	CLA	C1D-ND	2.63	1.41	1.37
42	17	311	A86	C-C1	2.63	1.56	1.50
30	C	506	CLA	MG-NB	-2.63	2.00	2.05
36	B	620	LMG	O4-C4	-2.63	1.36	1.43
39	C	517	DGD	O3G-C1D	-2.63	1.35	1.40
30	B	623	CLA	MG-ND	-2.63	2.00	2.05
30	B	610	CLA	C1D-ND	2.63	1.41	1.37
42	18	315	A86	C-C1	2.63	1.56	1.50
41	v	201	HEM	CAC-C3C	2.63	1.54	1.47
42	14	301	A86	C19-C18	2.63	1.56	1.52
30	b	608	CLA	C1D-ND	2.63	1.41	1.37
30	17	310	CLA	C3B-C4B	2.63	1.48	1.42
30	D	401	CLA	MG-ND	-2.63	2.00	2.05
30	d	401	CLA	MG-ND	-2.63	2.00	2.05
30	B	612	CLA	CMA-C3A	-2.63	1.47	1.53
39	C	517	DGD	O4E-C4E	-2.63	1.36	1.43
30	c	513	CLA	MG-NB	-2.63	2.00	2.05
41	v	201	HEM	C3C-C2C	-2.63	1.32	1.37
42	16	313	A86	C-C1	2.63	1.56	1.50
42	11	316	A86	C24-C1	2.63	1.51	1.45
30	b	622	CLA	MG-ND	-2.63	2.00	2.05
30	21	304	CLA	C4B-NB	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	21	313	A86	O-C13	-2.63	1.17	1.23
30	C	514	CLA	C3B-C4B	2.63	1.48	1.42
42	14	315	A86	C14-C15	2.63	1.57	1.52
30	19	303	CLA	C3B-C4B	2.62	1.48	1.42
30	12	308	CLA	CMD-C2D	-2.62	1.45	1.50
30	A	402	CLA	MG-NB	-2.62	2.00	2.05
30	C	507	CLA	C4B-NB	2.62	1.41	1.37
30	c	514	CLA	C3B-C4B	2.62	1.48	1.42
30	12	309	CLA	C3B-C4B	2.62	1.48	1.42
30	B	603	CLA	C1D-ND	2.62	1.41	1.37
30	c	503	CLA	C1B-NB	-2.62	1.34	1.37
30	18	311	CLA	C1B-C2B	2.62	1.49	1.43
31	A	403	PHO	C3B-C2B	-2.62	1.36	1.40
42	16	311	A86	O-C13	-2.62	1.17	1.23
42	17	313	A86	O-C13	-2.62	1.17	1.23
30	b	609	CLA	C4B-NB	2.62	1.41	1.37
30	20	208	CLA	C1B-C2B	2.62	1.49	1.43
30	20	209	CLA	MG-NB	-2.62	2.00	2.05
36	b	619	LMG	O4-C4	-2.62	1.36	1.43
42	16	310	A86	C-C1	2.62	1.56	1.50
30	b	615	CLA	CMB-C2B	-2.62	1.45	1.50
30	11	305	CLA	C3B-C4B	2.62	1.48	1.42
31	d	404	PHO	CAC-C3C	-2.62	1.46	1.51
42	19	312	A86	C24-C1	2.61	1.51	1.45
42	13	314	A86	C14-C15	2.61	1.57	1.52
30	b	604	CLA	C1B-NB	-2.61	1.34	1.37
33	a	405	SQD	O47-C7	2.61	1.41	1.34
42	18	315	A86	C14-C15	2.61	1.57	1.52
39	c	518	DGD	O3G-C1D	-2.61	1.35	1.40
42	11	313	A86	C14-C15	2.61	1.57	1.52
41	V	201	HEM	CAC-C3C	2.61	1.54	1.47
30	b	611	CLA	C1B-NB	-2.61	1.34	1.37
30	15	301	CLA	MG-NB	-2.61	2.00	2.05
30	20	204	CLA	MG-NB	-2.61	2.00	2.05
42	12	317	A86	C14-C15	2.61	1.57	1.52
42	13	312	A86	O-C13	-2.61	1.17	1.23
30	15	306	CLA	C3B-C4B	2.61	1.48	1.42
30	13	306	CLA	C3B-C4B	2.61	1.48	1.42
42	13	301	A86	C24-C1	2.61	1.51	1.45
30	17	307	CLA	CMD-C2D	-2.61	1.45	1.50
30	b	612	CLA	CMA-C3A	-2.61	1.47	1.53
42	13	314	A86	C-C1	2.61	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	614	CLA	MG-NB	-2.60	2.00	2.05
42	12	317	A86	O-C13	-2.60	1.17	1.23
42	18	302	A86	C24-C1	2.60	1.51	1.45
30	18	305	CLA	C3B-C4B	2.60	1.48	1.42
30	c	503	CLA	CMD-C2D	-2.60	1.45	1.50
42	17	311	A86	O-C13	-2.60	1.17	1.23
30	16	307	CLA	C4B-NB	2.60	1.41	1.37
30	B	610	CLA	CMD-C2D	-2.60	1.45	1.50
30	b	603	CLA	MG-ND	-2.60	2.00	2.05
30	16	305	CLA	CMD-C2D	-2.60	1.45	1.50
42	18	314	A86	O-C13	-2.60	1.17	1.23
30	b	615	CLA	MG-NB	-2.60	2.00	2.05
36	B	619	LMG	O7-C8	-2.60	1.40	1.46
42	17	314	A86	C-C1	2.60	1.56	1.50
42	20	213	A86	C24-C1	2.60	1.51	1.45
30	12	303	CLA	CMD-C2D	-2.60	1.45	1.50
42	11	311	A86	O-C13	-2.60	1.17	1.23
42	14	314	A86	O-C13	-2.60	1.17	1.23
42	16	312	A86	O-C13	-2.60	1.17	1.23
42	15	316	A86	C24-C1	2.60	1.51	1.45
42	17	311	A86	C24-C1	2.60	1.51	1.45
41	v	201	HEM	C2A-C3A	-2.60	1.31	1.38
42	15	312	A86	C14-C15	2.60	1.57	1.52
42	14	313	A86	O-C13	-2.60	1.17	1.23
30	15	308	CLA	C3B-C4B	2.60	1.48	1.42
30	D	405	CLA	MG-ND	-2.60	2.00	2.05
30	16	305	CLA	C4B-NB	2.59	1.41	1.37
30	19	305	CLA	MG-NB	-2.59	2.00	2.05
36	b	618	LMG	O7-C8	-2.59	1.40	1.46
30	C	503	CLA	CMD-C2D	-2.59	1.45	1.50
30	b	603	CLA	C1B-NB	-2.59	1.34	1.37
30	16	306	CLA	C4B-NB	2.59	1.41	1.37
30	15	306	CLA	C1B-C2B	2.59	1.49	1.43
42	15	311	A86	O-C13	-2.59	1.17	1.23
30	11	307	CLA	C4B-NB	2.59	1.41	1.37
30	18	310	CLA	MG-NB	-2.59	2.00	2.05
42	21	310	A86	C-C1	2.59	1.56	1.50
42	16	312	A86	C24-C1	2.59	1.51	1.45
42	15	316	A86	C-C1	2.59	1.56	1.50
30	W	102	CLA	C4B-NB	2.59	1.41	1.37
30	Z	102	CLA	MG-NB	-2.59	2.00	2.05
30	19	309	CLA	C3B-C4B	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z	102	CLA	C1B-C2B	2.59	1.49	1.43
30	c	505	CLA	CAC-C3C	-2.59	1.44	1.51
42	17	312	A86	O-C13	-2.59	1.17	1.23
30	b	613	CLA	CAA-C2A	-2.59	1.49	1.54
42	15	312	A86	O-C13	-2.59	1.17	1.23
30	Z	102	CLA	C3B-C4B	2.59	1.48	1.42
30	B	603	CLA	MG-ND	-2.58	2.00	2.05
30	B	604	CLA	C1B-NB	-2.58	1.34	1.37
30	B	608	CLA	C1D-ND	2.58	1.41	1.37
36	1	101	LMG	O1-C1	2.58	1.44	1.40
30	b	609	CLA	CMD-C2D	-2.58	1.45	1.50
42	11	312	A86	O-C13	-2.58	1.17	1.23
30	18	308	CLA	C1B-C2B	2.58	1.49	1.43
30	c	510	CLA	CMC-C2C	-2.58	1.45	1.50
30	b	610	CLA	C1D-ND	2.58	1.41	1.37
30	d	401	CLA	CMC-C2C	-2.58	1.45	1.50
30	B	605	CLA	MG-NB	-2.58	2.00	2.05
30	c	512	CLA	MG-ND	-2.58	2.00	2.05
30	B	610	CLA	MG-ND	-2.58	2.00	2.05
30	B	610	CLA	CMB-C2B	-2.58	1.45	1.50
36	c	519	LMG	O8-C9	-2.58	1.39	1.45
42	14	314	A86	C24-C1	2.58	1.51	1.45
30	B	604	CLA	CAC-C3C	-2.57	1.44	1.51
30	B	614	CLA	MG-NB	-2.57	2.00	2.05
30	C	512	CLA	MG-ND	-2.57	2.00	2.05
30	C	508	CLA	CMD-C2D	-2.57	1.45	1.50
30	11	303	CLA	MG-NB	-2.57	2.00	2.05
30	16	303	CLA	MG-NB	-2.57	2.00	2.05
30	D	405	CLA	CMC-C2C	-2.57	1.45	1.50
42	17	302	A86	C-C1	2.57	1.56	1.50
30	b	610	CLA	MG-ND	-2.57	2.00	2.05
42	15	315	A86	C24-C1	2.57	1.51	1.45
30	B	605	CLA	CMD-C2D	-2.57	1.45	1.50
42	12	317	A86	C24-C1	2.57	1.51	1.45
42	13	315	A86	C-C1	2.57	1.56	1.50
30	C	520	CLA	C3B-C4B	2.57	1.48	1.42
42	17	315	A86	C24-C1	2.57	1.51	1.45
30	B	615	CLA	CMB-C2B	-2.57	1.45	1.50
30	12	313	CLA	C4B-NB	2.57	1.40	1.37
30	B	613	CLA	CAA-C2A	-2.57	1.49	1.54
30	b	602	CLA	MG-NB	-2.57	2.00	2.05
30	11	304	CLA	MG-ND	-2.57	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	513	CLA	CMD-C2D	-2.57	1.45	1.50
30	c	508	CLA	C1B-NB	-2.57	1.34	1.37
30	C	510	CLA	CMC-C2C	-2.57	1.45	1.50
42	17	315	A86	O-C13	-2.57	1.17	1.23
42	19	312	A86	O-C13	-2.57	1.17	1.23
30	18	304	CLA	C1B-C2B	2.57	1.49	1.43
30	14	303	CLA	CMC-C2C	-2.57	1.45	1.50
42	12	316	A86	O-C13	-2.57	1.17	1.23
30	15	305	CLA	C1B-C2B	2.56	1.49	1.43
42	17	313	A86	C24-C1	2.56	1.51	1.45
30	B	603	CLA	C1B-NB	-2.56	1.34	1.37
42	19	312	A86	C-C1	2.56	1.56	1.50
30	20	207	CLA	C3B-C4B	2.56	1.48	1.42
30	12	312	CLA	CMD-C2D	-2.56	1.45	1.50
30	D	401	CLA	CMC-C2C	-2.56	1.45	1.50
30	14	304	CLA	C4B-NB	2.56	1.40	1.37
30	C	504	CLA	MG-NB	-2.56	2.00	2.05
42	11	316	A86	C-C1	2.56	1.56	1.50
30	b	608	CLA	CMD-C2D	-2.56	1.45	1.50
36	Q	301	LMG	O8-C9	-2.56	1.39	1.45
30	C	512	CLA	C3B-C4B	2.56	1.48	1.42
30	C	513	CLA	CMD-C2D	-2.56	1.45	1.50
30	14	310	CLA	C4B-NB	2.56	1.40	1.37
30	C	514	CLA	MG-NB	-2.56	2.00	2.05
36	D	408	LMG	O1-C7	-2.56	1.39	1.43
30	C	505	CLA	CAC-C3C	-2.56	1.44	1.51
30	B	608	CLA	CMD-C2D	-2.56	1.45	1.50
30	13	305	CLA	C4B-NB	2.55	1.40	1.37
30	13	309	CLA	C4B-NB	2.55	1.40	1.37
30	21	306	CLA	C1B-C2B	2.55	1.49	1.43
30	C	513	CLA	C3B-C4B	2.55	1.48	1.42
30	15	302	CLA	C1B-C2B	2.55	1.49	1.43
30	B	609	CLA	CMD-C2D	-2.55	1.45	1.50
30	21	307	CLA	C1B-C2B	2.55	1.49	1.43
30	c	506	CLA	MG-NB	-2.55	2.00	2.05
30	16	302	CLA	CMC-C2C	-2.55	1.45	1.50
42	12	315	A86	C-C1	2.55	1.56	1.50
42	20	212	A86	C35-C34	2.55	1.56	1.51
42	13	313	A86	C24-C1	2.55	1.51	1.45
30	b	610	CLA	CMD-C2D	-2.55	1.45	1.50
30	c	508	CLA	CMD-C2D	-2.55	1.45	1.50
30	12	308	CLA	MG-ND	-2.55	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	13	301	A86	C-C1	2.55	1.56	1.50
42	12	304	A86	C24-C1	2.55	1.51	1.45
36	W	101	LMG	O8-C9	-2.55	1.39	1.45
30	16	309	CLA	C4B-NB	2.55	1.40	1.37
42	15	315	A86	C-C1	2.54	1.56	1.50
30	b	605	CLA	CMD-C2D	-2.54	1.45	1.50
30	19	305	CLA	C3B-C4B	2.54	1.48	1.42
30	b	622	CLA	C4B-NB	2.54	1.40	1.37
42	21	314	A86	C24-C1	2.54	1.51	1.45
42	12	304	A86	C-C1	2.54	1.56	1.50
30	12	305	CLA	CMC-C2C	-2.54	1.45	1.50
30	16	306	CLA	CMB-C2B	-2.54	1.45	1.50
30	19	302	CLA	C1B-NB	-2.54	1.34	1.37
30	19	305	CLA	C4B-NB	2.54	1.40	1.37
30	B	623	CLA	C3B-C4B	2.54	1.48	1.42
30	z	101	CLA	MG-ND	-2.54	2.00	2.05
36	w	101	LMG	O8-C9	-2.54	1.39	1.45
30	14	310	CLA	CMD-C2D	-2.54	1.45	1.50
42	11	312	A86	C24-C1	2.54	1.51	1.45
30	14	302	CLA	CMD-C2D	-2.54	1.45	1.50
30	b	606	CLA	CMB-C2B	-2.54	1.45	1.50
30	B	602	CLA	MG-NB	-2.54	2.00	2.05
30	z	101	CLA	C4B-NB	2.54	1.40	1.37
30	13	305	CLA	MG-ND	-2.54	2.00	2.05
42	13	315	A86	C24-C1	2.54	1.51	1.45
39	c	518	DGD	O3G-C3G	-2.54	1.39	1.43
30	C	510	CLA	C1D-ND	2.54	1.40	1.37
30	11	308	CLA	C4B-NB	2.54	1.40	1.37
30	19	309	CLA	C4B-NB	2.54	1.40	1.37
42	18	313	A86	C-C1	2.54	1.56	1.50
35	A	408	LHG	O7-C5	-2.53	1.40	1.46
33	B	621	SQD	O47-C7	2.53	1.41	1.34
30	B	606	CLA	CMC-C2C	-2.53	1.45	1.50
30	20	203	CLA	MG-NB	-2.53	2.00	2.05
30	21	308	CLA	C1B-C2B	2.53	1.49	1.43
30	D	401	CLA	C1D-ND	2.53	1.40	1.37
36	12	301	LMG	O4-C4	-2.53	1.37	1.43
42	17	316	A86	O-C13	-2.53	1.18	1.23
35	a	407	LHG	O7-C5	-2.53	1.40	1.46
39	C	517	DGD	O3G-C3G	-2.53	1.39	1.43
30	11	301	CLA	CMC-C2C	-2.53	1.45	1.50
30	c	514	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	310	CLA	MG-NB	-2.53	2.00	2.05
30	18	306	CLA	MG-NB	-2.53	2.00	2.05
30	20	206	CLA	MG-NB	-2.53	2.00	2.05
30	d	406	CLA	CMC-C2C	-2.53	1.45	1.50
30	c	513	CLA	C3B-C4B	2.53	1.48	1.42
30	A	404	CLA	CMB-C2B	-2.53	1.45	1.50
30	B	606	CLA	CMB-C2B	-2.53	1.45	1.50
30	b	609	CLA	CMB-C2B	-2.53	1.45	1.50
30	13	309	CLA	CMD-C2D	-2.53	1.45	1.50
30	20	207	CLA	MG-NB	-2.53	2.00	2.05
42	15	312	A86	C24-C1	2.53	1.51	1.45
42	20	201	A86	C-C1	2.53	1.56	1.50
39	J	101	DGD	O1G-C1G	-2.53	1.39	1.45
30	a	403	CLA	CMC-C2C	-2.53	1.45	1.50
30	c	512	CLA	C3B-C4B	2.52	1.48	1.42
30	16	303	CLA	C4B-NB	2.52	1.40	1.37
30	b	614	CLA	CMD-C2D	-2.52	1.45	1.50
30	14	304	CLA	MG-NB	-2.52	2.00	2.05
37	12	302	LMU	O3'-C3'	2.52	1.48	1.43
30	B	605	CLA	CMB-C2B	-2.52	1.45	1.50
30	12	307	CLA	C4B-NB	2.52	1.40	1.37
30	C	509	CLA	CMD-C2D	-2.52	1.45	1.50
42	17	315	A86	C-C1	2.52	1.56	1.50
33	b	620	SQD	O47-C7	2.52	1.41	1.34
42	16	310	A86	C24-C1	2.52	1.51	1.45
42	15	314	A86	O-C13	-2.52	1.18	1.23
30	C	503	CLA	C1B-NB	-2.52	1.34	1.37
30	16	309	CLA	CMD-C2D	-2.52	1.45	1.50
30	18	301	CLA	MG-NB	-2.52	2.00	2.05
30	c	513	CLA	C4B-NB	2.52	1.40	1.37
30	20	204	CLA	C3B-C4B	2.52	1.48	1.42
30	c	504	CLA	MG-NB	-2.52	2.00	2.05
30	D	406	CLA	C1D-ND	2.52	1.40	1.37
30	19	309	CLA	MG-NB	-2.52	2.00	2.05
30	b	610	CLA	CMB-C2B	-2.52	1.45	1.50
30	d	407	CLA	CMD-C2D	-2.52	1.45	1.50
41	V	201	HEM	C2A-C3A	-2.51	1.32	1.38
30	20	204	CLA	C4B-NB	2.51	1.40	1.37
42	15	310	A86	C-C1	2.51	1.56	1.50
36	1	101	LMG	O7-C8	-2.51	1.40	1.46
33	A	406	SQD	O2-C2	-2.51	1.37	1.43
30	b	604	CLA	CAC-C3C	-2.51	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	406	CLA	MG-ND	-2.51	2.00	2.05
30	a	403	CLA	CMB-C2B	-2.51	1.45	1.50
30	16	304	CLA	MG-NB	-2.51	2.00	2.05
30	b	605	CLA	CMB-C2B	-2.51	1.45	1.50
30	12	311	CLA	C4B-NB	2.51	1.40	1.37
30	b	605	CLA	MG-NB	-2.51	2.00	2.05
33	a	405	SQD	O2-C2	-2.51	1.37	1.43
42	14	301	A86	O-C13	-2.51	1.18	1.23
30	C	508	CLA	CMB-C2B	-2.51	1.45	1.50
36	m	102	LMG	O4-C4	-2.51	1.37	1.43
30	11	315	CLA	CMD-C2D	-2.51	1.45	1.50
30	C	519	CLA	MG-ND	-2.50	2.00	2.05
30	19	303	CLA	MG-NB	-2.50	2.00	2.05
30	b	607	CLA	CMD-C2D	-2.50	1.45	1.50
30	16	308	CLA	MG-ND	-2.50	2.00	2.05
42	20	201	A86	O-C13	-2.50	1.18	1.23
30	B	615	CLA	MG-ND	-2.50	2.00	2.05
30	13	307	CLA	MG-NB	-2.50	2.00	2.05
30	14	306	CLA	MG-ND	-2.50	2.00	2.05
30	c	510	CLA	C1D-ND	2.50	1.40	1.37
30	14	310	CLA	MG-ND	-2.50	2.00	2.05
30	c	508	CLA	CMB-C2B	-2.50	1.45	1.50
30	C	503	CLA	CHC-C4B	-2.50	1.33	1.39
30	16	304	CLA	C4B-NB	2.50	1.40	1.37
30	21	309	CLA	C1B-C2B	2.50	1.49	1.43
30	C	507	CLA	C1B-NB	-2.50	1.34	1.37
30	c	514	CLA	CMC-C2C	-2.50	1.45	1.50
42	15	315	A86	O-C13	-2.50	1.18	1.23
30	11	308	CLA	CMD-C2D	-2.50	1.45	1.50
30	16	307	CLA	CMD-C2D	-2.50	1.45	1.50
30	C	508	CLA	CMC-C2C	-2.50	1.45	1.50
30	13	309	CLA	MG-ND	-2.50	2.00	2.05
30	20	206	CLA	C3B-C4B	2.50	1.48	1.42
42	12	319	A86	O-C13	-2.50	1.18	1.23
30	B	614	CLA	CMD-C2D	-2.50	1.45	1.50
30	13	302	CLA	CMC-C2C	-2.50	1.45	1.50
30	11	304	CLA	C1B-NB	-2.50	1.34	1.37
42	14	312	A86	C-C1	2.50	1.56	1.50
42	18	302	A86	C-C1	2.49	1.56	1.50
30	12	313	CLA	MG-ND	-2.49	2.00	2.05
30	d	407	CLA	C1D-ND	2.49	1.40	1.37
30	14	308	CLA	MG-NB	-2.49	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	622	CLA	C3B-C4B	2.49	1.48	1.42
30	14	306	CLA	CMD-C2D	-2.49	1.45	1.50
30	11	309	CLA	MG-NB	-2.49	2.00	2.05
30	12	303	CLA	MG-NB	-2.49	2.00	2.05
30	11	304	CLA	C4B-NB	2.49	1.40	1.37
30	12	308	CLA	C4B-NB	2.49	1.40	1.37
30	12	305	CLA	C4B-NB	2.49	1.40	1.37
42	13	315	A86	O-C13	-2.49	1.18	1.23
30	14	302	CLA	MG-NB	-2.49	2.00	2.05
30	b	602	CLA	C4B-NB	2.49	1.40	1.37
36	d	410	LMG	O1-C7	-2.49	1.39	1.43
30	b	606	CLA	CMC-C2C	-2.49	1.45	1.50
42	14	315	A86	C24-C1	2.49	1.51	1.45
30	W	102	CLA	MG-NB	-2.49	2.00	2.05
30	M	101	CLA	C3B-C4B	2.49	1.48	1.42
30	B	607	CLA	C1B-NB	-2.49	1.34	1.37
30	b	605	CLA	C4B-NB	2.49	1.40	1.37
30	B	607	CLA	CMB-C2B	-2.49	1.45	1.50
30	B	607	CLA	CMD-C2D	-2.49	1.45	1.50
30	b	601	CLA	CMB-C2B	-2.49	1.45	1.50
30	11	301	CLA	C1B-C2B	2.49	1.49	1.43
30	c	503	CLA	CHC-C4B	-2.49	1.33	1.39
30	c	509	CLA	CMD-C2D	-2.48	1.45	1.50
30	b	613	CLA	CMD-C2D	-2.48	1.45	1.50
30	c	510	CLA	CMD-C2D	-2.48	1.45	1.50
30	17	306	CLA	C3B-C4B	2.48	1.48	1.42
30	a	402	CLA	CMD-C2D	-2.48	1.45	1.50
30	c	508	CLA	CMC-C2C	-2.48	1.45	1.50
42	11	310	A86	C-C1	2.48	1.56	1.50
30	21	301	CLA	C1B-C2B	2.48	1.49	1.43
42	19	310	A86	C-C1	2.48	1.56	1.50
30	20	206	CLA	C4B-NB	2.48	1.40	1.37
30	20	209	CLA	CMB-C2B	-2.48	1.45	1.50
30	17	301	CLA	CMB-C2B	-2.48	1.45	1.50
30	C	512	CLA	C1B-NB	-2.48	1.34	1.37
42	21	312	A86	C-C1	2.48	1.56	1.50
36	M	102	LMG	O4-C4	-2.48	1.37	1.43
30	A	404	CLA	MG-ND	-2.48	2.00	2.05
30	18	309	CLA	MG-ND	-2.48	2.00	2.05
30	21	306	CLA	O2A-C1	-2.48	1.39	1.46
30	B	613	CLA	CMD-C2D	-2.47	1.45	1.50
30	17	305	CLA	C4B-NB	2.47	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	14	316	A86	O-C13	-2.47	1.18	1.23
42	15	316	A86	O-C13	-2.47	1.18	1.23
30	m	101	CLA	C3B-C4B	2.47	1.48	1.42
30	A	402	CLA	CMD-C2D	-2.47	1.45	1.50
30	12	308	CLA	C1B-NB	-2.47	1.34	1.37
42	21	313	A86	C24-C1	2.47	1.51	1.45
30	w	102	CLA	MG-NB	-2.47	2.00	2.05
42	12	304	A86	O-C13	-2.47	1.18	1.23
30	a	402	CLA	CMC-C2C	-2.47	1.45	1.50
30	B	613	CLA	CMC-C2C	-2.47	1.45	1.50
40	D	407	PL9	C31-C29	-2.47	1.46	1.51
30	b	615	CLA	MG-ND	-2.47	2.00	2.05
42	11	311	A86	C14-C15	2.47	1.57	1.52
30	b	613	CLA	CMC-C2C	-2.47	1.45	1.50
30	B	614	CLA	C1B-NB	-2.47	1.34	1.37
42	17	302	A86	C24-C1	2.47	1.51	1.45
30	11	308	CLA	MG-ND	-2.47	2.00	2.05
30	d	407	CLA	CMB-C2B	-2.47	1.45	1.50
30	16	303	CLA	C3B-C4B	2.47	1.48	1.42
42	18	315	A86	C24-C1	2.47	1.51	1.45
30	a	403	CLA	MG-ND	-2.46	2.00	2.05
30	18	303	CLA	C3B-C4B	2.46	1.48	1.42
30	M	101	CLA	CMB-C2B	-2.46	1.45	1.50
30	19	301	CLA	C3B-C4B	2.46	1.48	1.42
42	18	302	A86	O-C13	-2.46	1.18	1.23
30	B	623	CLA	C4B-NB	2.46	1.40	1.37
42	21	312	A86	C24-C1	2.46	1.51	1.45
30	18	307	CLA	C1B-C2B	2.46	1.49	1.43
30	13	302	CLA	C4B-NB	2.46	1.40	1.37
42	11	314	A86	O-C13	-2.46	1.18	1.23
30	C	503	CLA	CAC-C3C	-2.46	1.44	1.51
30	A	402	CLA	CMC-C2C	-2.46	1.45	1.50
30	17	301	CLA	MG-ND	-2.46	2.00	2.05
30	D	406	CLA	CMB-C2B	-2.46	1.45	1.50
30	13	304	CLA	C4B-NB	2.46	1.40	1.37
30	11	306	CLA	MG-NB	-2.46	2.00	2.05
30	B	605	CLA	C4B-NB	2.46	1.40	1.37
30	14	305	CLA	C4B-NB	2.46	1.40	1.37
30	w	102	CLA	C4B-NB	2.46	1.40	1.37
30	11	301	CLA	C4B-NB	2.46	1.40	1.37
30	16	302	CLA	C4B-NB	2.46	1.40	1.37
30	20	202	CLA	MG-NB	-2.46	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	309	CLA	C4B-NB	2.46	1.40	1.37
42	11	316	A86	O-C13	-2.46	1.18	1.23
30	b	607	CLA	C1B-NB	-2.46	1.34	1.37
30	c	506	CLA	C3B-C4B	2.46	1.48	1.42
30	b	622	CLA	CMB-C2B	-2.46	1.45	1.50
30	18	301	CLA	C3B-C4B	2.45	1.48	1.42
30	12	312	CLA	MG-NB	-2.45	2.00	2.05
30	c	507	CLA	C1D-ND	2.45	1.40	1.37
30	D	406	CLA	CMD-C2D	-2.45	1.45	1.50
30	C	505	CLA	MG-ND	-2.45	2.00	2.05
30	16	301	CLA	C3B-C4B	2.45	1.48	1.42
30	16	304	CLA	CMB-C2B	-2.45	1.45	1.50
30	B	609	CLA	CMB-C2B	-2.45	1.45	1.50
42	18	314	A86	C14-C15	2.45	1.57	1.52
30	11	302	CLA	MG-NB	-2.45	2.00	2.05
42	15	313	A86	C24-C1	2.45	1.51	1.45
39	j	101	DGD	O1G-C1G	-2.45	1.39	1.45
30	B	602	CLA	C4B-NB	2.45	1.40	1.37
30	D	406	CLA	C1B-NB	-2.45	1.34	1.37
30	11	302	CLA	C4B-NB	2.45	1.40	1.37
42	13	301	A86	O-C13	-2.45	1.18	1.23
30	12	313	CLA	CMD-C2D	-2.45	1.45	1.50
30	11	305	CLA	MG-NB	-2.45	2.00	2.05
39	C	516	DGD	O5D-C6D	-2.45	1.39	1.43
42	16	313	A86	O-C13	-2.45	1.18	1.23
42	13	311	A86	C-C1	2.45	1.55	1.50
30	b	610	CLA	C3B-C4B	2.45	1.48	1.42
30	C	514	CLA	CMC-C2C	-2.44	1.45	1.50
30	c	504	CLA	MG-ND	-2.44	2.00	2.05
30	19	308	CLA	C4B-NB	2.44	1.40	1.37
30	C	507	CLA	CMD-C2D	-2.44	1.45	1.50
30	16	302	CLA	CMB-C2B	-2.44	1.45	1.50
30	12	306	CLA	C4B-NB	2.44	1.40	1.37
30	C	505	CLA	CMD-C2D	-2.44	1.45	1.50
30	c	507	CLA	C1B-NB	-2.44	1.34	1.37
30	13	308	CLA	C4B-NB	2.44	1.40	1.37
30	13	308	CLA	C3B-C4B	2.44	1.48	1.42
30	14	306	CLA	C1B-NB	-2.44	1.34	1.37
30	17	308	CLA	MG-ND	-2.44	2.00	2.05
30	B	611	CLA	CMD-C2D	-2.44	1.45	1.50
30	12	309	CLA	MG-NB	-2.44	2.00	2.05
30	A	404	CLA	CMC-C2C	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	315	CLA	MG-NB	-2.44	2.00	2.05
42	14	313	A86	C14-C15	2.44	1.57	1.52
30	c	503	CLA	CAC-C3C	-2.44	1.44	1.51
30	W	102	CLA	CMC-C2C	-2.44	1.45	1.50
30	B	601	CLA	CMB-C2B	-2.44	1.45	1.50
30	d	407	CLA	C1B-NB	-2.44	1.34	1.37
30	19	302	CLA	C3B-C4B	2.44	1.48	1.42
42	13	314	A86	C24-C1	2.44	1.51	1.45
30	C	504	CLA	C4B-NB	2.44	1.40	1.37
30	14	303	CLA	C1B-C2B	2.44	1.49	1.43
30	m	101	CLA	CMB-C2B	-2.44	1.45	1.50
30	21	304	CLA	MG-NB	-2.44	2.01	2.05
30	b	611	CLA	CMD-C2D	-2.44	1.45	1.50
30	18	312	CLA	C1B-C2B	2.44	1.49	1.43
30	15	309	CLA	MG-NB	-2.44	2.01	2.05
30	d	401	CLA	C1B-NB	-2.44	1.34	1.37
30	11	303	CLA	C4B-NB	2.44	1.40	1.37
30	C	506	CLA	CMC-C2C	-2.44	1.45	1.50
30	c	506	CLA	CMC-C2C	-2.44	1.45	1.50
30	c	507	CLA	CMD-C2D	-2.43	1.45	1.50
42	19	311	A86	C-C1	2.43	1.55	1.50
30	18	311	CLA	CMD-C2D	-2.43	1.45	1.50
30	C	506	CLA	C3B-C4B	2.43	1.48	1.42
30	18	310	CLA	CMD-C2D	-2.43	1.45	1.50
30	18	310	CLA	C3B-C4B	2.43	1.48	1.42
30	13	303	CLA	MG-NB	-2.43	2.01	2.05
42	15	311	A86	C14-C15	2.43	1.57	1.52
30	b	605	CLA	C3B-C4B	2.43	1.48	1.42
31	D	403	PHO	C1D-C2D	2.43	1.42	1.39
42	13	312	A86	C14-C15	2.43	1.57	1.52
30	c	514	CLA	MG-ND	-2.43	2.01	2.05
40	d	408	PL9	C31-C29	-2.43	1.46	1.51
30	18	304	CLA	MG-NB	-2.43	2.01	2.05
30	C	511	CLA	CMC-C2C	-2.43	1.45	1.50
30	W	102	CLA	CMB-C2B	-2.43	1.45	1.50
30	13	310	CLA	C1B-C2B	2.43	1.49	1.43
30	B	607	CLA	MG-ND	-2.43	2.01	2.05
42	20	210	A86	O-C13	-2.43	1.18	1.23
30	12	306	CLA	MG-NB	-2.43	2.01	2.05
30	15	308	CLA	MG-NB	-2.43	2.01	2.05
30	21	302	CLA	MG-NB	-2.43	2.01	2.05
41	V	201	HEM	C3D-C2D	-2.42	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	504	CLA	MG-ND	-2.42	2.01	2.05
30	17	306	CLA	C4B-NB	2.42	1.40	1.37
42	16	311	A86	C14-C15	2.42	1.57	1.52
30	13	308	CLA	CMD-C2D	-2.42	1.45	1.50
42	12	318	A86	C24-C1	2.42	1.51	1.45
41	F	102	HEM	FE-ND	2.42	2.02	1.94
30	15	309	CLA	C1B-C2B	2.42	1.49	1.43
30	c	505	CLA	CMC-C2C	-2.42	1.45	1.50
30	13	307	CLA	CMB-C2B	-2.42	1.45	1.50
30	16	309	CLA	CMC-C2C	-2.42	1.45	1.50
30	18	312	CLA	MG-NB	-2.42	2.01	2.05
30	21	303	CLA	MG-NB	-2.42	2.01	2.05
30	12	311	CLA	C3B-C4B	2.42	1.48	1.42
30	C	513	CLA	C4B-NB	2.42	1.40	1.37
30	19	307	CLA	C1B-NB	-2.42	1.34	1.37
30	18	309	CLA	CMB-C2B	-2.42	1.45	1.50
30	c	505	CLA	MG-ND	-2.42	2.01	2.05
30	12	311	CLA	MG-ND	-2.42	2.01	2.05
30	12	310	CLA	CMB-C2B	-2.42	1.45	1.50
39	c	517	DGD	O5D-C6D	-2.42	1.39	1.43
30	B	610	CLA	C3B-C4B	2.42	1.48	1.42
30	14	307	CLA	MG-NB	-2.42	2.01	2.05
30	C	507	CLA	CMC-C2C	-2.42	1.45	1.50
30	c	504	CLA	C4B-NB	2.42	1.40	1.37
30	19	305	CLA	CMB-C2B	-2.41	1.45	1.50
30	12	305	CLA	C1B-C2B	2.41	1.48	1.43
30	14	309	CLA	C3B-C4B	2.41	1.48	1.42
41	f	102	HEM	FE-ND	2.41	2.02	1.94
30	c	505	CLA	CMD-C2D	-2.41	1.45	1.50
30	15	303	CLA	C1B-C2B	2.41	1.48	1.43
30	17	304	CLA	C4B-NB	2.41	1.40	1.37
30	D	402	CLA	MG-ND	-2.41	2.01	2.05
30	13	310	CLA	MG-NB	-2.41	2.01	2.05
30	b	614	CLA	C1B-NB	-2.41	1.34	1.37
30	B	602	CLA	C3B-C4B	2.41	1.48	1.42
30	c	502	CLA	C1B-NB	-2.41	1.34	1.37
41	v	201	HEM	C3D-C2D	-2.41	1.31	1.36
30	B	604	CLA	CHC-C4B	-2.41	1.34	1.39
30	w	102	CLA	CMB-C2B	-2.41	1.45	1.50
31	d	404	PHO	C1D-C2D	2.41	1.42	1.39
42	20	211	A86	C-C1	2.41	1.55	1.50
30	17	307	CLA	MG-NB	-2.41	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	313	A86	C24-C1	2.41	1.51	1.45
30	B	605	CLA	C3B-C4B	2.41	1.48	1.42
30	C	509	CLA	C1D-ND	2.41	1.40	1.37
30	D	402	CLA	CMB-C2B	-2.41	1.45	1.50
42	17	312	A86	C14-C15	2.41	1.57	1.52
30	20	206	CLA	C1B-C2B	2.41	1.48	1.43
30	21	302	CLA	C1B-C2B	2.41	1.48	1.43
30	c	502	CLA	MG-ND	-2.41	2.01	2.05
30	13	306	CLA	MG-NB	-2.41	2.01	2.05
30	b	604	CLA	CHC-C4B	-2.40	1.34	1.39
30	c	507	CLA	CMC-C2C	-2.40	1.45	1.50
30	D	401	CLA	C1B-NB	-2.40	1.34	1.37
30	12	314	CLA	MG-NB	-2.40	2.01	2.05
30	b	607	CLA	MG-ND	-2.40	2.01	2.05
30	20	202	CLA	C1B-C2B	2.40	1.48	1.43
30	13	305	CLA	C1B-NB	-2.40	1.34	1.37
30	17	301	CLA	C1B-C2B	2.40	1.48	1.43
30	14	311	CLA	MG-NB	-2.40	2.01	2.05
30	b	603	CLA	CMC-C2C	-2.40	1.45	1.50
30	C	512	CLA	C4B-NB	2.40	1.40	1.37
30	14	310	CLA	MG-NB	-2.40	2.01	2.05
30	21	306	CLA	MG-NB	-2.40	2.01	2.05
30	12	311	CLA	CMD-C2D	-2.40	1.45	1.50
30	13	302	CLA	C1B-C2B	2.40	1.48	1.43
30	13	307	CLA	C1B-C2B	2.40	1.48	1.43
30	C	514	CLA	CMD-C2D	-2.40	1.45	1.50
30	b	614	CLA	CMC-C2C	-2.40	1.45	1.50
30	17	301	CLA	CMD-C2D	-2.40	1.45	1.50
30	b	607	CLA	CMB-C2B	-2.40	1.45	1.50
30	11	308	CLA	MG-NB	-2.40	2.01	2.05
30	19	308	CLA	CMD-C2D	-2.39	1.45	1.50
30	C	519	CLA	C1B-C2B	2.39	1.48	1.43
30	D	405	CLA	C1B-NB	-2.39	1.34	1.37
30	14	306	CLA	C4B-NB	2.39	1.40	1.37
42	17	314	A86	C24-C1	2.39	1.51	1.45
30	12	313	CLA	CMC-C2C	-2.39	1.45	1.50
30	16	308	CLA	C3B-C4B	2.39	1.48	1.42
30	B	608	CLA	MG-NB	-2.39	2.01	2.05
30	14	309	CLA	O2A-C1	-2.39	1.39	1.46
30	c	512	CLA	C4B-NB	2.39	1.40	1.37
30	C	514	CLA	MG-ND	-2.39	2.01	2.05
30	w	102	CLA	CMC-C2C	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	303	CLA	CMD-C2D	-2.39	1.45	1.50
30	17	304	CLA	C1B-NB	-2.39	1.34	1.37
30	16	308	CLA	CMB-C2B	-2.39	1.45	1.50
32	b	623	BCR	C30-C25	-2.39	1.50	1.53
30	16	301	CLA	C1B-C2B	2.39	1.48	1.43
30	11	309	CLA	C1B-C2B	2.39	1.48	1.43
42	20	212	A86	O-C13	-2.39	1.18	1.23
42	21	310	A86	O4-C34	-2.39	1.40	1.46
30	b	602	CLA	C3B-C4B	2.39	1.48	1.42
32	B	624	BCR	C30-C25	-2.39	1.50	1.53
30	12	307	CLA	C1B-C2B	2.38	1.48	1.43
30	14	309	CLA	CMD-C2D	-2.38	1.45	1.50
30	18	309	CLA	C1B-NB	-2.38	1.34	1.37
30	w	103	CLA	MG-NB	-2.38	2.01	2.05
42	21	311	A86	C-C1	2.38	1.55	1.50
42	12	316	A86	C14-C15	2.38	1.57	1.52
30	14	303	CLA	C3B-C4B	2.38	1.48	1.42
30	d	406	CLA	C4B-NB	2.38	1.40	1.37
42	19	310	A86	C24-C1	2.38	1.51	1.45
30	17	309	CLA	CMD-C2D	-2.38	1.45	1.50
30	18	301	CLA	CMD-C2D	-2.38	1.45	1.50
30	12	310	CLA	C1B-C2B	2.38	1.48	1.43
30	14	310	CLA	CMC-C2C	-2.38	1.45	1.50
30	18	305	CLA	MG-NB	-2.38	2.01	2.05
42	16	313	A86	O4-C34	-2.38	1.40	1.46
30	c	514	CLA	CMD-C2D	-2.38	1.45	1.50
30	d	402	CLA	CMB-C2B	-2.38	1.45	1.50
42	12	315	A86	C14-C15	2.38	1.57	1.52
30	12	306	CLA	CMD-C2D	-2.38	1.45	1.50
30	b	612	CLA	CMB-C2B	-2.38	1.45	1.50
36	1	101	LMG	O4-C4	-2.38	1.37	1.43
30	d	402	CLA	MG-ND	-2.38	2.01	2.05
30	c	511	CLA	CMC-C2C	-2.38	1.45	1.50
30	16	309	CLA	MG-ND	-2.38	2.01	2.05
42	13	311	A86	O4-C34	-2.38	1.40	1.46
30	12	314	CLA	C1B-C2B	2.38	1.48	1.43
30	16	309	CLA	C3B-C4B	2.38	1.48	1.42
30	C	512	CLA	CMB-C2B	-2.38	1.45	1.50
30	11	308	CLA	CMC-C2C	-2.38	1.45	1.50
30	17	310	CLA	MG-NB	-2.38	2.01	2.05
30	11	307	CLA	C3B-C4B	2.38	1.48	1.42
30	B	601	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	611	CLA	MG-ND	-2.38	2.01	2.05
30	16	303	CLA	CMD-C2D	-2.38	1.45	1.50
30	c	502	CLA	CMC-C2C	-2.37	1.45	1.50
30	14	304	CLA	CMD-C2D	-2.37	1.45	1.50
30	21	303	CLA	C1B-C2B	2.37	1.48	1.43
30	c	512	CLA	C1B-NB	-2.37	1.34	1.37
30	B	623	CLA	CMB-C2B	-2.37	1.45	1.50
30	19	306	CLA	CMD-C2D	-2.37	1.45	1.50
30	14	303	CLA	C4B-NB	2.37	1.40	1.37
30	B	612	CLA	CMB-C2B	-2.37	1.45	1.50
42	12	319	A86	C14-C15	2.37	1.57	1.52
30	B	607	CLA	CMC-C2C	-2.37	1.45	1.50
42	18	314	A86	C-C1	2.37	1.55	1.50
30	C	502	CLA	MG-ND	-2.37	2.01	2.05
30	D	406	CLA	MG-ND	-2.37	2.01	2.05
30	11	302	CLA	C3B-C4B	2.37	1.48	1.42
30	19	301	CLA	C4B-NB	2.37	1.40	1.37
30	19	306	CLA	CMB-C2B	-2.37	1.45	1.50
42	21	310	A86	C24-C1	2.37	1.51	1.45
30	D	405	CLA	C3B-C4B	2.37	1.48	1.42
30	16	302	CLA	C1B-C2B	2.37	1.48	1.43
30	19	307	CLA	MG-ND	-2.37	2.01	2.05
30	11	302	CLA	CMD-C2D	-2.37	1.45	1.50
30	17	310	CLA	C1B-C2B	2.37	1.48	1.43
30	13	309	CLA	MG-NB	-2.37	2.01	2.05
30	13	303	CLA	C4B-NB	2.37	1.40	1.37
42	13	312	A86	C-C1	2.37	1.55	1.50
30	C	510	CLA	CMD-C2D	-2.37	1.45	1.50
30	B	614	CLA	CMC-C2C	-2.37	1.45	1.50
30	16	303	CLA	MG-ND	-2.37	2.01	2.05
30	17	304	CLA	C3B-C4B	2.37	1.48	1.42
30	13	303	CLA	C3B-C4B	2.37	1.48	1.42
30	b	622	CLA	C1B-NB	-2.36	1.34	1.37
42	13	311	A86	C14-C15	2.36	1.57	1.52
42	18	313	A86	C14-C15	2.36	1.57	1.52
30	B	603	CLA	CMC-C2C	-2.36	1.45	1.50
30	c	506	CLA	CMB-C2B	-2.36	1.45	1.50
36	d	410	LMG	O4-C4	-2.36	1.37	1.43
30	16	301	CLA	CMD-C2D	-2.36	1.45	1.50
30	C	507	CLA	C1D-ND	2.36	1.40	1.37
30	B	623	CLA	C1B-NB	-2.36	1.34	1.37
30	18	308	CLA	MG-NB	-2.36	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	311	CLA	C1B-C2B	2.36	1.48	1.43
30	19	302	CLA	CMD-C2D	-2.36	1.45	1.50
30	11	306	CLA	CMB-C2B	-2.36	1.45	1.50
30	19	308	CLA	C3B-C4B	2.36	1.48	1.42
30	13	309	CLA	CMC-C2C	-2.36	1.45	1.50
42	15	314	A86	C14-C15	2.36	1.57	1.52
30	14	305	CLA	C1B-C2B	2.36	1.48	1.43
30	C	512	CLA	CMC-C2C	-2.36	1.45	1.50
30	17	306	CLA	MG-ND	-2.36	2.01	2.05
30	C	511	CLA	C3B-C4B	2.36	1.48	1.42
30	21	301	CLA	MG-NB	-2.36	2.01	2.05
30	14	304	CLA	C1B-C2B	2.36	1.48	1.43
30	D	402	CLA	CMD-C2D	-2.36	1.45	1.50
30	11	307	CLA	CMD-C2D	-2.36	1.45	1.50
30	19	307	CLA	CMD-C2D	-2.36	1.45	1.50
30	18	303	CLA	C1B-C2B	2.35	1.48	1.43
30	11	302	CLA	C1B-C2B	2.35	1.48	1.43
30	19	308	CLA	C1B-C2B	2.35	1.48	1.43
33	B	621	SQD	O3-C3	-2.35	1.37	1.43
30	14	311	CLA	CMD-C2D	-2.35	1.45	1.50
39	c	518	DGD	O1G-C1G	-2.35	1.39	1.45
30	20	207	CLA	C1B-C2B	2.35	1.48	1.43
30	16	307	CLA	MG-ND	-2.35	2.01	2.05
30	C	505	CLA	CMC-C2C	-2.35	1.45	1.50
30	19	302	CLA	MG-ND	-2.35	2.01	2.05
30	14	308	CLA	C1B-C2B	2.35	1.48	1.43
33	B	621	SQD	O2-C2	-2.35	1.37	1.43
30	11	309	CLA	CMD-C2D	-2.35	1.45	1.50
30	17	303	CLA	C1B-C2B	2.35	1.48	1.43
39	J	101	DGD	O3D-C3D	-2.35	1.37	1.43
30	C	511	CLA	CAA-C2A	-2.35	1.49	1.54
30	12	307	CLA	CMD-C2D	-2.35	1.45	1.50
30	C	506	CLA	CMB-C2B	-2.35	1.45	1.50
30	17	303	CLA	C3B-C4B	2.35	1.48	1.42
30	21	308	CLA	MG-NB	-2.35	2.01	2.05
42	11	311	A86	C-C1	2.35	1.55	1.50
30	b	604	CLA	CMC-C2C	-2.35	1.45	1.50
30	B	611	CLA	MG-ND	-2.35	2.01	2.05
30	18	307	CLA	MG-NB	-2.35	2.01	2.05
31	d	404	PHO	C3B-CAB	-2.35	1.43	1.47
42	12	316	A86	C-C1	2.35	1.55	1.50
42	17	316	A86	C24-C1	2.35	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	302	CLA	C3B-C4B	2.35	1.48	1.42
42	11	310	A86	O4-C34	-2.35	1.40	1.46
30	17	304	CLA	MG-NB	-2.35	2.01	2.05
42	18	313	A86	O4-C34	-2.35	1.40	1.46
30	17	303	CLA	CMD-C2D	-2.35	1.45	1.50
30	19	301	CLA	CMD-C2D	-2.35	1.45	1.50
30	d	406	CLA	C1B-NB	-2.35	1.34	1.37
42	15	314	A86	C24-C1	2.35	1.51	1.45
42	14	316	A86	C24-C1	2.35	1.51	1.45
30	17	309	CLA	CMC-C2C	-2.35	1.45	1.50
42	15	311	A86	C-C1	2.35	1.55	1.50
30	17	308	CLA	CMD-C2D	-2.35	1.45	1.50
42	17	316	A86	C14-C15	2.34	1.57	1.52
33	b	620	SQD	O3-C3	-2.34	1.37	1.43
30	11	303	CLA	C1B-C2B	2.34	1.48	1.43
30	19	305	CLA	CMD-C2D	-2.34	1.45	1.50
30	c	511	CLA	C3B-C4B	2.34	1.48	1.42
30	16	306	CLA	C3B-C4B	2.34	1.48	1.42
42	14	312	A86	O4-C34	-2.34	1.40	1.46
30	C	502	CLA	C1B-NB	-2.34	1.34	1.37
33	B	621	SQD	O4-C4	-2.34	1.37	1.43
30	11	308	CLA	C3B-C4B	2.34	1.48	1.42
30	d	402	CLA	CMD-C2D	-2.34	1.45	1.50
30	c	512	CLA	CMB-C2B	-2.34	1.45	1.50
42	11	311	A86	C24-C1	2.34	1.51	1.45
33	b	620	SQD	O2-C2	-2.34	1.37	1.43
30	17	303	CLA	CMC-C2C	-2.34	1.45	1.50
42	14	301	A86	O4-C34	-2.34	1.40	1.46
30	19	301	CLA	MG-ND	-2.34	2.01	2.05
39	C	517	DGD	O1G-C1G	-2.34	1.39	1.45
30	11	301	CLA	C3B-C4B	2.34	1.48	1.42
30	16	306	CLA	C1B-C2B	2.34	1.48	1.43
30	W	102	CLA	CMD-C2D	-2.34	1.45	1.50
30	18	309	CLA	CMD-C2D	-2.34	1.45	1.50
42	14	301	A86	C24-C1	2.34	1.51	1.45
33	A	406	SQD	O3-C3	-2.34	1.37	1.43
30	11	306	CLA	C1B-C2B	2.34	1.48	1.43
30	15	303	CLA	MG-NB	-2.34	2.01	2.05
30	12	306	CLA	C3B-C4B	2.34	1.48	1.42
30	z	101	CLA	C1B-C2B	2.34	1.48	1.43
39	J	101	DGD	O2E-C2E	-2.33	1.37	1.43
30	15	304	CLA	MG-NB	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	15	314	A86	O4-C34	-2.33	1.40	1.46
42	15	310	A86	C14-C15	2.33	1.57	1.52
30	A	402	CLA	C3B-C4B	2.33	1.48	1.42
42	14	313	A86	C-C1	2.33	1.55	1.50
30	c	506	CLA	MG-ND	-2.33	2.01	2.05
42	14	312	A86	C14-C15	2.33	1.57	1.52
42	20	211	A86	C24-C1	2.33	1.51	1.45
39	c	517	DGD	O2E-C2E	-2.33	1.37	1.43
42	16	313	A86	C14-C15	2.33	1.57	1.52
30	C	504	CLA	C1B-C2B	2.33	1.48	1.43
30	M	101	CLA	CMC-C2C	-2.33	1.45	1.50
30	15	304	CLA	CMD-C2D	-2.33	1.45	1.50
30	12	313	CLA	MG-NB	-2.33	2.01	2.05
42	16	310	A86	O4-C34	-2.33	1.40	1.46
30	12	314	CLA	CMD-C2D	-2.33	1.45	1.50
42	11	314	A86	C14-C15	2.33	1.57	1.52
30	11	303	CLA	CMD-C2D	-2.33	1.45	1.50
30	c	513	CLA	CMB-C2B	-2.33	1.45	1.50
42	11	314	A86	O4-C34	-2.33	1.40	1.46
42	15	310	A86	O4-C34	-2.33	1.40	1.46
30	B	604	CLA	CMC-C2C	-2.33	1.45	1.50
30	20	203	CLA	C3B-C4B	2.33	1.48	1.42
30	16	303	CLA	CMC-C2C	-2.33	1.45	1.50
30	17	307	CLA	C3B-C4B	2.33	1.48	1.42
30	b	602	CLA	CMD-C2D	-2.33	1.45	1.50
42	13	301	A86	C14-C15	2.33	1.57	1.52
30	17	307	CLA	C1B-C2B	2.33	1.48	1.43
30	c	504	CLA	CMC-C2C	-2.33	1.45	1.50
42	12	316	A86	C24-C1	2.33	1.50	1.45
30	11	307	CLA	MG-ND	-2.33	2.01	2.05
36	D	408	LMG	O4-C4	-2.33	1.37	1.43
30	a	402	CLA	C3B-C4B	2.33	1.48	1.42
42	17	312	A86	C-C1	2.33	1.55	1.50
30	16	304	CLA	CMD-C2D	-2.33	1.45	1.50
30	20	203	CLA	C1B-C2B	2.33	1.48	1.43
30	15	308	CLA	MG-ND	-2.33	2.01	2.05
30	C	520	CLA	CMD-C2D	-2.33	1.45	1.50
30	B	614	CLA	C1B-C2B	2.33	1.48	1.43
31	A	403	PHO	C4D-CHA	2.32	1.43	1.39
30	17	305	CLA	C3B-C4B	2.32	1.48	1.42
30	12	310	CLA	CMD-C2D	-2.32	1.45	1.50
30	d	406	CLA	C3B-C4B	2.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	309	CLA	C3B-C4B	2.32	1.48	1.42
42	12	315	A86	O4-C34	-2.32	1.40	1.46
30	w	102	CLA	CMD-C2D	-2.32	1.45	1.50
30	13	307	CLA	CMD-C2D	-2.32	1.45	1.50
30	c	509	CLA	C1D-ND	2.32	1.40	1.37
42	12	319	A86	O4-C34	-2.32	1.40	1.46
30	13	308	CLA	MG-ND	-2.32	2.01	2.05
30	13	308	CLA	CMC-C2C	-2.32	1.45	1.50
30	16	308	CLA	CMD-C2D	-2.32	1.45	1.50
30	b	607	CLA	CMC-C2C	-2.32	1.45	1.50
42	20	211	A86	O4-C34	-2.32	1.40	1.46
30	14	305	CLA	CMD-C2D	-2.32	1.45	1.50
30	13	304	CLA	C1B-C2B	2.32	1.48	1.43
42	11	310	A86	C14-C15	2.32	1.57	1.52
30	B	602	CLA	CMB-C2B	-2.32	1.45	1.50
30	B	601	CLA	CMC-C2C	-2.32	1.45	1.50
30	A	402	CLA	MG-ND	-2.32	2.01	2.05
30	b	608	CLA	MG-NB	-2.32	2.01	2.05
30	13	303	CLA	C1B-C2B	2.32	1.48	1.43
30	18	301	CLA	C1B-C2B	2.32	1.48	1.43
30	20	208	CLA	MG-NB	-2.32	2.01	2.05
30	W	103	CLA	MG-NB	-2.31	2.01	2.05
30	11	303	CLA	C3B-C4B	2.31	1.48	1.42
30	14	308	CLA	CMB-C2B	-2.31	1.45	1.50
30	d	407	CLA	MG-ND	-2.31	2.01	2.05
30	b	601	CLA	MG-ND	-2.31	2.01	2.05
32	f	101	BCR	C30-C25	-2.31	1.50	1.53
30	c	502	CLA	C1B-C2B	2.31	1.48	1.43
36	12	301	LMG	O7-C8	-2.31	1.40	1.46
30	13	304	CLA	C3B-C4B	2.31	1.48	1.42
31	D	403	PHO	C3B-CAB	-2.31	1.43	1.47
30	19	306	CLA	C4B-NB	2.31	1.40	1.37
30	C	508	CLA	CHC-C4B	-2.31	1.34	1.39
30	B	607	CLA	C3B-C4B	2.31	1.48	1.42
33	b	620	SQD	O4-C4	-2.31	1.37	1.43
42	14	301	A86	C14-C15	2.31	1.57	1.52
30	17	303	CLA	CMB-C2B	-2.31	1.45	1.50
30	20	203	CLA	CMB-C2B	-2.31	1.45	1.50
36	12	301	LMG	O6-C5	-2.31	1.38	1.44
39	j	101	DGD	O2E-C2E	-2.31	1.37	1.43
30	21	307	CLA	MG-NB	-2.31	2.01	2.05
30	C	502	CLA	CMC-C2C	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	508	CLA	CAC-C3C	-2.31	1.45	1.51
42	18	314	A86	C24-C1	2.31	1.50	1.45
30	18	311	CLA	MG-ND	-2.31	2.01	2.05
30	C	504	CLA	CMC-C2C	-2.31	1.45	1.50
30	12	313	CLA	C1B-C2B	2.31	1.48	1.43
30	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
39	C	516	DGD	O2E-C2E	-2.31	1.37	1.43
30	19	301	CLA	CMC-C2C	-2.31	1.45	1.50
30	19	304	CLA	MG-ND	-2.31	2.01	2.05
42	18	302	A86	C14-C15	2.31	1.57	1.52
30	c	511	CLA	CAA-C2A	-2.31	1.49	1.54
30	C	504	CLA	CMB-C2B	-2.30	1.45	1.50
30	a	402	CLA	MG-ND	-2.30	2.01	2.05
30	14	309	CLA	CMB-C2B	-2.30	1.45	1.50
30	c	504	CLA	C1B-C2B	2.30	1.48	1.43
30	W	102	CLA	MG-ND	-2.30	2.01	2.05
30	13	309	CLA	C1B-C2B	2.30	1.48	1.43
30	14	309	CLA	MG-ND	-2.30	2.01	2.05
42	16	311	A86	C24-C1	2.30	1.50	1.45
30	b	606	CLA	CAC-C3C	-2.30	1.45	1.51
39	j	101	DGD	O3D-C3D	-2.30	1.37	1.43
30	12	305	CLA	C3B-C4B	2.30	1.48	1.42
42	13	315	A86	C14-C15	2.30	1.57	1.52
30	20	205	CLA	C3B-C4B	2.30	1.48	1.42
30	19	308	CLA	MG-ND	-2.30	2.01	2.05
30	19	304	CLA	C1B-NB	-2.30	1.35	1.37
42	21	311	A86	C24-C1	2.30	1.50	1.45
30	B	606	CLA	CAC-C3C	-2.30	1.45	1.51
30	12	307	CLA	C3B-C4B	2.30	1.48	1.42
30	17	306	CLA	C1B-NB	-2.30	1.35	1.37
42	15	311	A86	C24-C1	2.30	1.50	1.45
30	b	607	CLA	C3B-C4B	2.30	1.48	1.42
30	11	306	CLA	CMD-C2D	-2.30	1.45	1.50
30	16	306	CLA	MG-NB	-2.30	2.01	2.05
30	c	512	CLA	CMC-C2C	-2.30	1.45	1.50
30	17	304	CLA	CMB-C2B	-2.30	1.45	1.50
30	16	308	CLA	CMC-C2C	-2.30	1.45	1.50
30	18	305	CLA	C1B-C2B	2.30	1.48	1.43
42	14	316	A86	O4-C34	-2.29	1.40	1.46
30	14	302	CLA	C1B-C2B	2.29	1.48	1.43
30	15	304	CLA	C1B-C2B	2.29	1.48	1.43
30	a	403	CLA	C3B-C4B	2.29	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	11	314	A86	C24-C1	2.29	1.50	1.45
30	D	406	CLA	C3B-C4B	2.29	1.48	1.42
33	a	405	SQD	O3-C3	-2.29	1.37	1.43
30	c	508	CLA	CHC-C4B	-2.29	1.34	1.39
30	D	406	CLA	CMC-C2C	-2.29	1.45	1.50
30	19	303	CLA	CMB-C2B	-2.29	1.45	1.50
30	17	305	CLA	MG-ND	-2.29	2.01	2.05
30	C	520	CLA	C4B-NB	2.29	1.40	1.37
30	B	615	CLA	C4B-NB	2.29	1.40	1.37
33	A	406	SQD	O4-C4	-2.29	1.37	1.43
30	d	402	CLA	C3B-C4B	2.29	1.48	1.42
30	B	602	CLA	CMD-C2D	-2.29	1.45	1.50
30	19	303	CLA	C1B-C2B	2.29	1.48	1.43
31	d	403	PHO	C4D-CHA	2.29	1.43	1.39
30	20	203	CLA	CMD-C2D	-2.29	1.45	1.50
30	14	310	CLA	C1B-C2B	2.29	1.48	1.43
30	b	601	CLA	C3B-C4B	2.29	1.48	1.42
30	12	313	CLA	C3B-C4B	2.29	1.48	1.42
30	W	103	CLA	C1B-C2B	2.29	1.48	1.43
42	17	316	A86	O4-C34	-2.29	1.40	1.46
30	19	309	CLA	CMD-C2D	-2.29	1.46	1.50
30	12	306	CLA	C1B-C2B	2.29	1.48	1.43
30	A	404	CLA	C3B-C4B	2.29	1.48	1.42
30	16	304	CLA	C3B-C4B	2.29	1.48	1.42
30	D	402	CLA	C3B-C4B	2.28	1.48	1.42
30	14	309	CLA	CMC-C2C	-2.28	1.46	1.50
30	19	306	CLA	C1B-NB	-2.28	1.35	1.37
30	19	301	CLA	CMB-C2B	-2.28	1.46	1.50
30	b	601	CLA	C4B-NB	2.28	1.40	1.37
30	b	601	CLA	CMD-C2D	-2.28	1.46	1.50
30	D	405	CLA	C4B-NB	2.28	1.40	1.37
33	l	101	SQD	O2-C2	-2.28	1.37	1.43
42	16	311	A86	C-C1	2.28	1.55	1.50
30	a	402	CLA	CMB-C2B	-2.28	1.46	1.50
42	15	316	A86	C14-C15	2.28	1.57	1.52
30	12	311	CLA	CMC-C2C	-2.28	1.46	1.50
30	14	305	CLA	C3B-C4B	2.28	1.48	1.42
30	C	506	CLA	MG-ND	-2.28	2.01	2.05
30	M	101	CLA	MG-ND	-2.28	2.01	2.05
30	14	310	CLA	C3B-C4B	2.28	1.48	1.42
30	D	405	CLA	CMB-C2B	-2.28	1.46	1.50
30	b	602	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	21	314	A86	O4-C34	-2.28	1.40	1.46
36	B	619	LMG	O1-C7	-2.28	1.39	1.43
30	b	601	CLA	CMC-C2C	-2.28	1.46	1.50
40	d	405	PL9	C36-C34	-2.28	1.46	1.51
39	C	516	DGD	O4D-C4D	-2.28	1.37	1.43
30	B	608	CLA	CMC-C2C	-2.28	1.46	1.50
30	15	308	CLA	C1B-C2B	2.28	1.48	1.43
30	11	307	CLA	CMB-C2B	-2.28	1.46	1.50
30	B	601	CLA	C3B-C4B	2.28	1.48	1.42
30	19	306	CLA	MG-ND	-2.28	2.01	2.05
30	13	306	CLA	C1B-C2B	2.27	1.48	1.43
30	14	307	CLA	C1B-C2B	2.27	1.48	1.43
36	b	618	LMG	O1-C7	-2.27	1.39	1.43
30	18	304	CLA	CMB-C2B	-2.27	1.46	1.50
42	11	316	A86	C14-C15	2.27	1.57	1.52
32	F	101	BCR	C30-C25	-2.27	1.50	1.53
30	16	305	CLA	MG-ND	-2.27	2.01	2.05
39	c	517	DGD	O4D-C4D	-2.27	1.37	1.43
30	B	614	CLA	CMB-C2B	-2.27	1.46	1.50
30	C	512	CLA	CMD-C2D	-2.27	1.46	1.50
30	b	608	CLA	CMC-C2C	-2.27	1.46	1.50
30	13	310	CLA	CMD-C2D	-2.27	1.46	1.50
30	13	304	CLA	CMD-C2D	-2.27	1.46	1.50
30	20	206	CLA	C1B-NB	-2.27	1.35	1.37
30	19	307	CLA	CMB-C2B	-2.27	1.46	1.50
30	14	310	CLA	CMB-C2B	-2.27	1.46	1.50
30	21	304	CLA	C1B-C2B	2.27	1.48	1.43
42	14	313	A86	C24-C1	2.27	1.50	1.45
41	f	102	HEM	C2A-C3A	-2.27	1.32	1.38
30	14	304	CLA	C3B-C4B	2.27	1.48	1.42
39	h	102	DGD	O4D-C4D	-2.27	1.37	1.43
30	b	609	CLA	CMC-C2C	-2.27	1.46	1.50
30	19	305	CLA	MG-ND	-2.27	2.01	2.05
30	11	305	CLA	C1B-C2B	2.27	1.48	1.43
30	19	307	CLA	C4B-NB	2.27	1.40	1.37
30	20	204	CLA	C1B-C2B	2.27	1.48	1.43
36	b	618	LMG	O8-C9	-2.27	1.40	1.45
30	16	309	CLA	CMB-C2B	-2.27	1.46	1.50
30	16	307	CLA	CMB-C2B	-2.27	1.46	1.50
30	18	310	CLA	CMB-C2B	-2.27	1.46	1.50
30	B	601	CLA	MG-ND	-2.27	2.01	2.05
30	19	309	CLA	MG-ND	-2.27	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	13	312	A86	C24-C1	2.27	1.50	1.45
30	C	520	CLA	C1B-NB	-2.27	1.35	1.37
30	b	614	CLA	CMB-C2B	-2.27	1.46	1.50
30	18	309	CLA	CMC-C2C	-2.26	1.46	1.50
42	14	316	A86	C14-C15	2.26	1.57	1.52
30	13	308	CLA	CMB-C2B	-2.26	1.46	1.50
30	14	308	CLA	CMD-C2D	-2.26	1.46	1.50
30	c	513	CLA	MG-ND	-2.26	2.01	2.05
30	d	407	CLA	CMC-C2C	-2.26	1.46	1.50
30	17	304	CLA	CMD-C2D	-2.26	1.46	1.50
30	15	301	CLA	C1B-C2B	2.26	1.48	1.43
30	17	305	CLA	CMB-C2B	-2.26	1.46	1.50
42	15	315	A86	C14-C15	2.26	1.57	1.52
42	12	319	A86	C24-C1	2.26	1.50	1.45
36	Q	301	LMG	O4-C4	-2.26	1.37	1.43
30	19	304	CLA	CMB-C2B	-2.26	1.46	1.50
30	12	303	CLA	C1B-C2B	2.26	1.48	1.43
42	12	304	A86	C14-C15	2.26	1.57	1.52
42	21	311	A86	O4-C34	-2.26	1.40	1.46
30	12	309	CLA	C1B-C2B	2.26	1.48	1.43
30	12	311	CLA	CMB-C2B	-2.26	1.46	1.50
30	b	614	CLA	C1B-C2B	2.26	1.48	1.43
33	a	405	SQD	O4-C4	-2.26	1.37	1.43
30	b	615	CLA	C4B-NB	2.26	1.40	1.37
30	18	304	CLA	C3B-C4B	2.26	1.48	1.42
30	18	311	CLA	CMC-C2C	-2.26	1.46	1.50
30	C	508	CLA	CAC-C3C	-2.26	1.45	1.51
39	j	101	DGD	O2D-C2D	-2.26	1.37	1.43
30	C	502	CLA	C1B-C2B	2.26	1.48	1.43
41	F	102	HEM	C2A-C3A	-2.26	1.32	1.38
30	c	507	CLA	C3B-C4B	2.26	1.48	1.42
30	C	502	CLA	CMB-C2B	-2.26	1.46	1.50
30	18	301	CLA	CMB-C2B	-2.26	1.46	1.50
30	11	308	CLA	C1B-C2B	2.26	1.48	1.43
39	H	102	DGD	O4D-C4D	-2.25	1.37	1.43
30	11	306	CLA	C3B-C4B	2.25	1.48	1.42
42	17	311	A86	O4-C34	-2.25	1.41	1.46
42	18	314	A86	O4-C34	-2.25	1.41	1.46
30	18	306	CLA	CMD-C2D	-2.25	1.46	1.50
42	20	213	A86	O4-C34	-2.25	1.41	1.46
42	12	315	A86	C24-C1	2.25	1.50	1.45
30	16	305	CLA	C3B-C4B	2.25	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	21	305	CLA	C1B-C2B	2.25	1.48	1.43
30	11	307	CLA	CMC-C2C	-2.25	1.46	1.50
30	B	611	CLA	C3B-C4B	2.25	1.48	1.42
30	c	504	CLA	CMB-C2B	-2.25	1.46	1.50
30	20	208	CLA	CMC-C2C	-2.25	1.46	1.50
30	m	101	CLA	CMC-C2C	-2.25	1.46	1.50
42	20	201	A86	O4-C34	-2.25	1.41	1.46
30	18	301	CLA	MG-ND	-2.25	2.01	2.05
30	w	103	CLA	C1B-C2B	2.25	1.48	1.43
30	19	303	CLA	CMD-C2D	-2.25	1.46	1.50
39	J	101	DGD	O2D-C2D	-2.25	1.37	1.43
42	17	312	A86	O4-C34	-2.25	1.41	1.46
30	A	402	CLA	CMB-C2B	-2.25	1.46	1.50
30	16	306	CLA	CMC-C2C	-2.25	1.46	1.50
30	13	303	CLA	MG-ND	-2.25	2.01	2.05
36	b	619	LMG	O2-C2	-2.25	1.37	1.43
42	17	315	A86	O4-C34	-2.25	1.41	1.46
42	16	313	A86	C24-C1	2.25	1.50	1.45
30	11	315	CLA	C1B-C2B	2.24	1.48	1.43
30	17	305	CLA	C1B-C2B	2.24	1.48	1.43
30	19	302	CLA	CMB-C2B	-2.24	1.46	1.50
36	B	620	LMG	O2-C2	-2.24	1.37	1.43
30	17	305	CLA	CMC-C2C	-2.24	1.46	1.50
36	c	519	LMG	O4-C4	-2.24	1.37	1.43
30	m	101	CLA	MG-ND	-2.24	2.01	2.05
30	20	206	CLA	CMD-C2D	-2.24	1.46	1.50
30	C	513	CLA	MG-ND	-2.24	2.01	2.05
30	14	302	CLA	CMB-C2B	-2.24	1.46	1.50
42	14	313	A86	O4-C34	-2.24	1.41	1.46
30	A	402	CLA	C4B-NB	2.24	1.40	1.37
42	12	316	A86	O4-C34	-2.24	1.41	1.46
30	16	304	CLA	MG-ND	-2.24	2.01	2.05
30	a	403	CLA	CAB-C3B	-2.23	1.41	1.47
42	15	310	A86	C24-C1	2.23	1.50	1.45
30	b	606	CLA	MG-ND	-2.23	2.01	2.05
30	b	605	CLA	CMC-C2C	-2.23	1.46	1.50
30	b	609	CLA	MG-ND	-2.23	2.01	2.05
30	15	308	CLA	CMC-C2C	-2.23	1.46	1.50
36	b	619	LMG	O3-C3	-2.23	1.37	1.43
30	C	505	CLA	CHC-C4B	-2.23	1.34	1.39
30	C	504	CLA	C3B-C4B	2.23	1.48	1.42
42	17	312	A86	C24-C1	2.23	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	601	CLA	C4B-NB	2.23	1.40	1.37
30	C	513	CLA	CMB-C2B	-2.23	1.46	1.50
30	w	102	CLA	MG-ND	-2.23	2.01	2.05
37	B	625	LMU	O3'-C3'	2.23	1.48	1.43
30	17	304	CLA	C1B-C2B	2.23	1.48	1.43
30	B	609	CLA	CMC-C2C	-2.23	1.46	1.50
36	B	619	LMG	O8-C9	-2.23	1.40	1.45
30	c	504	CLA	C3B-C4B	2.23	1.48	1.42
30	14	303	CLA	CMD-C2D	-2.23	1.46	1.50
30	b	601	CLA	C1B-NB	-2.23	1.35	1.37
30	14	305	CLA	CMC-C2C	-2.23	1.46	1.50
42	11	310	A86	C24-C1	2.23	1.50	1.45
30	B	609	CLA	MG-ND	-2.23	2.01	2.05
30	b	622	CLA	CMC-C2C	-2.23	1.46	1.50
30	12	305	CLA	CMD-C2D	-2.23	1.46	1.50
30	15	308	CLA	CMD-C2D	-2.23	1.46	1.50
30	c	505	CLA	CHC-C4B	-2.23	1.34	1.39
36	b	618	LMG	O4-C4	-2.23	1.37	1.43
30	17	301	CLA	C4B-NB	2.23	1.40	1.37
42	11	311	A86	O4-C34	-2.23	1.41	1.46
39	C	517	DGD	O2E-C2E	-2.23	1.37	1.43
39	c	518	DGD	O2E-C2E	-2.23	1.37	1.43
42	13	312	A86	O4-C34	-2.23	1.41	1.46
30	c	513	CLA	CMC-C2C	-2.23	1.46	1.50
30	17	310	CLA	CMD-C2D	-2.23	1.46	1.50
30	17	309	CLA	MG-ND	-2.23	2.01	2.05
30	A	402	CLA	C1B-NB	-2.23	1.35	1.37
39	j	101	DGD	O6D-C5D	-2.23	1.38	1.44
30	c	502	CLA	CMB-C2B	-2.23	1.46	1.50
30	16	304	CLA	CMC-C2C	-2.23	1.46	1.50
30	11	302	CLA	MG-ND	-2.23	2.01	2.05
36	B	620	LMG	O3-C3	-2.22	1.37	1.43
30	15	301	CLA	CMD-C2D	-2.22	1.46	1.50
30	11	302	CLA	CMC-C2C	-2.22	1.46	1.50
30	b	611	CLA	CAC-C3C	-2.22	1.45	1.51
30	b	614	CLA	MG-ND	-2.22	2.01	2.05
30	B	605	CLA	C1B-NB	-2.22	1.35	1.37
30	20	209	CLA	MG-ND	-2.22	2.01	2.05
30	19	306	CLA	C1B-C2B	2.22	1.48	1.43
30	11	303	CLA	MG-ND	-2.22	2.01	2.05
30	C	513	CLA	CMC-C2C	-2.22	1.46	1.50
30	15	306	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	20	212	A86	C14-C15	2.22	1.57	1.52
30	D	405	CLA	CAA-C2A	-2.22	1.50	1.54
30	18	303	CLA	CMB-C2B	-2.22	1.46	1.50
42	15	311	A86	O4-C34	-2.22	1.41	1.46
30	16	304	CLA	C1B-C2B	2.22	1.48	1.43
30	18	304	CLA	CMD-C2D	-2.22	1.46	1.50
30	12	307	CLA	MG-ND	-2.22	2.01	2.05
30	c	512	CLA	CMD-C2D	-2.22	1.46	1.50
30	b	614	CLA	C3B-C4B	2.22	1.48	1.42
30	B	611	CLA	CAC-C3C	-2.22	1.45	1.51
33	L	103	SQD	O2-C2	-2.22	1.37	1.43
30	C	511	CLA	C1D-ND	2.21	1.40	1.37
30	13	302	CLA	CMD-C2D	-2.21	1.46	1.50
30	C	520	CLA	MG-ND	-2.21	2.01	2.05
30	19	308	CLA	CMC-C2C	-2.21	1.46	1.50
42	13	311	A86	C24-C1	2.21	1.50	1.45
30	11	303	CLA	CMC-C2C	-2.21	1.46	1.50
30	d	406	CLA	CMB-C2B	-2.21	1.46	1.50
30	15	301	CLA	CMB-C2B	-2.21	1.46	1.50
30	b	611	CLA	C3B-C4B	2.21	1.48	1.42
30	M	101	CLA	C1B-NB	-2.21	1.35	1.37
36	B	619	LMG	O4-C4	-2.21	1.37	1.43
30	17	309	CLA	O2A-CGA	2.21	1.38	1.30
30	12	303	CLA	CMB-C2B	-2.21	1.46	1.50
30	14	304	CLA	CMC-C2C	-2.21	1.46	1.50
30	13	309	CLA	CMB-C2B	-2.21	1.46	1.50
30	14	304	CLA	MG-ND	-2.21	2.01	2.05
30	a	402	CLA	C1B-C2B	2.21	1.48	1.43
30	20	206	CLA	MG-ND	-2.21	2.01	2.05
42	16	311	A86	O4-C34	-2.21	1.41	1.46
30	16	303	CLA	C1B-NB	-2.21	1.35	1.37
30	17	304	CLA	MG-ND	-2.20	2.01	2.05
30	d	406	CLA	CAA-C2A	-2.20	1.50	1.54
30	20	206	CLA	CMB-C2B	-2.20	1.46	1.50
30	c	513	CLA	C1B-NB	-2.20	1.35	1.37
30	z	101	CLA	CMB-C2B	-2.20	1.46	1.50
30	12	307	CLA	CMC-C2C	-2.20	1.46	1.50
30	d	402	CLA	CMC-C2C	-2.20	1.46	1.50
30	15	309	CLA	CMD-C2D	-2.20	1.46	1.50
30	B	606	CLA	MG-ND	-2.20	2.01	2.05
30	11	301	CLA	CMD-C2D	-2.20	1.46	1.50
30	14	306	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	20	209	CLA	C1B-NB	-2.20	1.35	1.37
30	C	507	CLA	C3B-C4B	2.20	1.47	1.42
30	d	407	CLA	C3B-C4B	2.20	1.47	1.42
30	15	306	CLA	CMC-C2C	-2.20	1.46	1.50
30	18	303	CLA	CMD-C2D	-2.20	1.46	1.50
30	11	315	CLA	CMB-C2B	-2.20	1.46	1.50
30	13	304	CLA	CMC-C2C	-2.20	1.46	1.50
42	14	312	A86	C24-C1	2.20	1.50	1.45
30	B	614	CLA	C3B-C4B	2.20	1.47	1.42
30	17	305	CLA	CMD-C2D	-2.20	1.46	1.50
30	17	304	CLA	CMC-C2C	-2.20	1.46	1.50
30	19	306	CLA	CMC-C2C	-2.20	1.46	1.50
30	16	303	CLA	C1B-C2B	2.20	1.48	1.43
30	16	307	CLA	CHC-C1C	2.20	1.43	1.38
30	A	404	CLA	CAB-C3B	-2.20	1.41	1.47
42	17	302	A86	O4-C34	-2.20	1.41	1.46
30	12	313	CLA	CMB-C2B	-2.20	1.46	1.50
30	21	302	CLA	CMD-C2D	-2.20	1.46	1.50
30	14	305	CLA	MG-ND	-2.19	2.01	2.05
30	15	305	CLA	MG-NB	-2.19	2.01	2.05
30	19	302	CLA	C1B-C2B	2.19	1.48	1.43
39	c	517	DGD	O2G-C2G	-2.19	1.41	1.46
30	14	302	CLA	CMC-C2C	-2.19	1.46	1.50
30	18	303	CLA	CMC-C2C	-2.19	1.46	1.50
30	12	312	CLA	C1B-C2B	2.19	1.48	1.43
30	21	302	CLA	CMB-C2B	-2.19	1.46	1.50
30	C	506	CLA	C4B-NB	2.19	1.40	1.37
40	D	404	PL9	C36-C34	-2.19	1.46	1.51
30	19	305	CLA	C1B-NB	-2.19	1.35	1.37
30	C	519	CLA	CMB-C2B	-2.19	1.46	1.50
30	18	312	CLA	CMD-C2D	-2.19	1.46	1.50
30	13	304	CLA	MG-ND	-2.19	2.01	2.05
30	15	303	CLA	CMD-C2D	-2.19	1.46	1.50
30	16	301	CLA	CMB-C2B	-2.19	1.46	1.50
30	15	309	CLA	CMB-C2B	-2.19	1.46	1.50
30	18	308	CLA	CMB-C2B	-2.19	1.46	1.50
30	B	609	CLA	C3B-C4B	2.19	1.47	1.42
30	b	609	CLA	C3B-C4B	2.19	1.47	1.42
30	11	302	CLA	C1B-NB	-2.19	1.35	1.37
30	14	302	CLA	MG-ND	-2.19	2.01	2.05
30	b	609	CLA	C1B-C2B	2.19	1.48	1.43
30	B	606	CLA	MG-NB	-2.19	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	312	CLA	CMC-C2C	-2.19	1.46	1.50
30	C	520	CLA	CMB-C2B	-2.19	1.46	1.50
30	12	305	CLA	CMB-C2B	-2.19	1.46	1.50
32	f	101	BCR	C33-C5	-2.18	1.47	1.50
30	12	312	CLA	CMB-C2B	-2.18	1.46	1.50
30	16	302	CLA	CMD-C2D	-2.18	1.46	1.50
30	18	308	CLA	CMD-C2D	-2.18	1.46	1.50
30	b	610	CLA	C4B-NB	2.18	1.40	1.37
30	15	305	CLA	CHC-C1C	2.18	1.43	1.38
30	15	307	CLA	CMC-C2C	-2.18	1.46	1.50
39	c	517	DGD	O3D-C3D	-2.18	1.37	1.43
30	B	601	CLA	C1B-NB	-2.18	1.35	1.37
32	F	101	BCR	C33-C5	-2.18	1.47	1.50
30	18	301	CLA	CMC-C2C	-2.18	1.46	1.50
30	b	605	CLA	C1B-NB	-2.18	1.35	1.37
31	d	403	PHO	CAA-C2A	-2.18	1.49	1.54
30	21	307	CLA	CMD-C2D	-2.18	1.46	1.50
30	14	308	CLA	C3B-C4B	2.18	1.47	1.42
30	20	207	CLA	CMD-C2D	-2.18	1.46	1.50
30	15	302	CLA	CMD-C2D	-2.18	1.46	1.50
30	C	510	CLA	CMA-C3A	-2.18	1.48	1.53
30	18	310	CLA	MG-ND	-2.18	2.01	2.05
30	11	303	CLA	C1B-NB	-2.18	1.35	1.37
30	D	405	CLA	C1B-C2B	2.18	1.48	1.43
39	C	516	DGD	O2G-C2G	-2.18	1.41	1.46
30	20	203	CLA	MG-ND	-2.18	2.01	2.05
30	15	307	CLA	CMB-C2B	-2.18	1.46	1.50
30	12	310	CLA	C3B-C4B	2.18	1.47	1.42
30	11	308	CLA	CMB-C2B	-2.18	1.46	1.50
30	16	302	CLA	C3B-C4B	2.17	1.47	1.42
30	21	309	CLA	MG-NB	-2.17	2.01	2.05
30	D	402	CLA	CMC-C2C	-2.17	1.46	1.50
30	11	301	CLA	CMB-C2B	-2.17	1.46	1.50
30	20	205	CLA	MG-ND	-2.17	2.01	2.05
42	17	314	A86	O4-C34	-2.17	1.41	1.46
30	15	301	CLA	CMC-C2C	-2.17	1.46	1.50
30	18	312	CLA	CMB-C2B	-2.17	1.46	1.50
30	B	614	CLA	MG-ND	-2.17	2.01	2.05
30	z	101	CLA	C3B-C4B	2.17	1.47	1.42
30	B	609	CLA	C1B-C2B	2.17	1.48	1.43
30	c	511	CLA	C1D-ND	2.17	1.40	1.37
30	14	303	CLA	CMB-C2B	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	613	CLA	CMB-C2B	-2.17	1.46	1.50
39	C	516	DGD	O3D-C3D	-2.17	1.37	1.43
30	b	606	CLA	MG-NB	-2.17	2.01	2.05
30	12	312	CLA	MG-ND	-2.17	2.01	2.05
30	C	519	CLA	C3B-C4B	2.17	1.47	1.42
39	J	101	DGD	O6D-C5D	-2.17	1.39	1.44
30	13	308	CLA	C1B-NB	-2.17	1.35	1.37
30	17	309	CLA	CMB-C2B	-2.17	1.46	1.50
30	19	303	CLA	CMC-C2C	-2.17	1.46	1.50
30	20	204	CLA	CMD-C2D	-2.17	1.46	1.50
30	11	305	CLA	CMD-C2D	-2.17	1.46	1.50
30	12	306	CLA	C1B-NB	-2.17	1.35	1.37
30	19	301	CLA	C1B-NB	-2.17	1.35	1.37
30	21	308	CLA	CMD-C2D	-2.17	1.46	1.50
30	D	405	CLA	C1D-ND	2.16	1.40	1.37
42	13	315	A86	O4-C34	-2.16	1.41	1.46
30	m	101	CLA	C4B-NB	2.16	1.40	1.37
30	C	502	CLA	CAC-C3C	-2.16	1.45	1.51
30	20	204	CLA	CMB-C2B	-2.16	1.46	1.50
30	12	307	CLA	CMB-C2B	-2.16	1.46	1.50
30	16	301	CLA	MG-ND	-2.16	2.01	2.05
30	18	308	CLA	MG-ND	-2.16	2.01	2.05
39	c	517	DGD	O4E-C4E	-2.16	1.37	1.43
30	b	613	CLA	C3B-C4B	2.16	1.47	1.42
30	13	307	CLA	C3B-C4B	2.16	1.47	1.42
42	18	313	A86	C24-C1	2.16	1.50	1.45
30	12	306	CLA	MG-ND	-2.16	2.01	2.05
30	12	313	CLA	C1B-NB	-2.16	1.35	1.37
32	c	520	BCR	C33-C5	-2.16	1.47	1.50
30	B	623	CLA	CMC-C2C	-2.16	1.46	1.50
30	11	303	CLA	CMB-C2B	-2.16	1.46	1.50
30	19	301	CLA	C1B-C2B	2.16	1.48	1.43
30	B	613	CLA	CMB-C2B	-2.16	1.46	1.50
30	14	305	CLA	CMB-C2B	-2.16	1.46	1.50
30	16	308	CLA	MG-NB	-2.16	2.01	2.05
30	17	303	CLA	MG-ND	-2.16	2.01	2.05
30	m	101	CLA	C1B-NB	-2.16	1.35	1.37
30	B	613	CLA	C3B-C4B	2.16	1.47	1.42
30	c	514	CLA	CMB-C2B	-2.16	1.46	1.50
36	1	101	LMG	O6-C5	-2.16	1.39	1.44
30	d	402	CLA	C1B-NB	-2.16	1.35	1.37
30	13	305	CLA	CMB-C2B	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	403	PHO	CAA-C2A	-2.15	1.49	1.54
30	14	307	CLA	CMB-C2B	-2.15	1.46	1.50
42	18	302	A86	O4-C34	-2.15	1.41	1.46
30	c	504	CLA	C1B-NB	-2.15	1.35	1.37
30	16	309	CLA	C1B-C2B	2.15	1.48	1.43
30	11	315	CLA	CMC-C2C	-2.15	1.46	1.50
30	11	304	CLA	CMB-C2B	-2.15	1.46	1.50
30	13	304	CLA	CMB-C2B	-2.15	1.46	1.50
30	17	309	CLA	C1B-C2B	2.15	1.48	1.43
30	C	519	CLA	C1B-NB	-2.15	1.35	1.37
30	12	306	CLA	CMC-C2C	-2.15	1.46	1.50
30	11	305	CLA	CMB-C2B	-2.15	1.46	1.50
30	C	520	CLA	CMC-C2C	-2.15	1.46	1.50
30	21	301	CLA	CMD-C2D	-2.15	1.46	1.50
42	13	314	A86	O4-C34	-2.15	1.41	1.46
42	19	310	A86	O4-C34	-2.15	1.41	1.46
30	13	303	CLA	CMC-C2C	-2.15	1.46	1.50
30	17	310	CLA	CMC-C2C	-2.15	1.46	1.50
36	B	620	LMG	O7-C8	-2.15	1.41	1.46
30	20	209	CLA	CMD-C2D	-2.15	1.46	1.50
30	16	305	CLA	C1B-C2B	2.15	1.48	1.43
30	13	306	CLA	CMC-C2C	-2.15	1.46	1.50
30	c	506	CLA	C4B-NB	2.15	1.40	1.37
42	20	210	A86	O4-C34	-2.15	1.41	1.46
30	M	101	CLA	C4B-NB	2.15	1.40	1.37
30	20	207	CLA	C1B-NB	-2.15	1.35	1.37
42	21	313	A86	O4-C34	-2.14	1.41	1.46
30	a	402	CLA	C1B-NB	-2.14	1.35	1.37
30	18	305	CLA	CMD-C2D	-2.14	1.46	1.50
31	D	403	PHO	C3B-C2B	-2.14	1.37	1.40
30	15	303	CLA	CMC-C2C	-2.14	1.46	1.50
30	15	302	CLA	MG-NB	-2.14	2.01	2.05
30	17	308	CLA	CHC-C4B	-2.14	1.34	1.39
30	18	305	CLA	CMC-C2C	-2.14	1.46	1.50
32	B	624	BCR	C33-C5	-2.14	1.47	1.50
30	20	207	CLA	MG-ND	-2.14	2.01	2.05
30	c	502	CLA	CAC-C3C	-2.14	1.45	1.51
30	15	309	CLA	MG-ND	-2.14	2.01	2.05
30	12	308	CLA	CMB-C2B	-2.14	1.46	1.50
30	15	307	CLA	CMD-C2D	-2.14	1.46	1.50
30	a	402	CLA	C4B-NB	2.14	1.40	1.37
30	11	307	CLA	C1B-NB	-2.14	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	19	302	CLA	C4B-NB	2.14	1.40	1.37
30	d	407	CLA	C4B-NB	2.14	1.40	1.37
30	14	309	CLA	C1B-NB	-2.14	1.35	1.37
30	z	101	CLA	CMC-C2C	-2.14	1.46	1.50
30	19	302	CLA	CMC-C2C	-2.14	1.46	1.50
30	A	402	CLA	C1B-C2B	2.14	1.48	1.43
30	D	406	CLA	C4B-NB	2.14	1.40	1.37
36	m	102	LMG	O8-C9	-2.13	1.40	1.45
30	15	308	CLA	CMB-C2B	-2.13	1.46	1.50
30	19	305	CLA	CMC-C2C	-2.13	1.46	1.50
30	13	303	CLA	C1B-NB	-2.13	1.35	1.37
30	C	511	CLA	CMB-C2B	-2.13	1.46	1.50
30	20	207	CLA	CMB-C2B	-2.13	1.46	1.50
30	a	403	CLA	C1D-ND	2.13	1.40	1.37
30	19	307	CLA	C1B-C2B	2.13	1.48	1.43
32	c	516	BCR	C38-C26	-2.13	1.47	1.50
42	14	315	A86	O4-C34	-2.13	1.41	1.46
30	13	310	CLA	CMB-C2B	-2.13	1.46	1.50
30	12	314	CLA	CMB-C2B	-2.13	1.46	1.50
30	12	314	CLA	MG-ND	-2.13	2.01	2.05
30	15	301	CLA	CHC-C1C	2.13	1.42	1.38
30	21	305	CLA	CMD-C2D	-2.13	1.46	1.50
30	12	303	CLA	MG-ND	-2.13	2.01	2.05
32	C	515	BCR	C33-C5	-2.13	1.47	1.50
30	c	510	CLA	CMA-C3A	-2.13	1.48	1.53
30	16	308	CLA	C1B-C2B	2.13	1.48	1.43
42	20	210	A86	C14-C15	2.13	1.56	1.52
30	C	503	CLA	C1B-C2B	2.13	1.48	1.43
30	12	309	CLA	CMB-C2B	-2.13	1.46	1.50
39	C	517	DGD	O2D-C2D	-2.13	1.38	1.43
30	d	401	CLA	CAC-C3C	-2.12	1.45	1.51
39	h	102	DGD	O3D-C3D	-2.12	1.38	1.43
30	11	315	CLA	MG-ND	-2.12	2.01	2.05
30	20	205	CLA	CMD-C2D	-2.12	1.46	1.50
30	17	308	CLA	C1B-NB	-2.12	1.35	1.37
31	d	404	PHO	C3B-C2B	-2.12	1.37	1.40
30	17	301	CLA	C1B-NB	-2.12	1.35	1.37
30	12	303	CLA	CMC-C2C	-2.12	1.46	1.50
30	13	302	CLA	CMB-C2B	-2.12	1.46	1.50
30	13	310	CLA	MG-ND	-2.12	2.01	2.05
30	15	306	CLA	MG-NB	-2.12	2.01	2.05
39	c	518	DGD	O2D-C2D	-2.12	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	519	CLA	CMD-C2D	-2.12	1.46	1.50
32	C	515	BCR	C38-C26	-2.12	1.47	1.50
30	11	305	CLA	CMC-C2C	-2.12	1.46	1.50
30	15	307	CLA	C1B-C2B	2.12	1.48	1.43
30	A	404	CLA	C1D-ND	2.12	1.40	1.37
30	14	306	CLA	CMC-C2C	-2.12	1.46	1.50
30	21	306	CLA	CMD-C2D	-2.12	1.46	1.50
30	18	312	CLA	MG-ND	-2.12	2.01	2.05
30	A	404	CLA	C1B-NB	-2.12	1.35	1.37
30	B	606	CLA	C5-C3	-2.12	1.46	1.51
33	L	103	SQD	O3-C3	-2.12	1.38	1.43
30	13	304	CLA	C1B-NB	-2.11	1.35	1.37
42	11	313	A86	O4-C34	-2.11	1.41	1.46
30	C	519	CLA	CMC-C2C	-2.11	1.46	1.50
30	D	401	CLA	CAC-C3C	-2.11	1.45	1.51
39	j	101	DGD	O4E-C4E	-2.11	1.38	1.43
30	19	307	CLA	C3B-C4B	2.11	1.47	1.42
42	12	318	A86	O4-C34	-2.11	1.41	1.46
39	j	101	DGD	O3G-C3G	-2.11	1.39	1.43
33	B	621	SQD	O47-C45	-2.11	1.41	1.46
42	15	315	A86	O4-C34	-2.11	1.41	1.46
39	j	101	DGD	O4D-C4D	-2.11	1.38	1.43
33	b	620	SQD	O47-C45	-2.11	1.41	1.46
30	B	603	CLA	C3B-C4B	2.11	1.47	1.42
30	C	514	CLA	C1B-C2B	2.11	1.48	1.43
30	b	606	CLA	C5-C3	-2.11	1.46	1.51
30	c	511	CLA	CMB-C2B	-2.11	1.46	1.50
30	b	605	CLA	CAC-C3C	-2.11	1.45	1.51
30	b	610	CLA	CAC-C3C	-2.11	1.45	1.51
30	19	307	CLA	CMC-C2C	-2.11	1.46	1.50
30	19	309	CLA	CMB-C2B	-2.11	1.46	1.50
32	Y	101	BCR	C33-C5	-2.11	1.47	1.50
30	18	305	CLA	CMB-C2B	-2.11	1.46	1.50
39	J	101	DGD	O4D-C4D	-2.10	1.38	1.43
30	14	307	CLA	CMD-C2D	-2.10	1.46	1.50
30	c	509	CLA	C3B-C4B	2.10	1.47	1.42
36	b	619	LMG	O7-C8	-2.10	1.41	1.46
40	d	408	PL9	C15-C14	-2.10	1.45	1.50
30	11	309	CLA	CMB-C2B	-2.10	1.46	1.50
30	13	309	CLA	C1B-NB	-2.10	1.35	1.37
30	15	307	CLA	MG-ND	-2.10	2.01	2.05
30	17	301	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	603	CLA	CHC-C4B	-2.10	1.34	1.39
42	13	301	A86	O4-C34	-2.10	1.41	1.46
30	20	207	CLA	CMC-C2C	-2.10	1.46	1.50
30	14	311	CLA	MG-ND	-2.10	2.01	2.05
30	C	511	CLA	CAC-C3C	-2.10	1.45	1.51
30	21	309	CLA	CMB-C2B	-2.10	1.46	1.50
30	C	504	CLA	C1B-NB	-2.10	1.35	1.37
30	b	608	CLA	MG-ND	-2.10	2.01	2.05
42	15	313	A86	O4-C34	-2.10	1.41	1.46
30	c	514	CLA	C1B-C2B	2.10	1.48	1.43
32	c	516	BCR	C33-C5	-2.10	1.47	1.50
30	21	301	CLA	CMC-C2C	-2.10	1.46	1.50
30	B	605	CLA	CAC-C3C	-2.10	1.45	1.51
39	J	101	DGD	O4E-C4E	-2.10	1.38	1.43
30	B	610	CLA	C4B-NB	2.10	1.40	1.37
30	14	311	CLA	CMB-C2B	-2.09	1.46	1.50
30	18	306	CLA	MG-ND	-2.09	2.01	2.05
30	b	602	CLA	CAC-C3C	-2.09	1.45	1.51
30	19	308	CLA	CMB-C2B	-2.09	1.46	1.50
30	19	306	CLA	C3B-C4B	2.09	1.47	1.42
30	12	309	CLA	CMC-C2C	-2.09	1.46	1.50
30	D	402	CLA	C1B-NB	-2.09	1.35	1.37
30	20	204	CLA	MG-ND	-2.09	2.01	2.05
30	c	511	CLA	CAC-C3C	-2.09	1.45	1.51
30	13	305	CLA	CMC-C2C	-2.09	1.46	1.50
30	21	308	CLA	CMB-C2B	-2.09	1.46	1.50
39	C	516	DGD	O4E-C4E	-2.09	1.38	1.43
30	A	404	CLA	C4B-NB	2.09	1.40	1.37
30	14	304	CLA	C1B-NB	-2.09	1.35	1.37
30	C	511	CLA	CHC-C1C	2.09	1.42	1.38
30	16	303	CLA	CMB-C2B	-2.09	1.46	1.50
30	15	304	CLA	CMC-C2C	-2.09	1.46	1.50
30	15	303	CLA	CMB-C2B	-2.09	1.46	1.50
30	17	307	CLA	CMB-C2B	-2.09	1.46	1.50
40	D	407	PL9	C15-C14	-2.09	1.45	1.50
30	b	603	CLA	CHC-C4B	-2.09	1.34	1.39
30	z	101	CLA	C1B-NB	-2.09	1.35	1.37
30	d	406	CLA	C1D-ND	2.09	1.40	1.37
39	c	517	DGD	O3G-C1D	-2.09	1.36	1.40
30	21	305	CLA	MG-NB	-2.08	2.01	2.05
30	Z	102	CLA	CMD-C2D	-2.08	1.46	1.50
42	11	316	A86	O4-C34	-2.08	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	103	SQD	O4-C4	-2.08	1.38	1.43
30	21	304	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	403	CLA	C4B-NB	2.08	1.40	1.37
30	12	306	CLA	CMB-C2B	-2.08	1.46	1.50
42	12	304	A86	O4-C34	-2.08	1.41	1.46
30	21	304	CLA	MG-ND	-2.08	2.01	2.05
36	M	102	LMG	O8-C9	-2.08	1.40	1.45
33	l	101	SQD	O3-C3	-2.08	1.38	1.43
30	21	303	CLA	CMB-C2B	-2.08	1.46	1.50
39	J	101	DGD	O3G-C3G	-2.08	1.39	1.43
30	C	513	CLA	C1B-NB	-2.08	1.35	1.37
30	21	306	CLA	CMB-C2B	-2.08	1.46	1.50
30	16	305	CLA	CMB-C2B	-2.08	1.46	1.50
30	21	302	CLA	CMC-C2C	-2.08	1.46	1.50
42	18	315	A86	O4-C34	-2.08	1.41	1.46
30	13	306	CLA	CMD-C2D	-2.08	1.46	1.50
30	21	305	CLA	C1B-NB	-2.08	1.35	1.37
30	20	204	CLA	CMC-C2C	-2.08	1.46	1.50
30	13	306	CLA	CMB-C2B	-2.07	1.46	1.50
30	18	307	CLA	CMB-C2B	-2.07	1.46	1.50
42	19	310	A86	C14-C15	2.07	1.56	1.52
30	12	307	CLA	C1B-NB	-2.07	1.35	1.37
33	A	406	SQD	O47-C45	-2.07	1.41	1.46
42	15	316	A86	O4-C34	-2.07	1.41	1.46
30	B	610	CLA	CAC-C3C	-2.07	1.45	1.51
30	d	406	CLA	C1B-C2B	2.07	1.48	1.43
30	14	304	CLA	CMB-C2B	-2.07	1.46	1.50
30	12	309	CLA	CMD-C2D	-2.07	1.46	1.50
30	b	611	CLA	C4B-NB	2.07	1.40	1.37
30	20	202	CLA	CMC-C2C	-2.07	1.46	1.50
30	16	309	CLA	C1B-NB	-2.07	1.35	1.37
30	C	514	CLA	CMB-C2B	-2.07	1.46	1.50
30	14	307	CLA	MG-ND	-2.07	2.01	2.05
30	17	310	CLA	MG-ND	-2.07	2.01	2.05
39	h	102	DGD	O2D-C2D	-2.07	1.38	1.43
32	h	101	BCR	C33-C5	-2.07	1.47	1.50
30	c	512	CLA	CHC-C1C	2.07	1.42	1.38
30	b	622	CLA	C1B-C2B	2.06	1.48	1.43
30	13	310	CLA	CMC-C2C	-2.06	1.46	1.50
30	17	306	CLA	CMB-C2B	-2.06	1.46	1.50
30	c	503	CLA	C1B-C2B	2.06	1.48	1.43
30	18	307	CLA	CHC-C1C	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	603	CLA	C3B-C4B	2.06	1.47	1.42
30	21	301	CLA	CMB-C2B	-2.06	1.46	1.50
33	l	101	SQD	O4-C4	-2.06	1.38	1.43
39	H	102	DGD	O3D-C3D	-2.06	1.38	1.43
30	11	309	CLA	CMC-C2C	-2.06	1.46	1.50
30	11	309	CLA	MG-ND	-2.06	2.01	2.05
30	15	302	CLA	CMC-C2C	-2.06	1.46	1.50
30	11	315	CLA	C1B-NB	-2.06	1.35	1.37
30	15	305	CLA	CMD-C2D	-2.06	1.46	1.50
36	M	102	LMG	O2-C2	-2.06	1.38	1.43
30	13	303	CLA	CMB-C2B	-2.06	1.46	1.50
30	17	310	CLA	CMB-C2B	-2.06	1.46	1.50
30	C	509	CLA	CHC-C4B	-2.06	1.34	1.39
30	13	307	CLA	C1B-NB	-2.06	1.35	1.37
30	14	305	CLA	C1B-NB	-2.06	1.35	1.37
30	17	305	CLA	C1B-NB	-2.06	1.35	1.37
30	d	402	CLA	C4B-NB	2.06	1.40	1.37
31	d	403	PHO	C3B-CAB	-2.06	1.43	1.47
32	c	515	BCR	C33-C5	-2.06	1.47	1.50
30	14	307	CLA	CMC-C2C	-2.06	1.46	1.50
30	C	509	CLA	C3B-C4B	2.06	1.47	1.42
30	b	615	CLA	CAC-C3C	-2.06	1.45	1.51
32	b	623	BCR	C33-C5	-2.05	1.47	1.50
30	B	623	CLA	C1D-ND	2.05	1.40	1.37
42	21	311	A86	C14-C15	2.05	1.56	1.52
30	19	304	CLA	CMD-C2D	-2.05	1.46	1.50
30	20	205	CLA	CMB-C2B	-2.05	1.46	1.50
30	20	205	CLA	CMC-C2C	-2.05	1.46	1.50
30	b	607	CLA	C4B-NB	2.05	1.40	1.37
30	17	307	CLA	MG-ND	-2.05	2.01	2.05
30	19	309	CLA	C1B-C2B	2.05	1.48	1.43
30	11	304	CLA	CMC-C2C	-2.05	1.46	1.50
32	Y	101	BCR	C34-C9	-2.05	1.46	1.50
30	11	305	CLA	MG-ND	-2.05	2.01	2.05
42	16	310	A86	C14-C15	2.05	1.56	1.52
30	21	303	CLA	MG-ND	-2.05	2.01	2.05
30	D	406	CLA	C1B-C2B	2.05	1.48	1.43
30	b	612	CLA	C1B-C2B	2.05	1.48	1.43
42	20	211	A86	C14-C15	2.05	1.56	1.52
30	c	511	CLA	CHC-C1C	2.05	1.42	1.38
30	w	102	CLA	C1B-C2B	2.05	1.48	1.43
30	z	101	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	20	208	CLA	CMD-C2D	-2.05	1.46	1.50
30	20	202	CLA	CMD-C2D	-2.05	1.46	1.50
30	20	202	CLA	CHC-C1C	2.05	1.42	1.38
30	W	102	CLA	C1B-C2B	2.05	1.48	1.43
30	b	614	CLA	CHC-C4B	-2.05	1.34	1.39
30	c	502	CLA	CHC-C4B	-2.05	1.34	1.39
30	B	608	CLA	MG-ND	-2.05	2.01	2.05
30	B	602	CLA	CAC-C3C	-2.04	1.45	1.51
30	11	308	CLA	C1B-NB	-2.04	1.35	1.37
40	D	404	PL9	C41-C39	-2.04	1.47	1.51
30	11	302	CLA	CMB-C2B	-2.04	1.46	1.50
30	21	304	CLA	CMC-C2C	-2.04	1.46	1.50
30	Z	102	CLA	CMB-C2B	-2.04	1.46	1.50
30	B	615	CLA	CAC-C3C	-2.04	1.45	1.51
30	21	309	CLA	O2A-CGA	2.04	1.37	1.30
30	12	308	CLA	CMC-C2C	-2.04	1.46	1.50
30	14	311	CLA	CMC-C2C	-2.04	1.46	1.50
36	c	519	LMG	O2-C2	-2.04	1.38	1.43
30	13	306	CLA	MG-ND	-2.04	2.01	2.05
42	17	302	A86	C35-C34	2.04	1.55	1.51
42	21	313	A86	C14-C15	2.04	1.56	1.52
31	A	403	PHO	C3B-CAB	-2.04	1.43	1.47
36	m	102	LMG	O2-C2	-2.03	1.38	1.43
39	H	102	DGD	O2D-C2D	-2.03	1.38	1.43
42	20	213	A86	C14-C15	2.03	1.56	1.52
42	21	314	A86	C14-C15	2.03	1.56	1.52
30	19	305	CLA	C1B-C2B	2.03	1.48	1.43
30	18	303	CLA	MG-ND	-2.03	2.01	2.05
30	16	306	CLA	CMD-C2D	-2.03	1.46	1.50
30	13	302	CLA	MG-ND	-2.03	2.01	2.05
30	21	309	CLA	CHC-C1C	2.03	1.42	1.38
30	c	509	CLA	CHC-C4B	-2.03	1.34	1.39
30	12	305	CLA	MG-ND	-2.03	2.01	2.05
36	w	101	LMG	C4-C5	2.03	1.57	1.53
30	b	603	CLA	C4B-NB	2.03	1.40	1.37
32	Z	101	BCR	C33-C5	-2.03	1.47	1.50
30	15	306	CLA	CMD-C2D	-2.03	1.46	1.50
36	w	101	LMG	O4-C4	-2.03	1.38	1.43
30	c	513	CLA	C1B-C2B	2.03	1.48	1.43
30	16	302	CLA	MG-ND	-2.03	2.01	2.05
32	H	101	BCR	C38-C26	-2.02	1.47	1.50
32	h	101	BCR	C38-C26	-2.02	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	21	309	CLA	CMC-C2C	-2.02	1.46	1.50
30	B	623	CLA	C1B-C2B	2.02	1.48	1.43
30	17	301	CLA	C3B-C4B	2.02	1.47	1.42
30	21	301	CLA	CHC-C1C	2.02	1.42	1.38
30	19	308	CLA	C1B-NB	-2.02	1.35	1.37
40	d	405	PL9	C41-C39	-2.02	1.47	1.51
30	C	502	CLA	CHC-C4B	-2.02	1.34	1.39
30	14	303	CLA	CHC-C1C	2.02	1.42	1.38
30	b	614	CLA	C4B-NB	2.02	1.40	1.37
30	21	306	CLA	CMC-C2C	-2.02	1.46	1.50
40	D	407	PL9	C16-C14	-2.02	1.47	1.51
30	B	614	CLA	CHC-C4B	-2.02	1.34	1.39
35	A	408	LHG	C8-C7	-2.02	1.44	1.50
30	B	607	CLA	C4B-NB	2.02	1.40	1.37
42	11	312	A86	C33-C34	2.02	1.55	1.51
30	15	307	CLA	CHC-C1C	2.02	1.42	1.38
30	d	407	CLA	C1B-C2B	2.02	1.48	1.43
30	12	310	CLA	C1B-NB	-2.02	1.35	1.37
30	12	311	CLA	C1B-NB	-2.02	1.35	1.37
30	C	510	CLA	C3B-C4B	2.02	1.47	1.42
30	20	209	CLA	CMC-C2C	-2.02	1.46	1.50
30	D	401	CLA	C3B-C4B	2.02	1.47	1.42
42	15	312	A86	C33-C34	2.02	1.55	1.51
30	18	311	CLA	CMB-C2B	-2.01	1.46	1.50
30	12	309	CLA	MG-ND	-2.01	2.01	2.05
30	11	301	CLA	CHC-C1C	2.01	1.42	1.38
30	c	505	CLA	C3B-C4B	2.01	1.47	1.42
30	19	303	CLA	MG-ND	-2.01	2.01	2.05
30	12	305	CLA	CHC-C1C	2.01	1.42	1.38
30	B	607	CLA	C1B-C2B	2.01	1.48	1.43
30	21	307	CLA	CMB-C2B	-2.01	1.46	1.50
30	18	305	CLA	CHC-C1C	2.01	1.42	1.38
30	c	510	CLA	C3B-C4B	2.01	1.47	1.42
35	a	407	LHG	C8-C7	-2.01	1.44	1.50
30	w	102	CLA	C1B-NB	-2.01	1.35	1.37
30	c	514	CLA	C4B-NB	2.01	1.40	1.37
30	17	304	CLA	CAC-C3C	-2.01	1.46	1.51
30	w	103	CLA	CMB-C2B	-2.01	1.46	1.50
30	11	306	CLA	C1B-NB	-2.01	1.35	1.37
30	15	305	CLA	CMB-C2B	-2.01	1.46	1.50
30	18	307	CLA	CMC-C2C	-2.01	1.46	1.50
42	17	313	A86	C33-C34	2.01	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Q	301	LMG	O2-C2	-2.01	1.38	1.43
30	11	301	CLA	MG-ND	-2.01	2.01	2.05
30	B	611	CLA	C4B-NB	2.01	1.40	1.37
30	15	301	CLA	MG-ND	-2.00	2.01	2.05
42	17	313	A86	C35-C34	2.00	1.55	1.51
30	18	306	CLA	CMB-C2B	-2.00	1.46	1.50
30	18	304	CLA	C1B-NB	-2.00	1.35	1.37
30	15	309	CLA	O2A-CGA	2.00	1.37	1.30
42	13	313	A86	C35-C34	2.00	1.55	1.51
30	18	307	CLA	CMD-C2D	-2.00	1.46	1.50
30	D	402	CLA	C4B-NB	2.00	1.40	1.37
30	b	601	CLA	C1B-C2B	2.00	1.48	1.43
30	w	103	CLA	CHC-C1C	2.00	1.42	1.38
30	18	312	CLA	O2A-CGA	2.00	1.37	1.30
30	17	309	CLA	MG-NB	-2.00	2.01	2.05

All (3400) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	17	311	A86	O1-C20-C19	55.34	154.95	113.38
42	17	315	A86	O1-C20-C19	55.32	154.94	113.38
42	18	313	A86	O1-C20-C19	55.08	154.75	113.38
42	20	210	A86	O1-C20-C19	55.05	154.74	113.38
42	11	310	A86	O1-C20-C19	55.03	154.72	113.38
42	13	311	A86	O1-C20-C19	55.00	154.70	113.38
42	15	310	A86	O1-C20-C19	55.00	154.70	113.38
42	12	315	A86	O1-C20-C19	54.99	154.69	113.38
42	14	312	A86	O1-C20-C19	54.99	154.69	113.38
42	11	313	A86	O1-C20-C19	54.26	154.14	113.38
42	12	318	A86	O1-C20-C19	54.24	154.13	113.38
42	14	315	A86	O1-C20-C19	54.24	154.13	113.38
42	17	314	A86	O1-C20-C19	54.24	154.12	113.38
42	18	315	A86	O1-C20-C19	54.23	154.12	113.38
42	15	313	A86	O1-C20-C19	54.21	154.11	113.38
42	13	314	A86	O1-C20-C19	54.17	154.07	113.38
42	20	212	A86	O1-C20-C19	54.09	154.02	113.38
42	19	312	A86	O1-C20-C19	53.41	153.50	113.38
42	16	310	A86	O1-C20-C19	53.36	153.47	113.38
42	17	302	A86	O1-C20-C19	52.82	153.06	113.38
42	17	316	A86	O1-C20-C19	52.61	152.90	113.38
42	11	314	A86	O1-C20-C19	52.58	152.88	113.38
42	14	316	A86	O1-C20-C19	52.54	152.85	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	14	301	A86	O1-C20-C19	52.52	152.83	113.38
42	15	314	A86	O1-C20-C19	52.51	152.83	113.38
42	12	319	A86	O1-C20-C19	52.47	152.80	113.38
42	16	313	A86	O1-C20-C19	52.46	152.79	113.38
42	17	312	A86	O1-C20-C19	51.99	152.44	113.38
42	14	313	A86	O1-C20-C19	51.99	152.44	113.38
42	12	316	A86	O1-C20-C19	51.96	152.42	113.38
42	13	312	A86	O1-C20-C19	51.94	152.40	113.38
42	18	314	A86	O1-C20-C19	51.89	152.37	113.38
42	16	311	A86	O1-C20-C19	51.89	152.36	113.38
42	11	311	A86	O1-C20-C19	51.86	152.34	113.38
42	15	311	A86	O1-C20-C19	51.86	152.34	113.38
42	20	201	A86	O1-C20-C19	51.61	152.15	113.38
42	21	314	A86	O1-C20-C19	51.51	152.08	113.38
42	20	213	A86	O1-C20-C19	51.49	152.06	113.38
42	19	310	A86	O1-C20-C19	50.72	151.48	113.38
42	11	312	A86	O1-C20-C19	50.68	151.46	113.38
42	15	312	A86	O1-C20-C19	50.62	151.41	113.38
42	17	313	A86	O1-C20-C19	50.60	151.39	113.38
42	16	312	A86	O1-C20-C19	50.57	151.37	113.38
42	13	313	A86	O1-C20-C19	50.55	151.36	113.38
42	14	314	A86	O1-C20-C19	50.54	151.35	113.38
42	12	317	A86	O1-C20-C19	50.53	151.34	113.38
42	21	311	A86	O1-C20-C19	49.05	150.23	113.38
42	20	211	A86	O1-C20-C19	49.01	150.20	113.38
42	21	313	A86	O1-C20-C19	48.91	150.12	113.38
42	21	310	A86	O1-C20-C19	48.60	149.89	113.38
42	12	304	A86	O1-C20-C19	48.00	149.44	113.38
42	13	301	A86	O1-C20-C19	47.99	149.43	113.38
42	11	316	A86	O1-C20-C19	47.97	149.42	113.38
42	18	302	A86	O1-C20-C19	47.97	149.41	113.38
42	13	315	A86	O1-C20-C19	47.96	149.41	113.38
42	15	316	A86	O1-C20-C19	47.95	149.40	113.38
42	15	315	A86	O1-C20-C19	47.92	149.38	113.38
42	19	311	A86	O1-C20-C19	46.13	148.03	113.38
42	21	312	A86	O1-C20-C19	45.21	147.35	113.38
42	18	302	A86	C17-C16-C15	11.87	121.27	109.16
42	12	304	A86	C17-C16-C15	11.87	121.27	109.16
42	15	315	A86	C17-C16-C15	11.86	121.26	109.16
42	11	316	A86	C17-C16-C15	11.85	121.25	109.16
42	13	301	A86	C17-C16-C15	11.85	121.25	109.16
42	13	315	A86	C17-C16-C15	11.83	121.23	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	316	A86	C17-C16-C15	11.80	121.20	109.16
42	17	315	A86	C21-C20-C19	-11.53	101.31	114.28
42	20	210	A86	O1-C20-C21	-11.37	101.43	115.06
42	11	313	A86	O1-C20-C21	-11.27	101.56	115.06
42	18	315	A86	O1-C20-C21	-11.26	101.57	115.06
42	17	314	A86	O1-C20-C21	-11.25	101.58	115.06
42	15	313	A86	O1-C20-C21	-11.24	101.59	115.06
42	12	318	A86	O1-C20-C21	-11.23	101.60	115.06
42	13	314	A86	O1-C20-C21	-11.20	101.63	115.06
42	14	315	A86	O1-C20-C21	-11.19	101.64	115.06
42	17	311	A86	O1-C20-C21	-11.19	101.65	115.06
42	17	315	A86	O1-C20-C21	-11.02	101.85	115.06
42	20	212	A86	O1-C20-C21	-10.96	101.92	115.06
42	11	310	A86	O1-C20-C21	-10.91	101.98	115.06
42	18	313	A86	O1-C20-C21	-10.91	101.99	115.06
42	17	316	A86	C21-C20-C19	-10.91	102.01	114.28
42	14	312	A86	O1-C20-C21	-10.90	101.99	115.06
42	12	315	A86	O1-C20-C21	-10.90	102.00	115.06
42	14	316	A86	C21-C20-C19	-10.88	102.04	114.28
42	13	311	A86	O1-C20-C21	-10.87	102.03	115.06
42	11	314	A86	C21-C20-C19	-10.87	102.06	114.28
42	16	313	A86	C21-C20-C19	-10.86	102.06	114.28
42	15	310	A86	O1-C20-C21	-10.86	102.05	115.06
42	17	302	A86	C21-C20-C19	-10.86	102.07	114.28
42	12	319	A86	C21-C20-C19	-10.84	102.09	114.28
42	14	301	A86	C21-C20-C19	-10.83	102.10	114.28
42	16	310	A86	O1-C20-C21	-10.82	102.10	115.06
42	15	314	A86	C21-C20-C19	-10.81	102.12	114.28
42	19	310	A86	C21-C20-C19	-10.73	102.21	114.28
42	15	310	A86	C21-C20-C19	-10.62	102.33	114.28
42	17	311	A86	C21-C20-C19	-10.62	102.34	114.28
42	18	313	A86	C21-C20-C19	-10.61	102.35	114.28
42	13	311	A86	C21-C20-C19	-10.60	102.36	114.28
42	12	315	A86	C21-C20-C19	-10.59	102.37	114.28
42	11	310	A86	C21-C20-C19	-10.58	102.38	114.28
42	14	312	A86	C21-C20-C19	-10.58	102.38	114.28
42	20	212	A86	C36-C31-C32	-10.57	109.21	119.70
42	11	312	A86	C21-C20-C19	-10.55	102.41	114.28
42	15	312	A86	C21-C20-C19	-10.54	102.43	114.28
42	17	313	A86	C21-C20-C19	-10.53	102.43	114.28
42	13	313	A86	C21-C20-C19	-10.53	102.43	114.28
42	16	312	A86	C21-C20-C19	-10.51	102.45	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	14	314	A86	C21-C20-C19	-10.50	102.46	114.28
42	12	317	A86	C21-C20-C19	-10.49	102.48	114.28
42	19	312	A86	O1-C20-C21	-10.37	102.64	115.06
42	19	312	A86	C21-C20-C19	-10.28	102.72	114.28
42	12	304	A86	C21-C20-C19	-10.14	102.87	114.28
42	15	315	A86	C21-C20-C19	-10.14	102.87	114.28
42	13	315	A86	C21-C20-C19	-10.14	102.87	114.28
42	20	210	A86	C21-C20-C19	-10.13	102.88	114.28
42	13	312	A86	O1-C20-C21	-10.13	102.92	115.06
42	12	316	A86	O1-C20-C21	-10.12	102.93	115.06
42	14	313	A86	O1-C20-C21	-10.12	102.93	115.06
42	18	314	A86	O1-C20-C21	-10.12	102.93	115.06
42	13	301	A86	C21-C20-C19	-10.11	102.91	114.28
42	11	316	A86	C21-C20-C19	-10.11	102.91	114.28
42	17	312	A86	O1-C20-C21	-10.10	102.95	115.06
42	16	311	A86	O1-C20-C21	-10.09	102.96	115.06
42	18	302	A86	C21-C20-C19	-10.09	102.93	114.28
42	15	316	A86	C21-C20-C19	-10.08	102.94	114.28
42	20	212	A86	C21-C20-C19	-10.06	102.96	114.28
42	11	311	A86	O1-C20-C21	-10.05	103.01	115.06
42	15	311	A86	O1-C20-C21	-10.05	103.01	115.06
42	21	314	A86	O1-C20-C21	-9.99	103.08	115.06
30	B	612	CLA	C4A-NA-C1A	9.98	111.19	106.71
42	20	213	A86	O1-C20-C21	-9.96	103.12	115.06
42	14	315	A86	C21-C20-C19	-9.91	103.13	114.28
42	19	311	A86	C36-C31-C32	-9.91	109.86	119.70
30	b	612	CLA	C4A-NA-C1A	9.90	111.16	106.71
42	17	312	A86	C21-C20-C19	-9.88	103.16	114.28
42	12	318	A86	C21-C20-C19	-9.88	103.17	114.28
42	13	314	A86	C21-C20-C19	-9.86	103.19	114.28
42	14	313	A86	C21-C20-C19	-9.86	103.19	114.28
42	11	311	A86	C21-C20-C19	-9.84	103.20	114.28
42	15	311	A86	C21-C20-C19	-9.84	103.20	114.28
42	15	313	A86	C21-C20-C19	-9.84	103.21	114.28
42	18	315	A86	C21-C20-C19	-9.84	103.22	114.28
42	17	314	A86	C21-C20-C19	-9.83	103.22	114.28
42	11	313	A86	C21-C20-C19	-9.83	103.22	114.28
42	12	316	A86	C21-C20-C19	-9.83	103.22	114.28
42	16	310	A86	C21-C20-C19	-9.82	103.23	114.28
42	13	312	A86	C21-C20-C19	-9.81	103.25	114.28
42	16	311	A86	C21-C20-C19	-9.81	103.25	114.28
42	18	314	A86	C21-C20-C19	-9.79	103.26	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	20	201	A86	C21-C20-C19	-9.77	103.29	114.28
42	17	302	A86	O1-C20-C21	-9.72	103.41	115.06
42	20	213	A86	C21-C20-C19	-9.62	103.45	114.28
42	21	314	A86	C21-C20-C19	-9.58	103.50	114.28
42	21	310	A86	C21-C20-C19	-9.50	103.60	114.28
42	17	315	A86	C36-C31-C32	-9.44	110.33	119.70
42	20	201	A86	O1-C20-C21	-9.41	103.78	115.06
42	11	314	A86	O1-C20-C21	-9.40	103.79	115.06
42	15	314	A86	O1-C20-C21	-9.40	103.80	115.06
42	14	301	A86	O1-C20-C21	-9.38	103.82	115.06
42	14	316	A86	O1-C20-C21	-9.36	103.84	115.06
42	12	319	A86	O1-C20-C21	-9.34	103.87	115.06
42	17	316	A86	O1-C20-C21	-9.34	103.87	115.06
42	16	313	A86	O1-C20-C21	-9.32	103.89	115.06
42	19	312	A86	C36-C31-C32	-9.30	110.47	119.70
42	21	311	A86	O1-C20-C21	-9.27	103.95	115.06
42	20	211	A86	O1-C20-C21	-9.24	103.99	115.06
42	21	313	A86	C21-C20-C19	-9.22	103.91	114.28
42	17	302	A86	C36-C31-C32	-9.20	110.56	119.70
42	21	311	A86	C21-C20-C19	-9.15	103.98	114.28
42	20	211	A86	C21-C20-C19	-9.15	103.99	114.28
42	19	310	A86	O1-C20-C21	-9.14	104.10	115.06
42	21	314	A86	C36-C31-C32	-9.13	110.64	119.70
42	20	213	A86	C36-C31-C32	-9.13	110.64	119.70
30	11	301	CLA	C4A-NA-C1A	9.12	110.80	106.71
30	13	302	CLA	C4A-NA-C1A	9.12	110.80	106.71
42	12	304	A86	C33-C32-C31	9.06	118.02	109.21
30	14	303	CLA	C4A-NA-C1A	9.06	110.78	106.71
42	15	315	A86	C33-C32-C31	9.05	118.00	109.21
42	19	311	A86	C21-C20-C19	-9.03	104.12	114.28
42	21	313	A86	O1-C20-C21	-9.03	104.24	115.06
30	16	302	CLA	C4A-NA-C1A	9.02	110.76	106.71
42	13	315	A86	C33-C32-C31	9.02	117.98	109.21
42	15	316	A86	C33-C32-C31	9.00	117.96	109.21
42	13	301	A86	C33-C32-C31	8.97	117.93	109.21
42	18	302	A86	C33-C32-C31	8.97	117.93	109.21
42	11	316	A86	C33-C32-C31	8.95	117.91	109.21
30	12	305	CLA	C4A-NA-C1A	8.91	110.71	106.71
30	c	510	CLA	C4A-NA-C1A	8.89	110.70	106.71
42	11	312	A86	O1-C20-C21	-8.87	104.43	115.06
42	16	312	A86	O1-C20-C21	-8.86	104.44	115.06
42	15	312	A86	O1-C20-C21	-8.84	104.47	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	317	A86	O1-C20-C21	-8.83	104.47	115.06
42	14	314	A86	O1-C20-C21	-8.83	104.47	115.06
30	C	510	CLA	C4A-NA-C1A	8.83	110.68	106.71
42	17	313	A86	O1-C20-C21	-8.83	104.47	115.06
42	13	313	A86	O1-C20-C21	-8.82	104.49	115.06
31	d	403	PHO	C4D-CHA-CBD	-8.81	104.53	108.52
31	A	403	PHO	C4D-CHA-CBD	-8.79	104.54	108.52
42	21	310	A86	O1-C20-C21	-8.73	104.60	115.06
42	17	313	A86	C33-C32-C31	8.59	117.56	109.21
42	13	313	A86	C33-C32-C31	8.58	117.55	109.21
42	14	314	A86	C33-C32-C31	8.55	117.52	109.21
30	C	520	CLA	C4A-NA-C1A	8.53	110.54	106.71
42	21	312	A86	C17-C16-C15	8.52	117.86	109.16
42	15	312	A86	C33-C32-C31	8.51	117.48	109.21
42	16	312	A86	C33-C32-C31	8.50	117.48	109.21
42	12	317	A86	C33-C32-C31	8.47	117.45	109.21
42	11	312	A86	C33-C32-C31	8.46	117.44	109.21
30	17	303	CLA	C4A-NA-C1A	8.45	110.51	106.71
42	20	201	A86	C36-C31-C32	-8.39	111.37	119.70
42	15	315	A86	C4-C5-C6	-8.38	115.35	127.31
42	13	315	A86	C4-C5-C6	-8.38	115.35	127.31
42	12	304	A86	C4-C5-C6	-8.36	115.38	127.31
42	13	301	A86	C4-C5-C6	-8.35	115.39	127.31
30	c	505	CLA	C4A-NA-C1A	8.34	110.46	106.71
42	15	316	A86	C4-C5-C6	-8.33	115.42	127.31
42	11	316	A86	C4-C5-C6	-8.33	115.42	127.31
42	14	314	A86	C17-C16-C15	8.32	117.65	109.16
42	18	302	A86	C4-C5-C6	-8.31	115.45	127.31
42	11	312	A86	C17-C16-C15	8.30	117.63	109.16
42	15	312	A86	C17-C16-C15	8.29	117.62	109.16
42	17	313	A86	C17-C16-C15	8.29	117.62	109.16
30	15	302	CLA	C4A-NA-C1A	8.27	110.42	106.71
42	17	302	A86	C4-C5-C6	-8.27	115.51	127.31
31	d	404	PHO	C4D-CHA-CBD	-8.26	104.78	108.52
30	13	307	CLA	C4A-NA-C1A	8.24	110.41	106.71
42	12	317	A86	C17-C16-C15	8.24	117.56	109.16
42	13	313	A86	C17-C16-C15	8.23	117.55	109.16
42	16	312	A86	C17-C16-C15	8.22	117.55	109.16
31	D	403	PHO	C4D-CHA-CBD	-8.21	104.80	108.52
30	D	406	CLA	C4A-NA-C1A	8.21	110.40	106.71
30	C	505	CLA	C4A-NA-C1A	8.20	110.39	106.71
30	b	609	CLA	C4A-NA-C1A	8.19	110.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	306	CLA	C4A-NA-C1A	8.19	110.39	106.71
30	A	402	CLA	C4A-NA-C1A	8.15	110.37	106.71
30	d	407	CLA	C4A-NA-C1A	8.14	110.36	106.71
30	15	301	CLA	C4A-NA-C1A	8.12	110.36	106.71
30	19	303	CLA	C4A-NA-C1A	8.12	110.36	106.71
30	12	310	CLA	C4A-NA-C1A	8.11	110.35	106.71
42	21	313	A86	C36-C31-C32	-8.07	111.69	119.70
30	B	609	CLA	C4A-NA-C1A	8.07	110.33	106.71
30	14	308	CLA	C4A-NA-C1A	8.06	110.33	106.71
30	C	502	CLA	C4A-NA-C1A	8.02	110.31	106.71
30	a	402	CLA	C4A-NA-C1A	8.01	110.31	106.71
30	16	306	CLA	C4A-NA-C1A	7.97	110.29	106.71
42	20	211	A86	C36-C31-C32	-7.97	111.78	119.70
42	21	312	A86	C21-C20-C19	-7.97	105.31	114.28
42	21	312	A86	O1-C20-C21	-7.97	105.51	115.06
42	21	311	A86	C36-C31-C32	-7.95	111.81	119.70
30	c	502	CLA	C4A-NA-C1A	7.94	110.27	106.71
42	11	310	A86	C33-C32-C31	7.92	116.91	109.21
30	15	307	CLA	C4A-NA-C1A	7.91	110.26	106.71
42	13	311	A86	C33-C32-C31	7.90	116.89	109.21
30	18	304	CLA	C4A-NA-C1A	7.88	110.25	106.71
42	15	310	A86	C33-C32-C31	7.85	116.84	109.21
30	C	514	CLA	C4A-NA-C1A	7.84	110.23	106.71
30	c	514	CLA	C4A-NA-C1A	7.82	110.22	106.71
42	12	315	A86	C33-C32-C31	7.82	116.81	109.21
42	14	312	A86	C33-C32-C31	7.80	116.80	109.21
30	20	206	CLA	C4A-NA-C1A	7.80	110.21	106.71
30	15	306	CLA	C4A-NA-C1A	7.80	110.21	106.71
42	18	313	A86	C33-C32-C31	7.79	116.78	109.21
30	16	303	CLA	C4A-NA-C1A	7.76	110.20	106.71
30	C	504	CLA	C4A-NA-C1A	7.76	110.19	106.71
30	14	305	CLA	C4A-NA-C1A	7.76	110.19	106.71
42	21	312	A86	C33-C32-C31	7.75	116.75	109.21
30	18	311	CLA	C4A-NA-C1A	7.70	110.17	106.71
30	13	304	CLA	C4A-NA-C1A	7.70	110.17	106.71
30	b	601	CLA	C4A-NA-C1A	7.66	110.15	106.71
30	18	305	CLA	C4A-NA-C1A	7.65	110.15	106.71
42	20	201	A86	C17-C16-C15	7.65	116.97	109.16
30	B	601	CLA	C4A-NA-C1A	7.65	110.15	106.71
30	11	303	CLA	C4A-NA-C1A	7.64	110.14	106.71
30	12	307	CLA	C4A-NA-C1A	7.64	110.14	106.71
30	19	308	CLA	C4A-NA-C1A	7.63	110.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	17	305	CLA	C4A-NA-C1A	7.63	110.14	106.71
30	b	608	CLA	C4A-NA-C1A	7.61	110.13	106.71
30	13	303	CLA	C4A-NA-C1A	7.61	110.13	106.71
42	17	315	A86	C4-C5-C6	-7.55	116.54	127.31
30	15	303	CLA	C4A-NA-C1A	7.54	110.10	106.71
30	b	613	CLA	C4A-NA-C1A	7.52	110.09	106.71
30	17	301	CLA	C4A-NA-C1A	7.52	110.09	106.71
30	20	204	CLA	C4A-NA-C1A	7.49	110.08	106.71
30	c	504	CLA	C4A-NA-C1A	7.49	110.07	106.71
30	14	304	CLA	C4A-NA-C1A	7.48	110.07	106.71
42	19	311	A86	O1-C20-C21	-7.45	106.14	115.06
30	18	308	CLA	C4A-NA-C1A	7.44	110.05	106.71
30	B	608	CLA	C4A-NA-C1A	7.44	110.05	106.71
30	C	512	CLA	C4A-NA-C1A	7.44	110.05	106.71
30	14	306	CLA	C4A-NA-C1A	7.43	110.05	106.71
30	B	603	CLA	C4A-NA-C1A	7.42	110.04	106.71
30	b	603	CLA	C4A-NA-C1A	7.40	110.03	106.71
42	14	301	A86	C17-C16-C15	7.39	116.70	109.16
30	20	203	CLA	C4A-NA-C1A	7.38	110.03	106.71
42	11	314	A86	C17-C16-C15	7.37	116.69	109.16
42	12	319	A86	C17-C16-C15	7.36	116.67	109.16
42	15	316	A86	O1-C20-C21	-7.35	106.25	115.06
42	15	314	A86	C17-C16-C15	7.35	116.66	109.16
42	14	316	A86	C17-C16-C15	7.35	116.66	109.16
30	B	611	CLA	C4A-NA-C1A	7.34	110.01	106.71
42	13	301	A86	O1-C20-C21	-7.34	106.26	115.06
42	16	313	A86	C17-C16-C15	7.34	116.65	109.16
30	b	611	CLA	C4A-NA-C1A	7.34	110.01	106.71
30	12	306	CLA	C4A-NA-C1A	7.34	110.00	106.71
42	12	304	A86	O1-C20-C21	-7.33	106.27	115.06
42	18	302	A86	O1-C20-C21	-7.33	106.27	115.06
30	11	302	CLA	C4A-NA-C1A	7.33	110.00	106.71
42	11	316	A86	O1-C20-C21	-7.33	106.28	115.06
42	13	315	A86	O1-C20-C21	-7.31	106.30	115.06
30	18	309	CLA	C4A-NA-C1A	7.30	109.99	106.71
30	c	509	CLA	C4A-NA-C1A	7.30	109.99	106.71
30	z	101	CLA	C4A-NA-C1A	7.30	109.99	106.71
42	17	316	A86	C17-C16-C15	7.30	116.61	109.16
42	16	311	A86	C33-C32-C31	7.29	116.30	109.21
30	12	308	CLA	C4A-NA-C1A	7.29	109.98	106.71
42	15	315	A86	O1-C20-C21	-7.28	106.33	115.06
30	12	309	CLA	C4A-NA-C1A	7.27	109.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	508	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	C	509	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	11	305	CLA	C4A-NA-C1A	7.27	109.97	106.71
42	14	313	A86	C33-C32-C31	7.27	116.27	109.21
30	B	607	CLA	C4A-NA-C1A	7.26	109.97	106.71
42	17	312	A86	C33-C32-C31	7.24	116.25	109.21
30	b	614	CLA	C4A-NA-C1A	7.24	109.96	106.71
30	16	304	CLA	C4A-NA-C1A	7.24	109.96	106.71
42	13	312	A86	C33-C32-C31	7.24	116.25	109.21
42	19	312	A86	C4-C5-C6	-7.24	116.98	127.31
42	18	314	A86	C33-C32-C31	7.23	116.24	109.21
42	11	313	A86	C33-C32-C31	7.22	116.23	109.21
42	13	314	A86	C33-C32-C31	7.22	116.23	109.21
42	20	210	A86	C36-C31-C32	-7.22	112.53	119.70
30	c	512	CLA	C4A-NA-C1A	7.22	109.95	106.71
30	20	207	CLA	C4A-NA-C1A	7.22	109.95	106.71
30	c	513	CLA	C4A-NA-C1A	7.21	109.95	106.71
42	11	311	A86	C33-C32-C31	7.20	116.21	109.21
30	12	312	CLA	C4A-NA-C1A	7.20	109.94	106.71
42	18	315	A86	C33-C32-C31	7.20	116.21	109.21
42	15	311	A86	C33-C32-C31	7.20	116.21	109.21
30	B	613	CLA	C4A-NA-C1A	7.20	109.94	106.71
30	D	405	CLA	C4A-NA-C1A	7.20	109.94	106.71
42	12	316	A86	C33-C32-C31	7.19	116.20	109.21
42	17	314	A86	C33-C32-C31	7.19	116.19	109.21
30	C	513	CLA	C4A-NA-C1A	7.18	109.94	106.71
42	15	313	A86	C33-C32-C31	7.18	116.19	109.21
30	Z	102	CLA	C4A-NA-C1A	7.18	109.93	106.71
42	12	318	A86	C33-C32-C31	7.17	116.18	109.21
30	d	406	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	13	306	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	11	315	CLA	C4A-NA-C1A	7.16	109.93	106.71
42	14	315	A86	C33-C32-C31	7.16	116.17	109.21
30	16	305	CLA	C4A-NA-C1A	7.16	109.92	106.71
30	13	305	CLA	C4A-NA-C1A	7.15	109.92	106.71
30	21	307	CLA	C4A-NA-C1A	7.14	109.92	106.71
30	B	606	CLA	C4A-NA-C1A	7.14	109.91	106.71
30	17	307	CLA	C4A-NA-C1A	7.14	109.91	106.71
30	A	404	CLA	C4A-NA-C1A	7.13	109.91	106.71
30	15	305	CLA	C4A-NA-C1A	7.13	109.91	106.71
30	21	302	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	C	503	CLA	C4A-NA-C1A	7.12	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	402	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	a	403	CLA	C4A-NA-C1A	7.11	109.90	106.71
30	18	303	CLA	C4A-NA-C1A	7.11	109.90	106.71
30	11	304	CLA	C4A-NA-C1A	7.10	109.90	106.71
30	d	402	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	B	623	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	b	607	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	C	519	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	21	308	CLA	C4A-NA-C1A	7.07	109.88	106.71
42	16	311	A86	C17-C16-C15	7.07	116.37	109.16
42	12	316	A86	C17-C16-C15	7.07	116.37	109.16
30	12	303	CLA	C4A-NA-C1A	7.07	109.88	106.71
30	17	309	CLA	C4A-NA-C1A	7.07	109.88	106.71
42	15	311	A86	C17-C16-C15	7.07	116.37	109.16
42	17	312	A86	C17-C16-C15	7.06	116.36	109.16
30	17	304	CLA	C4A-NA-C1A	7.06	109.88	106.71
42	11	311	A86	C17-C16-C15	7.05	116.36	109.16
42	13	312	A86	C17-C16-C15	7.05	116.35	109.16
30	14	307	CLA	C4A-NA-C1A	7.04	109.87	106.71
42	14	313	A86	C17-C16-C15	7.04	116.35	109.16
30	19	305	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	14	302	CLA	C4A-NA-C1A	7.01	109.86	106.71
30	B	614	CLA	C4A-NA-C1A	7.00	109.85	106.71
30	15	308	CLA	C4A-NA-C1A	7.00	109.85	106.71
30	21	306	CLA	C4A-NA-C1A	7.00	109.85	106.71
42	18	314	A86	C17-C16-C15	6.97	116.28	109.16
30	21	301	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	b	606	CLA	C4A-NA-C1A	6.93	109.82	106.71
30	c	508	CLA	C4A-NA-C1A	6.91	109.81	106.71
30	B	610	CLA	C4A-NA-C1A	6.90	109.81	106.71
30	18	310	CLA	C4A-NA-C1A	6.90	109.81	106.71
30	c	503	CLA	C4A-NA-C1A	6.89	109.81	106.71
30	18	306	CLA	C4A-NA-C1A	6.88	109.80	106.71
30	b	610	CLA	C4A-NA-C1A	6.88	109.80	106.71
42	21	310	A86	C3-C2-C1	-6.87	117.50	127.31
42	21	312	A86	C25-C26-C27	-6.86	117.52	127.31
42	17	311	A86	C33-C32-C31	6.86	115.88	109.21
30	19	302	CLA	C4A-NA-C1A	6.85	109.78	106.71
30	16	301	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	19	304	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	B	605	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	b	605	CLA	C4A-NA-C1A	6.80	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	21	303	CLA	C4A-NA-C1A	6.80	109.76	106.71
42	19	310	A86	C36-C31-C32	-6.79	112.95	119.70
30	D	401	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	d	401	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	15	304	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	20	208	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	B	602	CLA	C4A-NA-C1A	6.76	109.75	106.71
30	c	506	CLA	C4A-NA-C1A	6.76	109.75	106.71
42	19	311	A86	C17-C16-C15	6.75	116.05	109.16
30	19	307	CLA	C4A-NA-C1A	6.73	109.73	106.71
30	18	307	CLA	C4A-NA-C1A	6.73	109.73	106.71
30	20	202	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	B	604	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	b	604	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	C	506	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	16	308	CLA	C4A-NA-C1A	6.69	109.71	106.71
42	21	313	A86	C25-C26-C27	-6.67	117.79	127.31
30	21	309	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	b	622	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	b	602	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	18	301	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	21	305	CLA	C4A-NA-C1A	6.56	109.65	106.71
30	12	313	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	13	309	CLA	C4A-NA-C1A	6.55	109.65	106.71
42	21	311	A86	C3-C2-C1	-6.53	117.99	127.31
42	19	310	A86	C3-C2-C1	-6.52	118.00	127.31
30	11	307	CLA	C4A-NA-C1A	6.51	109.63	106.71
30	14	310	CLA	C4A-NA-C1A	6.51	109.63	106.71
30	17	306	CLA	C4A-NA-C1A	6.51	109.63	106.71
30	11	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
42	20	211	A86	C3-C2-C1	-6.49	118.04	127.31
30	13	308	CLA	C4A-NA-C1A	6.47	109.61	106.71
30	w	103	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	20	205	CLA	C4A-NA-C1A	6.43	109.60	106.71
42	17	302	A86	C33-C32-C31	6.42	115.45	109.21
42	14	314	A86	C4-C5-C6	-6.41	118.16	127.31
42	13	313	A86	C4-C5-C6	-6.41	118.17	127.31
42	12	317	A86	C4-C5-C6	-6.39	118.19	127.31
30	12	311	CLA	C4A-NA-C1A	6.38	109.58	106.71
42	17	313	A86	C4-C5-C6	-6.37	118.22	127.31
42	20	212	A86	C3-C2-C1	-6.37	118.22	127.31
42	16	312	A86	C4-C5-C6	-6.37	118.22	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	312	A86	C4-C5-C6	-6.34	118.26	127.31
30	14	309	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	20	209	CLA	C4A-NA-C1A	6.34	109.56	106.71
42	11	312	A86	C4-C5-C6	-6.32	118.29	127.31
30	W	103	CLA	C4A-NA-C1A	6.32	109.55	106.71
30	19	306	CLA	C4A-NA-C1A	6.31	109.54	106.71
30	19	309	CLA	C4A-NA-C1A	6.26	109.52	106.71
30	14	311	CLA	C4A-NA-C1A	6.22	109.50	106.71
30	21	304	CLA	C4A-NA-C1A	6.21	109.50	106.71
30	12	314	CLA	C4A-NA-C1A	6.21	109.50	106.71
42	16	310	A86	C33-C32-C31	6.19	115.22	109.21
42	20	210	A86	C4-C5-C6	-6.18	118.48	127.31
30	16	307	CLA	C4A-NA-C1A	6.16	109.47	106.71
30	11	309	CLA	C4A-NA-C1A	6.12	109.46	106.71
30	17	310	CLA	C4A-NA-C1A	6.11	109.45	106.71
30	13	310	CLA	C4A-NA-C1A	6.09	109.44	106.71
42	16	311	A86	C3-C2-C1	-6.09	118.62	127.31
42	18	314	A86	C3-C2-C1	-6.09	118.62	127.31
42	12	316	A86	C3-C2-C1	-6.08	118.63	127.31
42	21	311	A86	C25-C26-C27	-6.08	118.63	127.31
42	19	311	A86	C4-C5-C6	-6.07	118.65	127.31
42	15	311	A86	C3-C2-C1	-6.07	118.65	127.31
42	16	310	A86	C36-C31-C32	-6.07	113.68	119.70
30	W	102	CLA	C4A-NA-C1A	6.05	109.43	106.71
42	11	311	A86	C3-C2-C1	-6.05	118.67	127.31
42	14	313	A86	C3-C2-C1	-6.04	118.70	127.31
30	18	312	CLA	C4A-NA-C1A	6.02	109.41	106.71
42	17	312	A86	C3-C2-C1	-6.02	118.72	127.31
42	20	211	A86	C25-C26-C27	-6.02	118.72	127.31
42	13	312	A86	C3-C2-C1	-6.01	118.73	127.31
30	15	309	CLA	C4A-NA-C1A	6.00	109.40	106.71
30	w	102	CLA	C4A-NA-C1A	5.96	109.39	106.71
30	19	301	CLA	C4A-NA-C1A	5.95	109.38	106.71
42	19	312	A86	C25-C26-C27	-5.91	118.87	127.31
42	21	312	A86	C4-C5-C6	-5.85	118.97	127.31
42	18	315	A86	C17-C16-C15	5.83	115.11	109.16
42	13	314	A86	C17-C16-C15	5.81	115.09	109.16
42	12	318	A86	C17-C16-C15	5.81	115.09	109.16
42	11	313	A86	C17-C16-C15	5.80	115.08	109.16
42	15	313	A86	C17-C16-C15	5.79	115.07	109.16
42	14	315	A86	C17-C16-C15	5.78	115.06	109.16
42	21	312	A86	C36-C31-C32	-5.77	113.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	14	301	A86	C3-C2-C1	-5.74	119.11	127.31
42	17	314	A86	C17-C16-C15	5.74	115.02	109.16
42	17	316	A86	C3-C2-C1	-5.74	119.12	127.31
42	21	310	A86	C17-C16-C15	5.74	115.02	109.16
42	15	314	A86	C3-C2-C1	-5.73	119.13	127.31
30	m	101	CLA	C4A-NA-C1A	5.72	109.28	106.71
42	21	310	A86	C33-C32-C31	5.71	114.76	109.21
30	M	101	CLA	C4A-NA-C1A	5.71	109.27	106.71
42	11	314	A86	C3-C2-C1	-5.70	119.18	127.31
42	14	316	A86	C3-C2-C1	-5.69	119.19	127.31
42	20	211	A86	C17-C16-C15	5.68	114.96	109.16
42	16	313	A86	C3-C2-C1	-5.68	119.21	127.31
42	12	319	A86	C3-C2-C1	-5.68	119.21	127.31
42	21	311	A86	C17-C16-C15	5.64	114.91	109.16
42	17	311	A86	C4-C5-C6	-5.62	119.29	127.31
42	19	311	A86	C3-C2-C1	-5.60	119.32	127.31
42	21	313	A86	C17-C16-C15	5.55	114.83	109.16
42	20	212	A86	C33-C32-C31	5.48	114.54	109.21
42	17	312	A86	C4-C5-C6	-5.46	119.51	127.31
42	21	313	A86	C3-C2-C1	-5.46	119.52	127.31
42	21	312	A86	C3-C2-C1	-5.45	119.53	127.31
42	13	312	A86	C4-C5-C6	-5.44	119.55	127.31
42	18	314	A86	C4-C5-C6	-5.44	119.55	127.31
42	15	311	A86	C4-C5-C6	-5.43	119.55	127.31
42	16	311	A86	C4-C5-C6	-5.43	119.56	127.31
42	12	316	A86	C4-C5-C6	-5.43	119.57	127.31
42	14	313	A86	C4-C5-C6	-5.41	119.58	127.31
42	11	311	A86	C4-C5-C6	-5.41	119.59	127.31
42	15	316	A86	C25-C26-C27	-5.40	119.61	127.31
42	13	315	A86	C25-C26-C27	-5.38	119.63	127.31
42	12	304	A86	C25-C26-C27	-5.38	119.63	127.31
30	17	309	CLA	C2A-C1A-CHA	5.38	133.27	123.86
42	18	302	A86	C25-C26-C27	-5.38	119.64	127.31
42	15	315	A86	C25-C26-C27	-5.37	119.65	127.31
42	11	316	A86	C25-C26-C27	-5.37	119.65	127.31
42	17	316	A86	C33-C32-C31	5.36	114.42	109.21
42	13	301	A86	C25-C26-C27	-5.36	119.66	127.31
42	14	301	A86	C33-C32-C31	5.32	114.38	109.21
42	16	313	A86	C33-C32-C31	5.32	114.38	109.21
42	14	316	A86	C33-C32-C31	5.31	114.38	109.21
42	21	312	A86	C20-C19-C18	-5.31	102.24	112.75
42	12	319	A86	C33-C32-C31	5.31	114.37	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	11	314	A86	C33-C32-C31	5.30	114.36	109.21
42	15	314	A86	C33-C32-C31	5.30	114.36	109.21
42	20	210	A86	O4-C38-C39	5.29	120.81	111.09
33	l	101	SQD	O7-S-C6	5.26	113.19	106.94
42	17	314	A86	C3-C2-C1	-5.24	119.83	127.31
42	13	314	A86	C3-C2-C1	-5.24	119.83	127.31
30	16	309	CLA	C4A-NA-C1A	5.24	109.06	106.71
42	15	310	A86	C3-C2-C1	-5.24	119.83	127.31
42	13	311	A86	C3-C2-C1	-5.23	119.85	127.31
42	11	310	A86	C3-C2-C1	-5.21	119.87	127.31
42	12	315	A86	C3-C2-C1	-5.21	119.87	127.31
30	c	507	CLA	CAA-C2A-C3A	-5.21	98.52	112.78
30	C	507	CLA	CAA-C2A-C3A	-5.20	98.53	112.78
42	18	315	A86	C3-C2-C1	-5.19	119.91	127.31
42	14	315	A86	C3-C2-C1	-5.19	119.91	127.31
42	18	313	A86	C3-C2-C1	-5.18	119.92	127.31
42	12	318	A86	C3-C2-C1	-5.18	119.92	127.31
42	14	312	A86	C3-C2-C1	-5.17	119.94	127.31
42	15	313	A86	C3-C2-C1	-5.17	119.94	127.31
33	L	103	SQD	O7-S-C6	5.15	113.06	106.94
42	11	313	A86	C3-C2-C1	-5.14	119.97	127.31
42	14	313	A86	O4-C38-C39	5.10	120.48	111.09
42	20	213	A86	O4-C38-C39	5.10	120.48	111.09
42	18	314	A86	O4-C38-C39	5.10	120.48	111.09
42	21	314	A86	O4-C38-C39	5.10	120.47	111.09
42	16	310	A86	C25-C26-C27	-5.09	120.05	127.31
30	b	615	CLA	C4A-NA-C1A	5.09	108.99	106.71
42	12	316	A86	O4-C38-C39	5.09	120.45	111.09
30	c	511	CLA	C4A-NA-C1A	5.06	108.98	106.71
42	13	312	A86	O4-C38-C39	5.06	120.40	111.09
42	15	311	A86	O4-C38-C39	5.06	120.40	111.09
42	17	312	A86	O4-C38-C39	5.06	120.39	111.09
42	16	310	A86	C3-C2-C1	-5.05	120.10	127.31
42	11	311	A86	O4-C38-C39	5.05	120.38	111.09
42	16	311	A86	O4-C38-C39	5.04	120.37	111.09
42	20	201	A86	C12-C11-C13	5.04	124.49	116.02
30	B	615	CLA	C4A-NA-C1A	5.04	108.97	106.71
42	20	210	A86	C25-C26-C27	-5.04	120.12	127.31
42	19	310	A86	O4-C38-C39	5.03	120.35	111.09
42	20	201	A86	C3-C2-C1	-5.01	120.16	127.31
42	13	301	A86	O4-C38-C39	5.00	120.29	111.09
33	L	103	SQD	O6-C1-C2	5.00	116.11	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	316	A86	O4-C38-C39	4.99	120.28	111.09
30	17	308	CLA	C4A-NA-C1A	4.99	108.95	106.71
42	11	316	A86	O4-C38-C39	4.99	120.26	111.09
42	20	201	A86	O4-C38-C39	4.98	120.26	111.09
42	13	315	A86	O4-C38-C39	4.98	120.26	111.09
42	18	302	A86	O4-C38-C39	4.98	120.25	111.09
30	17	309	CLA	CAA-C2A-C1A	4.98	128.29	111.97
42	15	310	A86	C17-C16-C15	4.96	114.22	109.16
42	15	315	A86	O4-C38-C39	4.96	120.21	111.09
42	12	304	A86	O4-C38-C39	4.96	120.21	111.09
33	l	101	SQD	O6-C1-C2	4.96	116.04	108.30
42	13	311	A86	C17-C16-C15	4.96	114.22	109.16
30	C	507	CLA	C4A-NA-C1A	4.94	108.93	106.71
42	12	315	A86	C17-C16-C15	4.93	114.19	109.16
42	17	315	A86	O4-C38-C39	4.92	120.14	111.09
42	14	312	A86	C17-C16-C15	4.91	114.17	109.16
42	20	212	A86	O4-C38-C39	4.91	120.12	111.09
42	21	314	A86	C3-C2-C1	-4.90	120.31	127.31
30	c	507	CLA	C4A-NA-C1A	4.90	108.91	106.71
42	11	310	A86	C17-C16-C15	4.88	114.14	109.16
42	20	213	A86	C3-C2-C1	-4.88	120.34	127.31
30	C	511	CLA	C4A-NA-C1A	4.86	108.89	106.71
42	18	313	A86	C17-C16-C15	4.86	114.12	109.16
42	19	310	A86	C17-C16-C15	4.85	114.11	109.16
42	12	317	A86	O4-C38-C39	4.84	120.00	111.09
42	11	312	A86	O4-C38-C39	4.84	119.99	111.09
42	17	302	A86	O4-C38-C39	4.84	119.99	111.09
42	16	312	A86	O4-C38-C39	4.82	119.96	111.09
42	15	312	A86	O4-C38-C39	4.82	119.96	111.09
42	14	314	A86	O4-C38-C39	4.82	119.95	111.09
42	16	310	A86	O4-C38-C39	4.81	119.94	111.09
42	17	314	A86	O4-C38-C39	4.81	119.94	111.09
42	21	313	A86	O4-C38-C39	4.80	119.92	111.09
42	14	315	A86	O4-C38-C39	4.80	119.92	111.09
42	13	314	A86	O4-C38-C39	4.79	119.91	111.09
42	17	311	A86	O4-C38-C39	4.79	119.90	111.09
42	12	318	A86	O4-C38-C39	4.79	119.90	111.09
42	18	315	A86	O4-C38-C39	4.78	119.89	111.09
42	11	313	A86	O4-C38-C39	4.78	119.89	111.09
42	13	313	A86	O4-C38-C39	4.78	119.89	111.09
42	17	313	A86	O4-C38-C39	4.78	119.88	111.09
39	C	516	DGD	O3G-C3G-C2G	-4.77	99.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	313	A86	O4-C38-C39	4.76	119.86	111.09
42	11	314	A86	O4-C38-C39	4.76	119.84	111.09
42	17	316	A86	O4-C38-C39	4.75	119.83	111.09
42	12	319	A86	O4-C38-C39	4.75	119.82	111.09
42	14	301	A86	O4-C38-C39	4.75	119.82	111.09
42	14	316	A86	O4-C38-C39	4.74	119.82	111.09
39	c	517	DGD	O3G-C3G-C2G	-4.74	99.46	110.90
42	19	311	A86	O4-C38-C39	4.74	119.81	111.09
42	16	313	A86	O4-C38-C39	4.74	119.80	111.09
42	19	312	A86	O4-C38-C39	4.72	119.77	111.09
42	15	314	A86	O4-C38-C39	4.71	119.76	111.09
34	a	406	BCT	O2-C-O1	4.71	131.76	119.55
30	16	302	CLA	CBA-CAA-C2A	4.68	127.69	113.86
34	A	407	BCT	O2-C-O1	4.68	131.70	119.55
42	16	312	A86	C41-C32-C31	-4.68	106.28	110.47
42	16	310	A86	C17-C16-C15	4.67	113.93	109.16
42	13	312	A86	C25-C26-C27	-4.66	120.66	127.31
42	17	311	A86	C3-C2-C1	-4.65	120.67	127.31
42	11	311	A86	C25-C26-C27	-4.65	120.67	127.31
42	12	316	A86	C25-C26-C27	-4.63	120.70	127.31
42	15	312	A86	C41-C32-C31	-4.63	106.33	110.47
42	14	313	A86	C25-C26-C27	-4.63	120.70	127.31
42	17	312	A86	C25-C26-C27	-4.63	120.71	127.31
42	21	312	A86	O4-C38-C39	4.62	119.60	111.09
42	11	312	A86	C41-C32-C31	-4.61	106.34	110.47
42	20	213	A86	C17-C16-C15	4.61	113.86	109.16
42	15	311	A86	C25-C26-C27	-4.61	120.73	127.31
42	16	311	A86	C25-C26-C27	-4.59	120.75	127.31
42	18	314	A86	C25-C26-C27	-4.59	120.77	127.31
42	21	314	A86	C17-C16-C15	4.58	113.83	109.16
30	b	603	CLA	O2D-CGD-O1D	-4.58	114.89	123.84
42	21	310	A86	O4-C38-C39	4.57	119.50	111.09
42	12	317	A86	C41-C32-C31	-4.56	106.39	110.47
40	d	405	PL9	C7-C3-C4	4.56	120.58	116.88
31	d	404	PHO	C2B-C1B-NB	-4.55	106.38	109.53
42	13	313	A86	C41-C32-C31	-4.55	106.40	110.47
42	14	314	A86	C41-C32-C31	-4.55	106.40	110.47
42	14	315	A86	C25-C26-C27	-4.55	120.82	127.31
42	17	313	A86	C41-C32-C31	-4.54	106.41	110.47
42	12	318	A86	C25-C26-C27	-4.54	120.84	127.31
42	18	315	A86	C25-C26-C27	-4.54	120.84	127.31
42	15	310	A86	O4-C38-C39	4.53	119.42	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	603	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
42	17	314	A86	C25-C26-C27	-4.52	120.86	127.31
31	D	403	PHO	C2B-C1B-NB	-4.52	106.41	109.53
42	11	310	A86	O4-C38-C39	4.51	119.39	111.09
42	12	315	A86	O4-C38-C39	4.50	119.37	111.09
42	11	313	A86	C25-C26-C27	-4.50	120.89	127.31
31	A	403	PHO	C2B-C1B-NB	-4.49	106.43	109.53
42	13	314	A86	C25-C26-C27	-4.48	120.92	127.31
42	20	211	A86	O4-C38-C39	4.47	119.32	111.09
42	14	312	A86	O4-C38-C39	4.47	119.32	111.09
42	15	313	A86	C25-C26-C27	-4.47	120.93	127.31
42	13	311	A86	O4-C38-C39	4.47	119.31	111.09
42	18	313	A86	O4-C38-C39	4.45	119.28	111.09
31	d	403	PHO	C2B-C1B-NB	-4.45	106.45	109.53
42	21	311	A86	O4-C38-C39	4.45	119.28	111.09
42	20	212	A86	C4-C5-C6	-4.43	120.98	127.31
40	D	404	PL9	C7-C3-C4	4.43	120.48	116.88
42	17	315	A86	C33-C32-C31	4.42	113.50	109.21
30	16	307	CLA	CMB-C2B-C1B	-4.38	118.70	125.37
42	15	310	A86	C4-C5-C6	-4.33	121.13	127.31
35	B	622	LHG	O4-P-O5	4.33	133.64	112.24
42	13	301	A86	C20-C19-C18	-4.32	104.21	112.75
35	b	621	LHG	O4-P-O5	4.31	133.57	112.24
42	12	304	A86	C20-C19-C18	-4.31	104.23	112.75
42	11	310	A86	C4-C5-C6	-4.31	121.17	127.31
42	13	311	A86	C4-C5-C6	-4.30	121.17	127.31
30	A	404	CLA	C3B-C4B-NB	-4.30	106.53	110.52
42	13	315	A86	C20-C19-C18	-4.29	104.25	112.75
35	a	407	LHG	O4-P-O5	4.29	133.44	112.24
42	15	316	A86	C20-C19-C18	-4.29	104.27	112.75
42	15	315	A86	C20-C19-C18	-4.29	104.27	112.75
42	18	302	A86	C20-C19-C18	-4.29	104.27	112.75
35	A	408	LHG	O4-P-O5	4.28	133.39	112.24
42	12	315	A86	C4-C5-C6	-4.27	121.21	127.31
42	18	313	A86	C4-C5-C6	-4.27	121.21	127.31
42	11	316	A86	C20-C19-C18	-4.27	104.30	112.75
42	14	312	A86	C4-C5-C6	-4.27	121.22	127.31
42	17	315	A86	C25-C24-C1	-4.25	114.48	126.42
42	19	312	A86	C33-C32-C31	4.25	113.34	109.21
42	17	302	A86	C3-C2-C1	-4.24	121.26	127.31
42	17	315	A86	C3-C2-C1	-4.24	121.26	127.31
30	a	403	CLA	C3B-C4B-NB	-4.23	106.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	17	306	CLA	CMB-C2B-C1B	-4.20	118.98	125.37
35	d	409	LHG	O4-P-O5	4.18	132.91	112.24
35	L	101	LHG	O4-P-O5	4.17	132.86	112.24
30	16	307	CLA	C3B-C4B-NB	-4.16	106.66	110.52
42	17	314	A86	C41-C32-C31	-4.13	106.78	110.47
42	19	310	A86	C4-C5-C6	-4.12	121.42	127.31
42	13	314	A86	C41-C32-C31	-4.12	106.78	110.47
42	18	313	A86	C25-C26-C27	-4.12	121.43	127.31
42	20	210	A86	C3-C2-C1	-4.10	121.45	127.31
35	l	102	LHG	O4-P-O5	4.09	132.44	112.24
42	13	311	A86	C25-C26-C27	-4.08	121.49	127.31
42	11	313	A86	C41-C32-C31	-4.08	106.83	110.47
42	14	312	A86	C25-C26-C27	-4.07	121.50	127.31
30	C	520	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
33	l	101	SQD	O9-S-C6	4.07	111.77	106.94
35	L	102	LHG	O4-P-O5	4.06	132.33	112.24
42	15	310	A86	C25-C26-C27	-4.05	121.52	127.31
42	11	310	A86	C25-C26-C27	-4.05	121.53	127.31
42	12	318	A86	C41-C32-C31	-4.05	106.85	110.47
42	15	313	A86	C41-C32-C31	-4.04	106.86	110.47
42	18	315	A86	C41-C32-C31	-4.03	106.86	110.47
42	12	315	A86	C25-C26-C27	-4.03	121.56	127.31
33	L	103	SQD	O9-S-C6	4.03	111.73	106.94
30	15	301	CLA	C3B-C4B-NB	-4.02	106.78	110.52
42	15	314	A86	C25-C24-C1	-4.02	115.12	126.42
32	c	521	BCR	C24-C23-C22	-4.02	120.17	126.23
32	C	518	BCR	C24-C23-C22	-4.02	120.17	126.23
42	14	315	A86	C41-C32-C31	-4.01	106.89	110.47
42	14	316	A86	C25-C24-C1	-4.01	115.16	126.42
42	12	319	A86	C25-C24-C1	-4.01	115.17	126.42
42	14	301	A86	C25-C24-C1	-4.00	115.17	126.42
42	17	316	A86	C25-C24-C1	-4.00	115.17	126.42
33	B	621	SQD	O7-S-C6	4.00	111.69	106.94
42	11	314	A86	C25-C24-C1	-3.99	115.19	126.42
33	b	620	SQD	O7-S-C6	3.99	111.68	106.94
42	16	313	A86	C25-C24-C1	-3.98	115.24	126.42
37	B	625	LMU	O1'-C1'-C2'	3.98	114.51	108.30
30	b	622	CLA	CBA-CAA-C2A	3.97	125.58	113.86
30	11	308	CLA	C2A-C1A-CHA	3.96	130.79	123.86
32	B	618	BCR	C2-C1-C6	3.95	116.57	110.48
30	13	309	CLA	C2A-C1A-CHA	3.94	130.75	123.86
37	B	625	LMU	C1B-O1B-C4'	-3.94	108.21	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	313	CLA	C2A-C1A-CHA	3.94	130.74	123.86
42	13	311	A86	C41-C32-C31	-3.93	106.95	110.47
42	21	313	A86	C3-C4-C5	-3.93	115.42	123.47
32	b	617	BCR	C2-C1-C6	3.93	116.53	110.48
30	14	310	CLA	C2A-C1A-CHA	3.93	130.72	123.86
30	B	623	CLA	CBA-CAA-C2A	3.91	125.40	113.86
30	17	303	CLA	CHB-C4A-NA	3.90	129.91	124.51
32	B	616	BCR	C15-C16-C17	-3.90	115.48	123.47
30	16	303	CLA	C2A-C1A-CHA	3.89	130.66	123.86
42	21	312	A86	O1-C15-C14	-3.88	105.42	113.21
32	m	103	BCR	C15-C16-C17	-3.88	115.53	123.47
42	17	315	A86	C25-C26-C27	-3.87	121.78	127.31
42	11	310	A86	C41-C32-C31	-3.86	107.01	110.47
37	12	302	LMU	O1'-C1'-C2'	3.86	114.32	108.30
33	A	406	SQD	O47-C7-C8	3.85	119.80	111.50
42	12	315	A86	C41-C32-C31	-3.85	107.03	110.47
33	a	405	SQD	O47-C7-C8	3.84	119.79	111.50
33	l	101	SQD	C4-C3-C2	3.84	117.53	110.82
42	15	310	A86	C41-C32-C31	-3.84	107.03	110.47
31	D	403	PHO	CMB-C2B-C3B	3.84	131.87	124.68
39	C	517	DGD	O6D-C1D-O3G	-3.84	100.87	109.97
39	c	518	DGD	O6D-C1D-O3G	-3.84	100.88	109.97
39	h	102	DGD	C1D-C2D-C3D	-3.84	102.01	110.00
42	14	312	A86	C41-C32-C31	-3.83	107.04	110.47
42	21	312	A86	C12-C11-C13	3.82	122.44	116.02
31	d	404	PHO	CMB-C2B-C3B	3.82	131.82	124.68
42	20	210	A86	C9-C8-C6	-3.80	115.74	126.42
33	L	103	SQD	C4-C3-C2	3.80	117.45	110.82
42	18	313	A86	C41-C32-C31	-3.79	107.08	110.47
30	15	308	CLA	C2A-C1A-CHA	3.79	130.48	123.86
37	12	302	LMU	C1B-O1B-C4'	-3.79	108.60	117.96
30	C	520	CLA	CHB-C4A-NA	3.78	129.74	124.51
39	H	102	DGD	C1D-C2D-C3D	-3.78	102.12	110.00
42	13	311	A86	C12-C11-C13	3.78	122.38	116.02
42	20	210	A86	C33-C32-C31	3.77	112.88	109.21
42	12	315	A86	C12-C11-C13	3.77	122.35	116.02
42	20	213	A86	C33-C32-C31	3.77	112.87	109.21
33	b	620	SQD	O9-S-O7	-3.76	100.93	113.95
30	16	302	CLA	CHB-C4A-NA	3.76	129.71	124.51
33	B	621	SQD	O9-S-O7	-3.76	100.95	113.95
42	20	201	A86	C25-C26-C27	-3.75	121.95	127.31
42	15	310	A86	C12-C11-C13	3.75	122.33	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	21	314	A86	C33-C32-C31	3.75	112.86	109.21
30	c	509	CLA	CMB-C2B-C1B	-3.75	119.67	125.37
42	17	313	A86	C25-C26-C27	-3.74	121.97	127.31
42	11	314	A86	C4-C5-C6	-3.74	121.98	127.31
30	13	305	CLA	CMB-C2B-C1B	-3.74	119.68	125.37
42	11	310	A86	C12-C11-C13	3.74	122.30	116.02
30	c	511	CLA	CMB-C2B-C1B	-3.73	119.68	125.37
42	16	311	A86	C41-C32-C31	-3.73	107.13	110.47
42	14	312	A86	C12-C11-C13	3.73	122.29	116.02
42	18	313	A86	C12-C11-C13	3.73	122.29	116.02
30	C	511	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
42	15	314	A86	C4-C5-C6	-3.73	121.99	127.31
30	C	509	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
42	12	317	A86	C25-C26-C27	-3.73	121.99	127.31
33	B	621	SQD	O47-C7-C8	3.72	119.53	111.50
33	b	620	SQD	O47-C7-C8	3.72	119.53	111.50
30	16	309	CLA	CAA-C2A-C3A	-3.72	102.59	112.78
42	16	313	A86	C4-C5-C6	-3.71	122.01	127.31
42	12	316	A86	C41-C32-C31	-3.71	107.15	110.47
42	15	312	A86	C25-C26-C27	-3.71	122.02	127.31
42	14	301	A86	C4-C5-C6	-3.71	122.02	127.31
42	20	213	A86	C25-C24-C1	-3.70	116.01	126.42
42	14	313	A86	C41-C32-C31	-3.70	107.16	110.47
42	14	316	A86	C4-C5-C6	-3.70	122.03	127.31
30	16	302	CLA	CAA-C2A-C1A	3.70	124.10	111.97
42	13	313	A86	C25-C26-C27	-3.70	122.03	127.31
30	11	304	CLA	CMB-C2B-C1B	-3.70	119.74	125.37
42	17	316	A86	C4-C5-C6	-3.70	122.04	127.31
42	11	312	A86	C25-C26-C27	-3.69	122.04	127.31
42	21	314	A86	C25-C24-C1	-3.69	116.04	126.42
30	13	305	CLA	CHB-C1B-NB	3.69	128.17	124.26
30	18	306	CLA	CMB-C2B-C1B	-3.69	119.75	125.37
30	b	622	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
30	14	306	CLA	CHB-C1B-NB	3.69	128.16	124.26
33	L	103	SQD	O47-C7-C8	3.69	119.45	111.50
42	14	314	A86	C25-C26-C27	-3.69	122.05	127.31
42	15	311	A86	C41-C32-C31	-3.69	107.17	110.47
33	l	101	SQD	O47-C7-C8	3.68	119.44	111.50
33	L	103	SQD	O5-C5-C4	3.68	116.38	109.69
30	a	403	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
30	A	404	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
33	a	405	SQD	O9-S-C6	3.67	111.31	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	319	A86	C4-C5-C6	-3.67	122.07	127.31
30	12	308	CLA	CMB-C2B-C1B	-3.67	119.77	125.37
42	17	312	A86	C41-C32-C31	-3.67	107.19	110.47
30	14	306	CLA	CMB-C2B-C1B	-3.67	119.78	125.37
33	A	406	SQD	O9-S-C6	3.67	111.30	106.94
42	11	311	A86	C41-C32-C31	-3.66	107.19	110.47
30	11	304	CLA	CHB-C1B-NB	3.66	128.13	124.26
42	13	312	A86	C41-C32-C31	-3.65	107.20	110.47
42	18	314	A86	C41-C32-C31	-3.65	107.20	110.47
42	16	312	A86	C25-C26-C27	-3.65	122.10	127.31
39	J	101	DGD	O3G-C3G-C2G	-3.65	102.10	110.90
30	12	308	CLA	CHB-C1B-NB	3.65	128.12	124.26
30	17	310	CLA	CAA-C2A-C3A	-3.64	102.80	112.78
30	16	307	CLA	CHB-C1B-NB	3.64	128.11	124.26
33	a	405	SQD	O9-S-O7	-3.64	101.35	113.95
30	B	623	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
30	15	302	CLA	CHB-C4A-NA	3.64	129.54	124.51
33	A	406	SQD	O5-C5-C4	3.63	116.30	109.69
42	16	313	A86	C12-C11-C13	3.63	122.12	116.02
33	l	101	SQD	O5-C5-C4	3.63	116.28	109.69
42	17	302	A86	C17-C16-C15	3.62	112.86	109.16
33	A	406	SQD	O9-S-O7	-3.62	101.42	113.95
39	j	101	DGD	O3G-C3G-C2G	-3.62	102.17	110.90
42	17	311	A86	C41-C32-C31	-3.61	107.24	110.47
30	17	308	CLA	CHB-C1B-NB	3.61	128.08	124.26
42	15	314	A86	C12-C11-C13	3.60	122.08	116.02
42	11	314	A86	C12-C11-C13	3.60	122.07	116.02
33	a	405	SQD	O5-C5-C4	3.60	116.23	109.69
33	A	406	SQD	O6-C1-C2	3.60	113.92	108.30
33	a	405	SQD	O6-C1-C2	3.60	113.92	108.30
30	16	305	CLA	CMB-C2B-C1B	-3.60	119.89	125.37
30	17	306	CLA	CHB-C1B-NB	3.60	128.06	124.26
42	19	310	A86	C25-C24-C1	-3.59	116.32	126.42
39	J	101	DGD	O6D-C1D-O3G	-3.59	101.47	109.97
42	17	316	A86	C12-C11-C13	3.59	122.05	116.02
42	19	310	A86	C25-C26-C27	-3.58	122.20	127.31
30	12	314	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
30	c	505	CLA	CHB-C4A-NA	3.58	129.46	124.51
39	j	101	DGD	O6D-C1D-O3G	-3.58	101.50	109.97
42	14	316	A86	C12-C11-C13	3.58	122.03	116.02
30	13	310	CLA	CAA-C2A-C3A	-3.58	102.98	112.78
42	14	301	A86	C12-C11-C13	3.57	122.02	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	511	CLA	C3B-C4B-NB	-3.57	107.20	110.52
42	17	311	A86	C25-C26-C27	-3.57	122.22	127.31
42	14	301	A86	C36-C31-C32	-3.57	116.16	119.70
42	12	319	A86	C12-C11-C13	3.56	122.01	116.02
42	21	310	A86	C25-C26-C27	-3.56	122.23	127.31
42	17	316	A86	C36-C31-C32	-3.56	116.16	119.70
30	14	311	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
30	11	309	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
42	15	314	A86	C36-C31-C32	-3.56	116.17	119.70
42	19	312	A86	C17-C16-C15	3.55	112.79	109.16
30	13	302	CLA	CHB-C4A-NA	3.55	129.43	124.51
30	12	305	CLA	CHB-C4A-NA	3.55	129.42	124.51
30	c	511	CLA	C3B-C4B-NB	-3.55	107.22	110.52
42	12	319	A86	C36-C31-C32	-3.55	116.17	119.70
30	17	309	CLA	CBA-CAA-C2A	3.55	124.33	113.86
42	21	312	A86	C4-C3-C2	-3.54	116.21	123.47
42	14	314	A86	C36-C31-C32	-3.54	116.19	119.70
42	12	317	A86	C3-C2-C1	-3.53	122.27	127.31
42	13	313	A86	C36-C31-C32	-3.53	116.19	119.70
36	d	410	LMG	C1-C2-C3	-3.53	102.64	110.00
30	14	303	CLA	CHB-C4A-NA	3.53	129.40	124.51
42	16	313	A86	C36-C31-C32	-3.53	116.19	119.70
42	17	313	A86	C36-C31-C32	-3.53	116.20	119.70
33	L	103	SQD	O9-S-O7	-3.53	101.74	113.95
36	D	408	LMG	C1-C2-C3	-3.53	102.65	110.00
30	C	505	CLA	CHB-C4A-NA	3.53	129.39	124.51
42	15	316	A86	C4-C3-C2	-3.52	116.26	123.47
42	14	316	A86	C36-C31-C32	-3.52	116.20	119.70
30	d	407	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
32	Z	101	BCR	C15-C16-C17	-3.52	116.27	123.47
32	c	515	BCR	C15-C16-C17	-3.52	116.27	123.47
33	b	620	SQD	O8-S-C6	3.51	111.34	105.74
30	11	301	CLA	CHB-C4A-NA	3.51	129.37	124.51
32	Z	101	BCR	C11-C10-C9	-3.51	122.30	127.31
42	19	312	A86	C3-C2-C1	-3.51	122.30	127.31
42	11	316	A86	C4-C3-C2	-3.51	116.29	123.47
42	21	313	A86	C12-C11-C13	3.50	121.91	116.02
39	c	518	DGD	O3G-C3G-C2G	-3.50	102.45	110.90
42	15	312	A86	C3-C2-C1	-3.50	122.31	127.31
33	l	101	SQD	O9-S-O7	-3.50	101.84	113.95
32	C	518	BCR	C15-C16-C17	-3.50	116.31	123.47
30	D	406	CLA	O2D-CGD-O1D	-3.49	117.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	13	315	A86	C4-C3-C2	-3.49	116.33	123.47
42	15	312	A86	C36-C31-C32	-3.49	116.24	119.70
42	16	312	A86	C36-C31-C32	-3.49	116.24	119.70
42	21	311	A86	C12-C11-C13	3.49	121.88	116.02
42	11	314	A86	C36-C31-C32	-3.48	116.24	119.70
42	20	211	A86	C12-C11-C13	3.48	121.87	116.02
42	15	310	A86	C34-O4-C38	-3.48	111.41	117.90
42	16	312	A86	C3-C2-C1	-3.48	122.34	127.31
42	11	310	A86	C34-O4-C38	-3.48	111.41	117.90
42	15	315	A86	C4-C3-C2	-3.48	116.35	123.47
42	11	312	A86	C3-C2-C1	-3.48	122.35	127.31
42	14	314	A86	C3-C2-C1	-3.48	122.35	127.31
32	a	404	BCR	C15-C16-C17	-3.48	116.35	123.47
42	12	304	A86	C4-C3-C2	-3.48	116.35	123.47
33	B	621	SQD	O8-S-C6	3.48	111.28	105.74
30	17	304	CLA	C2A-C1A-CHA	3.47	129.93	123.86
42	18	302	A86	C4-C3-C2	-3.47	116.36	123.47
32	A	405	BCR	C15-C16-C17	-3.47	116.36	123.47
42	13	313	A86	C3-C2-C1	-3.47	122.36	127.31
42	17	313	A86	C3-C2-C1	-3.46	122.36	127.31
42	14	313	A86	C36-C31-C32	-3.46	116.26	119.70
42	18	313	A86	C34-O4-C38	-3.46	111.45	117.90
42	11	316	A86	C3-C2-C1	-3.46	122.38	127.31
42	13	301	A86	C4-C3-C2	-3.46	116.39	123.47
42	12	315	A86	C34-O4-C38	-3.46	111.46	117.90
42	11	312	A86	C36-C31-C32	-3.46	116.27	119.70
42	17	302	A86	C25-C26-C27	-3.45	122.38	127.31
42	21	310	A86	C20-C19-C18	-3.45	105.92	112.75
32	c	521	BCR	C15-C16-C17	-3.45	116.41	123.47
30	18	309	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
42	19	311	A86	C12-C11-C13	3.45	121.82	116.02
42	13	311	A86	C34-O4-C38	-3.45	111.47	117.90
30	18	311	CLA	C2A-C1A-CHA	3.45	129.89	123.86
32	c	515	BCR	C11-C10-C9	-3.45	122.39	127.31
39	C	517	DGD	O3G-C3G-C2G	-3.45	102.58	110.90
42	17	316	A86	C20-C19-C18	-3.44	105.94	112.75
42	14	312	A86	C34-O4-C38	-3.44	111.48	117.90
42	16	311	A86	C36-C31-C32	-3.44	116.28	119.70
42	18	302	A86	C3-C2-C1	-3.44	122.40	127.31
31	D	403	PHO	O1D-CGD-CBD	3.44	130.47	124.74
30	18	306	CLA	CHB-C1B-NB	3.44	127.90	124.26
42	16	313	A86	C20-C19-C18	-3.44	105.95	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	317	A86	C36-C31-C32	-3.43	116.29	119.70
42	13	301	A86	C3-C2-C1	-3.43	122.41	127.31
42	15	316	A86	C3-C2-C1	-3.43	122.41	127.31
42	12	319	A86	C20-C19-C18	-3.43	105.96	112.75
42	11	314	A86	C20-C19-C18	-3.43	105.97	112.75
39	c	517	DGD	O5D-C6D-C5D	-3.43	102.71	109.05
42	21	312	A86	C41-C32-C31	-3.42	107.41	110.47
42	15	314	A86	C20-C19-C18	-3.42	105.98	112.75
42	12	304	A86	C3-C2-C1	-3.42	122.43	127.31
42	13	315	A86	C3-C2-C1	-3.42	122.43	127.31
30	20	205	CLA	CHB-C1B-NB	3.42	127.88	124.26
42	11	316	A86	C40-C32-C31	-3.42	107.41	110.47
42	12	316	A86	C36-C31-C32	-3.41	116.31	119.70
42	17	312	A86	C36-C31-C32	-3.41	116.31	119.70
42	18	302	A86	C40-C32-C31	-3.41	107.42	110.47
42	14	316	A86	C20-C19-C18	-3.41	106.00	112.75
42	15	316	A86	C40-C32-C31	-3.41	107.42	110.47
30	19	302	CLA	CMB-C2B-C1B	-3.41	120.18	125.37
42	15	315	A86	C3-C2-C1	-3.41	122.44	127.31
42	17	302	A86	C9-C8-C6	-3.41	116.84	126.42
42	19	312	A86	C9-C10-C11	-3.41	116.59	126.61
42	21	310	A86	C4-C5-C6	-3.41	122.45	127.31
42	14	314	A86	C26-C25-C24	-3.41	112.58	123.22
42	14	301	A86	C20-C19-C18	-3.41	106.01	112.75
30	C	514	CLA	CHB-C4A-NA	3.41	129.22	124.51
42	16	312	A86	C26-C25-C24	-3.41	112.59	123.22
30	13	302	CLA	C1-C2-C3	-3.40	120.16	126.04
42	11	312	A86	C26-C25-C24	-3.40	112.60	123.22
32	B	618	BCR	C24-C23-C22	-3.40	121.09	126.23
42	13	313	A86	C26-C25-C24	-3.40	112.60	123.22
42	13	312	A86	C36-C31-C32	-3.40	116.32	119.70
42	17	313	A86	C26-C25-C24	-3.40	112.61	123.22
30	b	610	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
30	c	514	CLA	CHB-C4A-NA	3.40	129.21	124.51
30	12	305	CLA	C1-C2-C3	-3.40	120.17	126.04
30	16	307	CLA	CHB-C4A-NA	3.39	129.21	124.51
32	b	617	BCR	C24-C23-C22	-3.39	121.11	126.23
31	d	404	PHO	O1D-CGD-CBD	3.39	130.39	124.74
30	15	307	CLA	CHB-C4A-NA	3.39	129.20	124.51
30	15	306	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
42	15	311	A86	C36-C31-C32	-3.39	116.34	119.70
42	12	317	A86	C26-C25-C24	-3.38	112.66	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	312	A86	C26-C25-C24	-3.38	112.67	123.22
39	C	516	DGD	O5D-C6D-C5D	-3.37	102.81	109.05
30	13	303	CLA	CHB-C4A-NA	3.37	129.17	124.51
30	C	511	CLA	CMB-C2B-C3B	3.37	134.75	126.59
42	13	315	A86	C40-C32-C31	-3.37	107.46	110.47
30	B	610	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
42	12	304	A86	C40-C32-C31	-3.37	107.46	110.47
30	d	401	CLA	C3B-C4B-NB	-3.37	107.39	110.52
30	14	303	CLA	C1-C2-C3	-3.36	120.22	126.04
42	18	314	A86	C36-C31-C32	-3.36	116.36	119.70
30	b	614	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
30	B	614	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
30	c	511	CLA	CMB-C2B-C3B	3.36	134.73	126.59
30	B	612	CLA	CHB-C4A-NA	3.36	129.16	124.51
40	d	405	PL9	C7-C3-C2	-3.36	118.88	123.30
30	16	308	CLA	C2A-C1A-CHA	3.36	129.73	123.86
39	H	102	DGD	O3G-C3G-C2G	-3.35	102.81	110.90
42	11	311	A86	C36-C31-C32	-3.35	116.37	119.70
30	b	612	CLA	CHB-C4A-NA	3.35	129.15	124.51
42	21	310	A86	C34-O4-C38	-3.35	111.65	117.90
32	a	404	BCR	C15-C14-C13	-3.35	122.53	127.31
30	c	512	CLA	C3B-C4B-NB	-3.35	107.41	110.52
42	13	314	A86	C3-C4-C5	-3.35	116.61	123.47
30	11	301	CLA	C1-C2-C3	-3.35	120.25	126.04
39	h	102	DGD	O3G-C3G-C2G	-3.34	102.83	110.90
30	18	303	CLA	CHB-C4A-NA	3.34	129.13	124.51
30	18	303	CLA	C3B-C4B-NB	-3.34	107.41	110.52
30	14	304	CLA	CHB-C4A-NA	3.34	129.13	124.51
42	18	315	A86	C3-C4-C5	-3.34	116.63	123.47
42	12	318	A86	C3-C4-C5	-3.34	116.64	123.47
30	14	309	CLA	CHB-C4A-NA	3.33	129.12	124.51
30	B	601	CLA	CHB-C4A-NA	3.33	129.12	124.51
30	D	401	CLA	C3B-C4B-NB	-3.33	107.42	110.52
42	17	314	A86	C3-C4-C5	-3.33	116.65	123.47
30	B	613	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
42	15	315	A86	C40-C32-C31	-3.33	107.49	110.47
30	11	307	CLA	CHB-C4A-NA	3.33	129.11	124.51
30	b	601	CLA	CHB-C4A-NA	3.33	129.11	124.51
30	13	308	CLA	CHB-C4A-NA	3.33	129.11	124.51
42	14	315	A86	C3-C4-C5	-3.32	116.67	123.47
30	d	401	CLA	CHB-C1B-NB	3.32	127.77	124.26
42	19	311	A86	C28-C27-C26	-3.32	118.28	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	613	CLA	CMB-C2B-C1B	-3.32	120.32	125.37
30	12	306	CLA	CHB-C4A-NA	3.31	129.09	124.51
42	13	301	A86	C40-C32-C31	-3.31	107.51	110.47
32	A	405	BCR	C15-C14-C13	-3.31	122.59	127.31
42	15	313	A86	C3-C4-C5	-3.31	116.70	123.47
42	11	313	A86	C3-C4-C5	-3.31	116.70	123.47
30	15	301	CLA	CHB-C4A-NA	3.30	129.08	124.51
30	C	512	CLA	C3B-C4B-NB	-3.30	107.46	110.52
30	17	303	CLA	C3B-C4B-NB	-3.29	107.47	110.52
30	C	512	CLA	CHB-C4A-NA	3.29	129.06	124.51
30	12	313	CLA	CHB-C4A-NA	3.29	129.06	124.51
30	21	305	CLA	CMB-C2B-C1B	-3.28	120.37	125.37
30	11	302	CLA	CHB-C4A-NA	3.28	129.05	124.51
30	16	306	CLA	CHB-C4A-NA	3.28	129.05	124.51
30	c	512	CLA	CHB-C4A-NA	3.28	129.05	124.51
33	l	101	SQD	C1-O5-C5	3.28	120.12	113.69
30	D	401	CLA	CHB-C1B-NB	3.28	127.73	124.26
42	11	313	A86	C12-C11-C13	3.27	121.52	116.02
42	12	318	A86	C12-C11-C13	3.27	121.52	116.02
42	15	313	A86	C12-C11-C13	3.27	121.52	116.02
40	D	404	PL9	C7-C3-C2	-3.27	119.00	123.30
30	20	209	CLA	CHB-C1B-NB	3.27	127.72	124.26
42	17	314	A86	C12-C11-C13	3.27	121.52	116.02
40	D	407	PL9	C7-C8-C9	-3.27	121.35	126.79
30	a	403	CLA	CHB-C4A-NA	3.26	129.03	124.51
42	20	201	A86	C10-C9-C8	-3.26	113.03	123.22
30	A	404	CLA	CHB-C4A-NA	3.26	129.03	124.51
33	L	103	SQD	C1-O5-C5	3.26	120.09	113.69
42	14	315	A86	C12-C11-C13	3.26	121.50	116.02
30	M	101	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
42	18	315	A86	C12-C11-C13	3.26	121.49	116.02
30	18	309	CLA	CHB-C1B-NB	3.25	127.70	124.26
40	d	408	PL9	C7-C8-C9	-3.25	121.38	126.79
30	b	604	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
30	c	509	CLA	CHB-C1B-NB	3.25	127.70	124.26
42	14	315	A86	C10-C9-C8	-3.25	113.08	123.22
42	13	314	A86	C12-C11-C13	3.25	121.48	116.02
30	12	311	CLA	CHB-C4A-NA	3.25	129.00	124.51
30	C	506	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
33	a	405	SQD	O8-S-C6	3.24	110.90	105.74
32	A	405	BCR	C24-C23-C22	-3.24	121.34	126.23
42	15	316	A86	C36-C31-C32	-3.24	116.48	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	508	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	C	509	CLA	CHB-C1B-NB	3.23	127.68	124.26
30	15	306	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	C	505	CLA	C3C-C4C-NC	-3.23	106.95	110.57
30	B	608	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
33	A	406	SQD	O8-S-C6	3.23	110.89	105.74
30	16	307	CLA	CMB-C2B-C3B	3.23	134.41	126.59
30	17	306	CLA	CMB-C2B-C3B	3.23	134.41	126.59
42	18	315	A86	C10-C9-C8	-3.23	113.14	123.22
30	17	308	CLA	CHB-C4A-NA	3.23	128.97	124.51
30	11	308	CLA	CHB-C4A-NA	3.23	128.97	124.51
37	B	625	LMU	O5B-C5B-C4B	3.22	115.55	109.69
42	15	313	A86	C10-C9-C8	-3.22	113.16	123.22
30	m	101	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
42	11	313	A86	C10-C9-C8	-3.22	113.17	123.22
30	13	309	CLA	CHB-C4A-NA	3.22	128.96	124.51
42	20	211	A86	C4-C3-C2	-3.22	116.88	123.47
42	12	304	A86	C36-C31-C32	-3.22	116.50	119.70
42	12	318	A86	C10-C9-C8	-3.22	113.18	123.22
30	14	310	CLA	CHB-C4A-NA	3.22	128.96	124.51
42	17	312	A86	C12-C11-C13	3.21	121.42	116.02
42	13	312	A86	C12-C11-C13	3.21	121.42	116.02
30	20	206	CLA	CHB-C4A-NA	3.21	128.96	124.51
42	15	311	A86	C12-C11-C13	3.21	121.42	116.02
30	c	506	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	B	609	CLA	CHB-C4A-NA	3.21	128.95	124.51
30	B	604	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	b	608	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	b	609	CLA	CHB-C4A-NA	3.21	128.95	124.51
42	15	315	A86	C36-C31-C32	-3.21	116.51	119.70
30	B	605	CLA	CHB-C4A-NA	3.21	128.94	124.51
30	c	507	CLA	CMB-C2B-C1B	-3.20	120.49	125.37
42	17	314	A86	C10-C9-C8	-3.20	113.22	123.22
30	C	507	CLA	CMB-C2B-C1B	-3.20	120.49	125.37
30	19	304	CLA	CHB-C4A-NA	3.20	128.94	124.51
30	B	608	CLA	CHB-C4A-NA	3.20	128.94	124.51
42	11	311	A86	C12-C11-C13	3.20	121.40	116.02
42	20	210	A86	C12-C11-C13	3.20	121.40	116.02
30	13	304	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
30	b	608	CLA	CHB-C4A-NA	3.20	128.94	124.51
42	13	314	A86	C10-C9-C8	-3.20	113.23	123.22
30	b	605	CLA	CHB-C4A-NA	3.20	128.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	516	DGD	O6D-C1D-O3G	-3.20	102.40	109.97
42	13	301	A86	C36-C31-C32	-3.20	116.52	119.70
30	15	302	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
42	13	315	A86	C36-C31-C32	-3.20	116.52	119.70
30	16	303	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
32	a	404	BCR	C24-C23-C22	-3.19	121.41	126.23
42	21	311	A86	C4-C3-C2	-3.19	116.94	123.47
42	12	316	A86	C12-C11-C13	3.19	121.38	116.02
37	12	302	LMU	C3'-C4'-C5'	3.19	118.23	110.93
42	20	210	A86	C41-C32-C31	-3.19	107.62	110.47
42	20	212	A86	C17-C16-C15	3.18	112.41	109.16
30	C	514	CLA	CMB-C2B-C1B	-3.18	120.52	125.37
42	14	313	A86	C12-C11-C13	3.18	121.37	116.02
42	11	316	A86	C36-C31-C32	-3.18	116.54	119.70
42	20	211	A86	C4-C5-C6	-3.18	122.77	127.31
30	12	307	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
30	c	508	CLA	CHB-C4A-NA	3.18	128.90	124.51
30	11	303	CLA	CAA-C2A-C3A	-3.17	104.08	112.78
42	21	311	A86	C4-C5-C6	-3.17	122.78	127.31
37	12	302	LMU	O5B-C5B-C4B	3.17	115.46	109.69
42	18	314	A86	C12-C11-C13	3.17	121.35	116.02
30	16	303	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
30	c	505	CLA	C3C-C4C-NC	-3.17	107.02	110.57
42	21	313	A86	C7-C6-C8	3.17	123.07	118.08
30	14	305	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
42	16	310	A86	C41-C32-C31	-3.17	107.64	110.47
39	c	517	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
30	b	607	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
30	14	306	CLA	CHB-C4A-NA	3.16	128.88	124.51
30	12	308	CLA	CHB-C4A-NA	3.15	128.87	124.51
42	14	301	A86	C10-C9-C8	-3.14	113.41	123.22
37	B	625	LMU	C3'-C4'-C5'	3.14	118.13	110.93
30	17	309	CLA	CHB-C4A-NA	3.14	128.86	124.51
42	14	316	A86	C10-C9-C8	-3.14	113.41	123.22
42	16	313	A86	C10-C9-C8	-3.14	113.42	123.22
42	12	319	A86	C10-C9-C8	-3.14	113.42	123.22
42	15	314	A86	C10-C9-C8	-3.14	113.42	123.22
30	c	514	CLA	CMB-C2B-C1B	-3.14	120.59	125.37
30	w	103	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
30	W	103	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
42	21	310	A86	C25-C24-C1	-3.13	117.62	126.42
42	16	311	A86	C12-C11-C13	3.13	121.28	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	405	CLA	CAA-C2A-C3A	-3.13	104.21	112.78
42	21	314	A86	C3-C4-C5	-3.13	117.07	123.47
30	15	304	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
30	17	303	CLA	CHB-C1B-NB	3.13	127.57	124.26
30	d	406	CLA	CAA-C2A-C3A	-3.12	104.22	112.78
30	15	307	CLA	C3B-C4B-NB	-3.12	107.62	110.52
42	17	316	A86	C10-C9-C8	-3.12	113.48	123.22
42	18	302	A86	C36-C31-C32	-3.12	116.60	119.70
42	11	314	A86	C10-C9-C8	-3.12	113.49	123.22
30	18	304	CLA	CHB-C4A-NA	3.11	128.82	124.51
42	20	213	A86	C3-C4-C5	-3.11	117.09	123.47
42	19	311	A86	C40-C32-C31	-3.11	107.69	110.47
30	14	310	CLA	CAA-C2A-C1A	3.11	122.17	111.97
32	B	624	BCR	C7-C8-C9	-3.11	121.54	126.23
30	d	402	CLA	C3B-C4B-NB	-3.11	107.63	110.52
30	B	607	CLA	CMB-C2B-C1B	-3.10	120.64	125.37
30	17	308	CLA	C4-C3-C5	3.10	120.49	115.27
42	21	310	A86	C36-C31-C32	-3.10	116.62	119.70
42	20	213	A86	C4-C5-C6	-3.10	122.89	127.31
30	13	309	CLA	CAA-C2A-C1A	3.10	122.12	111.97
30	16	303	CLA	CHB-C4A-NA	3.09	128.79	124.51
42	17	302	A86	C40-C32-C31	-3.09	107.70	110.47
30	b	622	CLA	CAA-C2A-C1A	3.09	122.11	111.97
30	11	308	CLA	CAA-C2A-C1A	3.09	122.11	111.97
30	20	204	CLA	CHB-C4A-NA	3.09	128.79	124.51
30	b	611	CLA	CHB-C1B-NB	3.09	127.53	124.26
30	12	313	CLA	CAA-C2A-C1A	3.09	122.10	111.97
30	C	510	CLA	CMB-C2B-C1B	-3.08	120.67	125.37
30	13	305	CLA	CHB-C4A-NA	3.08	128.77	124.51
42	21	314	A86	C4-C5-C6	-3.08	122.92	127.31
30	B	611	CLA	CHB-C1B-NB	3.07	127.51	124.26
30	15	304	CLA	CHB-C1B-NB	3.07	127.51	124.26
30	12	305	CLA	C3B-C4B-NB	-3.07	107.66	110.52
30	c	505	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	b	610	CLA	C3B-C4B-NB	-3.07	107.66	110.52
30	18	311	CLA	CHB-C4A-NA	3.07	128.76	124.51
42	20	212	A86	C25-C24-C1	-3.07	117.79	126.42
41	v	201	HEM	CAC-C3C-C4C	3.07	132.31	124.90
30	b	609	CLA	CHC-C4B-NB	3.07	127.51	124.26
32	a	408	BCR	C11-C10-C9	-3.07	122.93	127.31
32	c	515	BCR	C24-C23-C22	-3.07	121.60	126.23
32	A	409	BCR	C11-C10-C9	-3.07	122.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	302	CLA	CHB-C1B-NB	3.07	127.50	124.26
42	16	310	A86	C26-C25-C24	-3.06	113.66	123.22
30	11	304	CLA	C2A-C1A-CHA	3.06	129.21	123.86
41	V	201	HEM	CAC-C3C-C4C	3.06	132.28	124.90
33	l	101	SQD	C3-C4-C5	3.06	115.70	110.24
32	b	616	BCR	C15-C14-C13	-3.06	122.95	127.31
30	11	304	CLA	CHB-C4A-NA	3.06	128.74	124.51
30	14	305	CLA	CBA-CAA-C2A	3.06	122.88	113.86
30	19	304	CLA	C2A-C1A-CHA	3.05	129.20	123.86
30	12	307	CLA	CBA-CAA-C2A	3.05	122.88	113.86
30	C	508	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
39	C	516	DGD	C1D-C2D-C3D	-3.05	103.64	110.00
30	11	301	CLA	C3B-C4B-NB	-3.05	107.68	110.52
37	B	625	LMU	O5'-C5'-C4'	3.05	116.19	109.75
30	B	623	CLA	CAA-C2A-C1A	3.05	121.97	111.97
35	A	408	LHG	O8-C23-C24	3.05	121.48	111.91
42	17	302	A86	C12-C11-C13	3.05	121.15	116.02
30	11	303	CLA	CBA-CAA-C2A	3.05	122.87	113.86
30	c	508	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
30	c	507	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
30	13	305	CLA	C2A-C1A-CHA	3.05	129.19	123.86
30	B	612	CLA	CHC-C4B-NB	3.05	127.48	124.26
30	b	612	CLA	CHC-C4B-NB	3.04	127.48	124.26
30	13	308	CLA	C3B-C4B-NB	-3.04	107.69	110.52
42	13	314	A86	C36-C31-C32	-3.04	116.68	119.70
30	13	304	CLA	CBA-CAA-C2A	3.04	122.84	113.86
33	L	103	SQD	C3-C4-C5	3.04	115.67	110.24
32	C	515	BCR	C11-C10-C9	-3.04	122.97	127.31
30	11	306	CLA	CHC-C4B-NB	3.04	127.48	124.26
35	a	407	LHG	O8-C23-C24	3.04	121.45	111.91
30	D	402	CLA	C3B-C4B-NB	-3.04	107.69	110.52
33	B	621	SQD	O9-S-C6	3.03	110.54	106.94
30	d	402	CLA	CHB-C4A-NA	3.03	128.70	124.51
32	B	617	BCR	C15-C14-C13	-3.03	122.99	127.31
30	12	311	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	13	308	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	19	304	CLA	CHB-C1B-NB	3.03	127.46	124.26
42	21	310	A86	C12-C11-C13	3.03	121.10	116.02
30	c	508	CLA	C2A-C1A-CHA	3.02	129.15	123.86
30	11	307	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
42	21	313	A86	C10-C9-C8	-3.02	113.78	123.22
30	W	102	CLA	O2D-CGD-O1D	-3.02	117.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	608	CLA	C3B-C4B-NB	-3.02	107.71	110.52
30	13	302	CLA	C3B-C4B-NB	-3.02	107.71	110.52
30	18	309	CLA	C3B-C4B-NB	-3.02	107.71	110.52
42	17	302	A86	C41-C32-C31	-3.02	107.77	110.47
30	19	303	CLA	CHB-C4A-NA	3.02	128.69	124.51
30	b	614	CLA	CHB-C4A-NA	3.02	128.69	124.51
30	19	302	CLA	CHB-C4A-NA	3.02	128.69	124.51
34	a	406	BCT	O3-C-O1	-3.02	111.71	119.55
30	C	502	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
30	14	309	CLA	C3B-C4B-NB	-3.02	107.71	110.52
30	B	609	CLA	CHC-C4B-NB	3.02	127.45	124.26
30	17	304	CLA	CHB-C4A-NA	3.02	128.69	124.51
42	11	313	A86	C36-C31-C32	-3.02	116.70	119.70
39	C	517	DGD	CDB-CCB-CBB	-3.02	99.11	114.42
42	19	312	A86	C9-C8-C6	-3.02	117.94	126.42
39	c	517	DGD	C1D-C2D-C3D	-3.02	103.72	110.00
42	17	311	A86	C9-C10-C11	-3.02	117.74	126.61
30	12	311	CLA	C3B-C4B-NB	-3.01	107.72	110.52
34	A	407	BCT	O3-C-O1	-3.01	111.73	119.55
30	C	519	CLA	C3B-C4B-NB	-3.01	107.72	110.52
30	14	306	CLA	C2A-C1A-CHA	3.01	129.13	123.86
30	d	407	CLA	CHB-C4A-NA	3.01	128.68	124.51
30	B	610	CLA	C3B-C4B-NB	-3.01	107.72	110.52
42	18	315	A86	C36-C31-C32	-3.01	116.71	119.70
42	20	213	A86	C10-C9-C8	-3.01	113.83	123.22
39	c	518	DGD	CDB-CCB-CBB	-3.01	99.16	114.42
30	C	505	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
42	12	317	A86	C35-C34-C33	3.01	115.12	109.88
30	20	207	CLA	CHB-C4A-NA	3.01	128.67	124.51
42	18	314	A86	C3-C4-C5	-3.01	117.32	123.47
42	13	313	A86	C35-C34-C33	3.01	115.12	109.88
30	c	510	CLA	CMB-C2B-C1B	-3.00	120.79	125.37
40	d	405	PL9	C41-C39-C38	-3.00	115.04	121.12
30	C	512	CLA	CAA-CBA-CGA	-3.00	104.48	113.25
32	c	516	BCR	C11-C10-C9	-3.00	123.03	127.31
30	14	309	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	15	302	CLA	C2A-C1A-CHA	3.00	129.11	123.86
42	21	314	A86	C10-C9-C8	-3.00	113.85	123.22
30	c	512	CLA	CAA-CBA-CGA	-3.00	104.49	113.25
30	11	307	CLA	C3B-C4B-NB	-3.00	107.73	110.52
42	17	313	A86	C35-C34-C33	3.00	115.11	109.88
30	C	507	CLA	O2D-CGD-O1D	-3.00	117.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	20	208	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
42	21	310	A86	C3-C4-C5	-3.00	117.33	123.47
42	11	313	A86	C25-C24-C1	-3.00	118.00	126.42
30	b	601	CLA	C3B-C4B-NB	-2.99	107.74	110.52
30	13	308	CLA	CHB-C1B-NB	2.99	127.43	124.26
32	Z	101	BCR	C24-C23-C22	-2.99	121.71	126.23
30	w	102	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
30	19	309	CLA	CHB-C4A-NA	2.99	128.65	124.51
42	14	314	A86	C35-C34-C33	2.99	115.09	109.88
37	12	302	LMU	O5'-C5'-C4'	2.99	116.06	109.75
42	17	312	A86	C3-C4-C5	-2.99	117.35	123.47
30	b	614	CLA	O2D-CGD-CBD	2.99	116.58	111.27
33	a	405	SQD	O48-C23-C24	2.99	121.29	111.91
30	14	303	CLA	C3B-C4B-NB	-2.99	107.74	110.52
42	15	313	A86	C25-C24-C1	-2.99	118.02	126.42
42	18	315	A86	C25-C24-C1	-2.99	118.03	126.42
30	17	306	CLA	CHB-C4A-NA	2.99	128.64	124.51
33	A	406	SQD	O48-C23-C24	2.99	121.28	111.91
30	12	308	CLA	C2A-C1A-CHA	2.99	129.08	123.86
42	12	318	A86	C36-C31-C32	-2.98	116.73	119.70
42	12	318	A86	C25-C24-C1	-2.98	118.03	126.42
42	14	315	A86	C25-C24-C1	-2.98	118.03	126.42
30	18	311	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
40	D	404	PL9	C41-C39-C38	-2.98	115.08	121.12
33	b	620	SQD	O9-S-C6	2.98	110.48	106.94
30	D	406	CLA	CHB-C4A-NA	2.98	128.63	124.51
42	17	315	A86	C7-C6-C5	-2.98	118.75	122.92
42	15	313	A86	C36-C31-C32	-2.98	116.74	119.70
42	13	314	A86	C25-C24-C1	-2.98	118.05	126.42
35	B	622	LHG	O8-C23-C24	2.98	121.25	111.91
42	15	316	A86	C7-C6-C5	-2.98	118.75	122.92
42	16	312	A86	C35-C34-C33	2.98	115.07	109.88
35	b	621	LHG	O8-C23-C24	2.98	121.24	111.91
42	13	301	A86	C7-C6-C5	-2.97	118.76	122.92
30	D	402	CLA	CHB-C4A-NA	2.97	128.62	124.51
30	19	305	CLA	CHB-C4A-NA	2.97	128.62	124.51
42	11	316	A86	C7-C6-C5	-2.97	118.76	122.92
32	c	516	BCR	C15-C16-C17	-2.97	117.39	123.47
32	A	405	BCR	C11-C10-C9	-2.97	123.07	127.31
30	B	614	CLA	O2D-CGD-CBD	2.97	116.54	111.27
30	12	311	CLA	C1-C2-C3	-2.97	120.91	126.04
42	12	304	A86	C7-C6-C5	-2.97	118.77	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	406	CLA	C3B-C4B-NB	-2.96	107.77	110.52
42	14	313	A86	C3-C4-C5	-2.96	117.40	123.47
30	B	615	CLA	CHB-C1B-NB	2.96	127.39	124.26
30	15	304	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	14	309	CLA	CHB-C1B-NB	2.96	127.39	124.26
42	17	315	A86	C17-C16-C15	2.96	112.19	109.16
36	b	619	LMG	O6-C1-O1	-2.96	102.96	109.97
30	b	608	CLA	C3B-C4B-NB	-2.96	107.77	110.52
42	16	311	A86	C3-C4-C5	-2.96	117.41	123.47
32	B	624	BCR	C11-C10-C9	-2.96	123.09	127.31
42	15	311	A86	C3-C4-C5	-2.96	117.41	123.47
42	18	302	A86	C7-C6-C5	-2.96	118.78	122.92
30	C	508	CLA	C2A-C1A-CHA	2.96	129.03	123.86
42	13	312	A86	C3-C4-C5	-2.96	117.42	123.47
30	13	307	CLA	CHC-C4B-NB	2.95	127.39	124.26
42	14	315	A86	C36-C31-C32	-2.95	116.76	119.70
42	15	312	A86	C35-C34-C33	2.95	115.03	109.88
42	20	201	A86	C4-C5-C6	-2.95	123.09	127.31
32	C	515	BCR	C15-C16-C17	-2.95	117.42	123.47
30	15	307	CLA	CHB-C1B-NB	2.95	127.38	124.26
42	11	311	A86	C3-C4-C5	-2.95	117.43	123.47
42	17	314	A86	C25-C24-C1	-2.95	118.13	126.42
30	13	310	CLA	C3B-C4B-NB	-2.95	107.78	110.52
42	19	312	A86	C7-C6-C5	-2.95	118.79	122.92
30	b	612	CLA	C3B-C4B-NB	-2.95	107.78	110.52
30	20	208	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	15	301	CLA	CHB-C1B-NB	2.95	127.38	124.26
30	B	614	CLA	CHB-C4A-NA	2.95	128.59	124.51
36	B	620	LMG	O6-C1-O1	-2.95	102.99	109.97
30	b	604	CLA	CHB-C4A-NA	2.95	128.59	124.51
42	11	312	A86	C35-C34-C33	2.95	115.02	109.88
30	b	615	CLA	CHB-C1B-NB	2.95	127.38	124.26
42	17	314	A86	C36-C31-C32	-2.94	116.77	119.70
42	14	315	A86	C7-C6-C8	2.94	122.72	118.08
30	12	308	CLA	CMB-C2B-C3B	2.94	133.72	126.59
30	B	612	CLA	C3B-C4B-NB	-2.94	107.78	110.52
42	15	315	A86	C7-C6-C5	-2.94	118.80	122.92
42	15	312	A86	C12-C11-C13	2.94	120.96	116.02
42	12	316	A86	C3-C4-C5	-2.94	117.45	123.47
30	18	306	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	b	613	CLA	CMB-C2B-C3B	2.94	133.71	126.59
30	15	305	CLA	CHB-C4A-NA	2.94	128.58	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	16	313	A86	C41-C32-C31	-2.94	107.84	110.47
42	14	314	A86	C12-C11-C13	2.94	120.96	116.02
30	11	305	CLA	CHB-C4A-NA	2.94	128.57	124.51
30	12	309	CLA	CHB-C4A-NA	2.94	128.57	124.51
30	13	305	CLA	CMB-C2B-C3B	2.94	133.70	126.59
30	z	101	CLA	C3B-C4B-NB	-2.94	107.79	110.52
42	17	313	A86	C12-C11-C13	2.93	120.95	116.02
42	12	317	A86	C12-C11-C13	2.93	120.95	116.02
30	12	303	CLA	CHB-C4A-NA	2.93	128.57	124.51
42	15	314	A86	C41-C32-C31	-2.93	107.85	110.47
30	21	302	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	11	304	CLA	CMB-C2B-C3B	2.93	133.69	126.59
30	15	303	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	21	305	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	C	506	CLA	C2D-C1D-ND	-2.93	107.94	110.10
30	16	305	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	19	305	CLA	C3B-C4B-NB	-2.93	107.80	110.52
30	c	502	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	16	306	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	12	311	CLA	CHB-C1B-NB	2.93	127.36	124.26
30	14	308	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	B	604	CLA	CHB-C4A-NA	2.92	128.56	124.51
42	13	315	A86	C7-C6-C5	-2.92	118.83	122.92
30	B	613	CLA	CMB-C2B-C3B	2.92	133.67	126.59
31	d	403	PHO	O1D-CGD-CBD	2.92	129.61	124.74
42	16	312	A86	C12-C11-C13	2.92	120.93	116.02
30	11	306	CLA	CHB-C4A-NA	2.92	128.55	124.51
30	19	309	CLA	C3B-C4B-NB	-2.92	107.81	110.52
42	17	316	A86	C41-C32-C31	-2.92	107.86	110.47
30	19	309	CLA	CHB-C1B-NB	2.92	127.34	124.26
30	14	306	CLA	CMB-C2B-C3B	2.92	133.65	126.59
42	13	313	A86	C12-C11-C13	2.92	120.92	116.02
30	16	301	CLA	CHB-C4A-NA	2.92	128.54	124.51
30	C	513	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	A	404	CLA	CHB-C1B-NB	2.91	127.34	124.26
42	11	312	A86	C12-C11-C13	2.91	120.92	116.02
31	A	403	PHO	O1D-CGD-CBD	2.91	129.59	124.74
30	17	309	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
32	b	623	BCR	C7-C8-C9	-2.91	121.83	126.23
42	16	311	A86	C34-O4-C38	-2.91	112.47	117.90
30	12	310	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	13	306	CLA	CHB-C4A-NA	2.91	128.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	305	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	c	510	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	12	307	CLA	CHB-C4A-NA	2.91	128.54	124.51
32	a	404	BCR	C11-C10-C9	-2.91	123.16	127.31
42	17	314	A86	C7-C6-C8	2.91	122.66	118.08
30	b	613	CLA	CHB-C4A-NA	2.91	128.53	124.51
42	13	314	A86	C7-C6-C8	2.91	122.66	118.08
30	12	312	CLA	CHB-C4A-NA	2.91	128.53	124.51
30	16	309	CLA	C3B-C4B-NB	-2.91	107.82	110.52
42	11	313	A86	C7-C6-C8	2.91	122.66	118.08
30	14	308	CLA	CHC-C4B-NB	2.91	127.33	124.26
30	11	307	CLA	C1-C2-C3	-2.90	121.02	126.04
30	13	304	CLA	CHB-C4A-NA	2.90	128.53	124.51
30	11	303	CLA	CHB-C4A-NA	2.90	128.52	124.51
30	B	607	CLA	CHB-C4A-NA	2.90	128.52	124.51
30	16	305	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
42	18	315	A86	C7-C6-C8	2.90	122.65	118.08
30	17	308	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
30	13	308	CLA	C1-C2-C3	-2.90	121.03	126.04
42	11	314	A86	C41-C32-C31	-2.90	107.88	110.47
30	17	310	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
42	12	318	A86	C7-C6-C8	2.89	122.64	118.08
30	12	310	CLA	CHC-C4B-NB	2.89	127.32	124.26
30	16	302	CLA	CMA-C3A-C2A	-2.89	102.16	113.83
30	13	307	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
42	13	312	A86	C34-O4-C38	-2.89	112.50	117.90
30	C	507	CLA	CHB-C1B-NB	2.89	127.32	124.26
30	d	407	CLA	C3B-C4B-NB	-2.89	107.83	110.52
36	b	619	LMG	O3-C3-C2	-2.89	103.67	110.35
30	C	502	CLA	CHC-C4B-NB	2.89	127.32	124.26
42	17	312	A86	C34-O4-C38	-2.89	112.51	117.90
30	11	315	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	c	502	CLA	CHC-C4B-NB	2.89	127.31	124.26
30	15	308	CLA	CHB-C4A-NA	2.89	128.51	124.51
32	Y	101	BCR	C24-C23-C22	-2.89	121.87	126.23
42	13	314	A86	C4-C5-C6	-2.89	123.19	127.31
42	11	311	A86	C34-O4-C38	-2.89	112.52	117.90
42	19	310	A86	C33-C32-C31	2.89	112.02	109.21
42	12	316	A86	C34-O4-C38	-2.89	112.52	117.90
30	C	510	CLA	O2D-CGD-CBD	2.89	116.40	111.27
30	a	403	CLA	CHB-C1B-NB	2.89	127.31	124.26
42	14	313	A86	C34-O4-C38	-2.89	112.52	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	520	BCR	C16-C15-C14	-2.88	117.56	123.47
30	B	601	CLA	C3B-C4B-NB	-2.88	107.84	110.52
30	A	402	CLA	C7-C6-C5	-2.88	105.53	113.36
39	J	101	DGD	O2D-C2D-C1D	-2.88	103.04	110.05
30	c	513	CLA	CHB-C4A-NA	2.88	128.50	124.51
30	c	511	CLA	C2D-C1D-ND	-2.88	107.98	110.10
32	b	623	BCR	C11-C10-C9	-2.88	123.19	127.31
42	14	301	A86	C41-C32-C31	-2.88	107.89	110.47
42	15	311	A86	C34-O4-C38	-2.88	112.53	117.90
30	c	510	CLA	O2D-CGD-CBD	2.88	116.39	111.27
39	j	101	DGD	O2D-C2D-C1D	-2.88	103.05	110.05
30	b	610	CLA	CHB-C1B-NB	2.88	127.31	124.26
30	c	506	CLA	C2D-C1D-ND	-2.88	107.98	110.10
36	B	620	LMG	O3-C3-C2	-2.88	103.69	110.35
42	15	313	A86	C7-C6-C8	2.88	122.61	118.08
30	c	512	CLA	C2A-C1A-CHA	2.88	128.89	123.86
42	17	314	A86	C4-C5-C6	-2.88	123.20	127.31
30	C	512	CLA	C2A-C1A-CHA	2.88	128.89	123.86
42	15	313	A86	C4-C5-C6	-2.88	123.20	127.31
30	19	308	CLA	CHB-C4A-NA	2.88	128.49	124.51
30	C	520	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
30	14	304	CLA	C2A-C1A-CHA	2.88	128.89	123.86
42	17	315	A86	C3-C4-C5	-2.88	117.58	123.47
30	B	613	CLA	CHB-C4A-NA	2.88	128.49	124.51
31	A	403	PHO	C2D-C1D-ND	-2.88	107.54	109.53
42	18	314	A86	C34-O4-C38	-2.88	112.54	117.90
42	11	313	A86	C4-C5-C6	-2.88	123.21	127.31
30	18	308	CLA	CHB-C4A-NA	2.88	128.49	124.51
30	B	610	CLA	CHB-C1B-NB	2.87	127.30	124.26
30	b	622	CLA	C3B-C4B-NB	-2.87	107.85	110.52
42	14	316	A86	C41-C32-C31	-2.87	107.90	110.47
30	b	602	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	b	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	11	302	CLA	C2A-C1A-CHA	2.87	128.88	123.86
42	20	201	A86	C-C1-C2	-2.87	118.90	122.92
30	14	311	CLA	C3B-C4B-NB	-2.87	107.85	110.52
42	12	319	A86	C41-C32-C31	-2.87	107.91	110.47
32	c	520	BCR	C24-C23-C22	-2.87	121.90	126.23
30	B	623	CLA	C3B-C4B-NB	-2.87	107.86	110.52
32	Y	101	BCR	C16-C15-C14	-2.87	117.60	123.47
30	B	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	a	402	CLA	C7-C6-C5	-2.87	105.58	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	602	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
30	B	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
32	Y	101	BCR	C11-C10-C9	-2.86	123.22	127.31
42	14	315	A86	C4-C5-C6	-2.86	123.22	127.31
30	D	405	CLA	CMB-C2B-C1B	-2.86	121.01	125.37
30	14	302	CLA	CHB-C4A-NA	2.86	128.47	124.51
42	18	315	A86	C4-C5-C6	-2.86	123.23	127.31
30	19	301	CLA	C4D-C3D-CAD	-2.86	104.73	108.10
30	11	307	CLA	CHB-C1B-NB	2.86	127.28	124.26
30	14	309	CLA	C1-C2-C3	-2.86	121.10	126.04
30	13	303	CLA	C2A-C1A-CHA	2.86	128.85	123.86
30	12	314	CLA	C3B-C4B-NB	-2.85	107.87	110.52
30	19	301	CLA	C1-C2-C3	-2.85	121.11	126.04
32	c	516	BCR	C15-C14-C13	-2.85	123.24	127.31
30	18	306	CLA	CMB-C2B-C3B	2.85	133.49	126.59
30	14	307	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	14	311	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	13	307	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	16	303	CLA	CMB-C2B-C3B	2.85	133.49	126.59
39	J	101	DGD	O5D-C6D-C5D	-2.85	103.78	109.05
30	12	310	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	b	607	CLA	CHB-C4A-NA	2.84	128.44	124.51
42	20	201	A86	C33-C32-C31	2.84	111.97	109.21
30	17	307	CLA	CHB-C4A-NA	2.84	128.44	124.51
39	j	101	DGD	O5D-C6D-C5D	-2.84	103.79	109.05
32	C	515	BCR	C15-C14-C13	-2.84	123.26	127.31
30	b	611	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
42	11	310	A86	C3-C4-C5	-2.83	117.67	123.47
30	21	301	CLA	CHB-C4A-NA	2.83	128.43	124.51
42	14	312	A86	C3-C4-C5	-2.83	117.67	123.47
39	h	102	DGD	CDB-CCB-CBB	-2.83	100.05	114.42
30	b	601	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
42	18	313	A86	C3-C4-C5	-2.83	117.68	123.47
31	d	403	PHO	C2D-C1D-ND	-2.83	107.57	109.53
30	16	305	CLA	CMB-C2B-C3B	2.83	133.44	126.59
39	J	101	DGD	C3G-C2G-C1G	-2.83	105.10	111.79
30	18	305	CLA	CHB-C4A-NA	2.83	128.42	124.51
30	20	202	CLA	CHB-C4A-NA	2.82	128.42	124.51
42	21	314	A86	C25-C26-C27	-2.82	123.28	127.31
30	15	307	CLA	C2A-C1A-CHA	2.82	128.80	123.86
42	19	312	A86	C40-C32-C31	-2.82	107.95	110.47
30	12	306	CLA	C2A-C1A-CHA	2.82	128.79	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	607	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	11	306	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
42	13	311	A86	C3-C4-C5	-2.82	117.70	123.47
30	C	510	CLA	CHB-C4A-NA	2.82	128.41	124.51
39	H	102	DGD	CDB-CCB-CBB	-2.82	100.11	114.42
30	B	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	13	310	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	12	314	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	C	511	CLA	CHB-C1B-NB	2.81	127.24	124.26
30	c	507	CLA	CHB-C1B-NB	2.81	127.24	124.26
30	16	305	CLA	CHB-C1B-NB	2.81	127.24	124.26
42	12	315	A86	C3-C4-C5	-2.81	117.71	123.47
30	c	509	CLA	CHB-C4A-NA	2.81	128.40	124.51
42	15	310	A86	C3-C4-C5	-2.81	117.72	123.47
32	a	408	BCR	C15-C16-C17	-2.81	117.72	123.47
32	c	520	BCR	C11-C10-C9	-2.81	123.30	127.31
31	A	403	PHO	CMB-C2B-C3B	2.81	129.93	124.68
30	C	511	CLA	C2D-C1D-ND	-2.81	108.03	110.10
42	12	318	A86	C4-C5-C6	-2.81	123.31	127.31
42	21	313	A86	C8-C6-C5	-2.81	114.64	118.94
42	20	213	A86	C25-C26-C27	-2.81	123.31	127.31
30	20	204	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
40	D	407	PL9	C40-C39-C41	2.80	119.99	115.27
30	21	303	CLA	C3B-C4B-NB	-2.80	107.91	110.52
42	20	212	A86	C3-C4-C5	-2.80	117.73	123.47
30	B	601	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
40	D	404	PL9	C40-C39-C41	2.80	119.99	115.27
30	c	511	CLA	CHB-C1B-NB	2.80	127.22	124.26
30	B	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	B	602	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	C	509	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	21	308	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	c	509	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	11	315	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
42	21	312	A86	C26-C25-C24	-2.80	114.48	123.22
40	d	408	PL9	C40-C39-C41	2.80	119.98	115.27
30	B	603	CLA	O2D-CGD-CBD	2.80	116.24	111.27
30	11	309	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	12	312	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
30	12	303	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
30	21	303	CLA	CHB-C4A-NA	2.79	128.38	124.51
30	C	503	CLA	CHB-C4A-NA	2.79	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	18	301	CLA	CHB-C4A-NA	2.79	128.38	124.51
32	B	616	BCR	C7-C8-C9	-2.79	122.01	126.23
32	m	103	BCR	C7-C8-C9	-2.79	122.01	126.23
36	c	519	LMG	O6-C1-O1	-2.79	103.36	109.97
30	d	406	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
30	21	301	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	b	606	CLA	C1-C2-C3	-2.79	121.22	126.04
31	d	403	PHO	CMB-C2B-C3B	2.79	129.90	124.68
30	b	622	CLA	CMD-C2D-C1D	-2.79	119.80	124.71
30	21	309	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
42	19	311	A86	C33-C32-C31	2.79	111.92	109.21
36	Q	301	LMG	O6-C1-O1	-2.78	103.38	109.97
30	c	506	CLA	CHB-C1B-NB	2.78	127.20	124.26
30	14	302	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
42	16	310	A86	C40-C32-C31	-2.78	107.98	110.47
32	A	409	BCR	C15-C16-C17	-2.78	117.77	123.47
30	18	311	CLA	CAA-C2A-C1A	2.78	121.09	111.97
40	d	405	PL9	C40-C39-C41	2.78	119.95	115.27
30	16	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
42	17	315	A86	C41-C32-C31	-2.78	107.98	110.47
30	b	610	CLA	CHB-C4A-NA	2.78	128.35	124.51
30	20	209	CLA	C3B-C4B-NB	-2.78	107.94	110.52
42	20	211	A86	C20-C19-C18	-2.78	107.26	112.75
39	J	101	DGD	CDB-CCB-CBB	-2.78	100.33	114.42
42	20	213	A86	C12-C11-C13	2.78	120.68	116.02
30	B	607	CLA	CHB-C1B-NB	2.77	127.19	124.26
30	14	308	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
42	20	211	A86	C10-C9-C8	-2.77	114.56	123.22
42	19	311	A86	C19-C18-C17	2.77	116.13	110.77
39	j	101	DGD	C3G-C2G-C1G	-2.77	105.23	111.79
30	b	603	CLA	O2D-CGD-CBD	2.77	116.19	111.27
42	21	311	A86	C20-C19-C18	-2.77	107.27	112.75
42	17	302	A86	C7-C6-C5	-2.77	119.04	122.92
33	a	405	SQD	C1-O5-C5	2.77	119.13	113.69
30	17	305	CLA	CHB-C4A-NA	2.77	128.34	124.51
30	15	309	CLA	C3B-C4B-NB	-2.77	107.95	110.52
30	19	307	CLA	C3B-C4B-NB	-2.77	107.95	110.52
30	15	308	CLA	CAA-C2A-C1A	2.77	121.05	111.97
32	b	616	BCR	C11-C10-C9	-2.77	123.36	127.31
30	b	602	CLA	CHB-C4A-NA	2.77	128.34	124.51
33	A	406	SQD	C1-O5-C5	2.77	119.12	113.69
39	j	101	DGD	CDB-CCB-CBB	-2.77	100.38	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	303	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	d	402	CLA	O2D-CGD-CBD	2.76	116.18	111.27
30	21	307	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
30	16	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
42	21	311	A86	C10-C9-C8	-2.76	114.59	123.22
30	B	615	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
42	21	314	A86	C12-C11-C13	2.76	120.66	116.02
30	b	615	CLA	C3B-C4B-NB	-2.76	107.95	110.52
30	11	304	CLA	C3A-C2A-C1A	2.76	105.47	101.34
30	B	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	C	506	CLA	CHB-C1B-NB	2.76	127.18	124.26
30	17	304	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
30	b	605	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
30	b	603	CLA	CHB-C4A-NA	2.75	128.32	124.51
30	c	502	CLA	CHB-C4A-NA	2.75	128.32	124.51
39	C	516	DGD	C3G-C2G-C1G	-2.75	105.28	111.79
30	11	303	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
30	B	606	CLA	CHB-C4A-NA	2.75	128.32	124.51
30	C	502	CLA	CHB-C4A-NA	2.75	128.32	124.51
30	b	615	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	12	307	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	B	603	CLA	CHB-C4A-NA	2.75	128.32	124.51
30	18	312	CLA	C3B-C4B-NB	-2.75	107.96	110.52
42	20	201	A86	C4-C3-C2	-2.75	117.85	123.47
30	19	307	CLA	CHB-C4A-NA	2.75	128.31	124.51
30	C	502	CLA	CMB-C2B-C1B	-2.75	121.19	125.37
30	B	609	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	13	304	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	D	402	CLA	O2D-CGD-CBD	2.75	116.15	111.27
30	14	305	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
30	C	509	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
30	17	306	CLA	C3B-C4B-NB	-2.74	107.97	110.52
30	12	303	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
42	19	311	A86	C-C1-C2	-2.74	119.09	122.92
30	17	308	CLA	C2D-C1D-ND	-2.74	108.09	110.10
30	W	102	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	21	302	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	19	303	CLA	CAA-CBA-CGA	2.74	121.25	113.25
30	C	520	CLA	CHB-C1B-NB	2.74	127.15	124.26
30	c	502	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
30	b	609	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
30	a	402	CLA	CMB-C2B-C1B	-2.73	121.20	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	21	303	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
30	18	304	CLA	CHC-C4B-NB	2.73	127.15	124.26
30	11	309	CLA	C3B-C4B-NB	-2.73	107.98	110.52
42	21	313	A86	C26-C25-C24	-2.73	114.69	123.22
30	17	306	CLA	C2D-C1D-ND	-2.73	108.09	110.10
30	16	304	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	17	301	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	15	305	CLA	C3B-C4B-NB	-2.73	107.98	110.52
42	16	310	A86	C12-C11-C13	2.73	120.61	116.02
30	C	514	CLA	CMB-C2B-C3B	2.73	133.20	126.59
30	Z	102	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	16	301	CLA	C3B-C4B-NB	-2.73	107.98	110.52
30	18	306	CLA	CHB-C4A-NA	2.73	128.28	124.51
32	B	617	BCR	C11-C10-C9	-2.73	123.42	127.31
30	c	514	CLA	CMB-C2B-C3B	2.73	133.19	126.59
30	b	607	CLA	CHB-C1B-NB	2.73	127.14	124.26
39	c	517	DGD	C3G-C2G-C1G	-2.72	105.34	111.79
30	18	307	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
32	C	515	BCR	C28-C27-C26	-2.72	109.21	114.08
30	b	606	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	18	309	CLA	C2A-C1A-CHA	2.72	128.62	123.86
30	20	205	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
36	b	618	LMG	C1-C2-C3	-2.72	104.33	110.00
30	19	302	CLA	CMB-C2B-C3B	2.72	133.18	126.59
30	z	101	CLA	CHB-C4A-NA	2.72	128.27	124.51
30	14	307	CLA	C3B-C4B-NB	-2.72	107.99	110.52
30	17	308	CLA	C3B-C4B-NB	-2.72	107.99	110.52
30	15	307	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
36	B	619	LMG	C1-C2-C3	-2.72	104.33	110.00
30	c	507	CLA	C2A-C1A-CHA	2.72	128.61	123.86
42	21	310	A86	C41-C32-C31	-2.72	108.04	110.47
41	f	102	HEM	CMB-C2B-C1B	-2.72	120.90	125.04
30	20	209	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	20	206	CLA	C2A-C1A-CHA	2.71	128.61	123.86
30	B	606	CLA	C1-C2-C3	-2.71	121.35	126.04
30	18	307	CLA	C3B-C4B-NB	-2.71	108.00	110.52
30	C	507	CLA	C2A-C1A-CHA	2.71	128.60	123.86
30	w	102	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	B	615	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	C	520	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	c	504	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	19	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	j	101	DGD	O3G-C1D-C2D	-2.70	104.09	108.30
30	21	307	CLA	C3B-C4B-NB	-2.70	108.01	110.52
30	A	402	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
30	c	508	CLA	O1D-CGD-CBD	2.70	130.01	124.48
30	13	305	CLA	C3A-C2A-C1A	2.70	105.38	101.34
30	c	503	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	21	306	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	d	402	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
36	1	101	LMG	O3-C3-C2	-2.70	104.12	110.35
30	16	303	CLA	CAA-C2A-C1A	2.70	120.81	111.97
30	C	506	CLA	CHB-C4A-NA	2.69	128.24	124.51
30	18	307	CLA	CHB-C4A-NA	2.69	128.24	124.51
42	14	314	A86	C3-C4-C5	-2.69	117.95	123.47
30	C	519	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	D	402	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
42	19	310	A86	C3-C4-C5	-2.69	117.96	123.47
30	c	506	CLA	CHB-C4A-NA	2.69	128.24	124.51
32	c	516	BCR	C28-C27-C26	-2.69	109.27	114.08
30	B	604	CLA	C2D-C1D-ND	-2.69	108.12	110.10
36	12	301	LMG	O3-C3-C2	-2.69	104.13	110.35
30	19	307	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	19	302	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	14	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
42	16	312	A86	C3-C4-C5	-2.69	117.96	123.47
36	d	410	LMG	O1-C7-C8	-2.69	104.41	110.90
39	J	101	DGD	O3G-C1D-C2D	-2.69	104.11	108.30
30	C	504	CLA	CAA-CBA-CGA	-2.69	105.40	113.25
30	18	312	CLA	CHB-C4A-NA	2.69	128.23	124.51
30	20	205	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	C	504	CLA	CHB-C4A-NA	2.69	128.23	124.51
30	21	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
30	c	504	CLA	CAA-CBA-CGA	-2.68	105.41	113.25
30	C	502	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
30	b	604	CLA	C1-C2-C3	-2.68	121.40	126.04
30	17	306	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
30	C	508	CLA	O1D-CGD-CBD	2.68	129.97	124.48
30	m	101	CLA	C3B-C4B-NB	-2.68	108.03	110.52
40	D	407	PL9	C22-C23-C24	-2.68	121.20	127.66
30	C	510	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
32	B	616	BCR	C11-C10-C9	-2.68	123.48	127.31
42	17	313	A86	C20-C19-C18	-2.68	107.45	112.75
30	c	502	CLA	CAA-C2A-C3A	-2.68	105.44	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	m	103	BCR	C11-C10-C9	-2.68	123.49	127.31
30	18	304	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
30	B	606	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
30	15	309	CLA	CHB-C4A-NA	2.67	128.21	124.51
42	12	317	A86	C3-C4-C5	-2.67	118.00	123.47
30	12	308	CLA	C3A-C2A-C1A	2.67	105.34	101.34
30	20	209	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
40	d	408	PL9	C22-C23-C24	-2.67	121.23	127.66
30	b	606	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
42	15	312	A86	C3-C4-C5	-2.67	118.00	123.47
36	D	408	LMG	O1-C7-C8	-2.67	104.46	110.90
30	13	306	CLA	C3B-C4B-NB	-2.67	108.04	110.52
30	c	510	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
30	16	302	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
42	14	315	A86	C8-C6-C5	-2.67	114.85	118.94
30	20	209	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	B	604	CLA	C1-C2-C3	-2.67	121.43	126.04
42	21	310	A86	C10-C9-C8	-2.67	114.90	123.22
32	c	521	BCR	C11-C10-C9	-2.66	123.51	127.31
30	11	305	CLA	C3B-C4B-NB	-2.66	108.04	110.52
42	11	312	A86	C20-C19-C18	-2.66	107.48	112.75
30	20	205	CLA	CHC-C4B-NB	2.66	127.08	124.26
42	13	313	A86	C3-C4-C5	-2.66	118.02	123.47
32	c	521	BCR	C27-C26-C25	2.66	126.60	122.73
30	21	309	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	d	401	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	20	203	CLA	CHB-C4A-NA	2.66	128.19	124.51
42	11	312	A86	C3-C4-C5	-2.66	118.02	123.47
42	17	313	A86	C3-C4-C5	-2.66	118.02	123.47
30	z	101	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	B	623	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	18	309	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	D	401	CLA	CHB-C4A-NA	2.66	128.19	124.51
42	15	312	A86	C20-C19-C18	-2.66	107.49	112.75
30	14	302	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
42	16	312	A86	C20-C19-C18	-2.66	107.49	112.75
30	b	604	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
30	C	514	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	b	613	CLA	C3B-C4B-NB	-2.66	108.05	110.52
30	20	204	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	c	517	DGD	C1E-O6E-C5E	2.65	118.90	113.69
30	b	622	CLA	O2D-CGD-O1D	-2.65	118.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	309	CLA	C3B-C4B-NB	-2.65	108.05	110.52
30	21	302	CLA	C3B-C4B-NB	-2.65	108.05	110.52
30	b	622	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	16	308	CLA	O2A-CGA-O1A	-2.65	116.69	123.30
30	16	302	CLA	C3B-C4B-NB	-2.65	108.06	110.52
32	B	616	BCR	C24-C23-C22	-2.65	122.23	126.23
30	16	305	CLA	CHC-C4B-NB	2.65	127.06	124.26
30	b	614	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
30	19	303	CLA	C1-O2A-CGA	2.65	123.39	116.44
39	H	102	DGD	O6D-C1D-O3G	-2.65	103.71	109.97
30	11	315	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
30	18	310	CLA	CHC-C4B-NB	2.65	127.06	124.26
30	21	309	CLA	CAA-C2A-C1A	-2.65	103.31	111.97
30	C	519	CLA	CHB-C4A-NA	2.64	128.17	124.51
42	18	315	A86	C8-C6-C5	-2.64	114.88	118.94
30	14	306	CLA	C3A-C2A-C1A	2.64	105.30	101.34
30	17	309	CLA	O2A-CGA-O1A	-2.64	116.72	123.30
39	C	517	DGD	CBB-CAB-C9B	-2.64	101.02	114.42
30	19	308	CLA	CMB-C2B-C1B	-2.64	121.35	125.37
42	11	313	A86	C8-C6-C5	-2.64	114.89	118.94
30	B	610	CLA	O2D-CGD-CBD	2.64	115.96	111.27
30	M	101	CLA	C3B-C4B-NB	-2.64	108.07	110.52
30	z	101	CLA	CHC-C4B-NB	2.64	127.05	124.26
30	c	514	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
42	17	314	A86	C8-C6-C5	-2.64	114.89	118.94
41	F	102	HEM	CMB-C2B-C1B	-2.64	121.02	125.04
30	B	614	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
30	W	102	CLA	C3B-C4B-NB	-2.64	108.07	110.52
30	b	606	CLA	CAA-CBA-CGA	-2.64	105.55	113.25
30	11	304	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	21	308	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
42	19	311	A86	O-C13-C14	-2.63	116.31	121.66
30	12	312	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
42	14	314	A86	C20-C19-C18	-2.63	107.54	112.75
42	13	313	A86	C20-C19-C18	-2.63	107.54	112.75
30	20	202	CLA	C3B-C4B-NB	-2.63	108.07	110.52
32	C	518	BCR	C11-C10-C9	-2.63	123.55	127.31
30	14	311	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	d	406	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
42	20	210	A86	C17-C16-C15	2.63	111.85	109.16
30	c	512	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
31	A	403	PHO	O2D-CGD-O1D	-2.63	118.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	317	A86	C20-C19-C18	-2.63	107.54	112.75
30	12	308	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	13	310	CLA	CHB-C4A-NA	2.63	128.15	124.51
42	13	314	A86	C8-C6-C5	-2.63	114.90	118.94
35	L	102	LHG	C20-C19-C18	-2.63	101.08	114.42
30	15	307	CLA	C1-C2-C3	-2.63	121.50	126.04
30	17	307	CLA	C2D-C1D-ND	-2.63	108.17	110.10
30	17	301	CLA	CHC-C4B-NB	2.63	127.04	124.26
39	h	102	DGD	O6D-C1D-O3G	-2.63	103.75	109.97
39	h	102	DGD	C3G-C2G-C1G	-2.63	105.58	111.79
42	15	313	A86	C8-C6-C5	-2.62	114.91	118.94
35	l	102	LHG	C20-C19-C18	-2.62	101.10	114.42
30	17	310	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	b	610	CLA	O2D-CGD-CBD	2.62	115.93	111.27
36	Q	301	LMG	O2-C2-C1	-2.62	103.68	110.05
31	d	403	PHO	O2D-CGD-O1D	-2.62	118.71	123.84
30	17	306	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
39	c	518	DGD	O2D-C2D-C1D	-2.62	103.68	110.05
30	15	305	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
40	D	407	PL9	C31-C32-C33	-2.62	103.28	111.88
30	B	612	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
30	14	306	CLA	O2D-CGD-CBD	2.62	115.92	111.27
30	B	604	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
30	D	405	CLA	CAA-CBA-CGA	-2.62	105.60	113.25
30	21	305	CLA	CBB-CAB-C3B	-2.62	114.60	127.62
30	b	604	CLA	C2D-C1D-ND	-2.62	108.17	110.10
30	21	306	CLA	C3B-C4B-NB	-2.62	108.09	110.52
32	Y	101	BCR	C28-C27-C26	-2.62	109.41	114.08
30	M	101	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	21	302	CLA	C2A-C1A-CHA	2.62	128.43	123.86
39	c	518	DGD	CBB-CAB-C9B	-2.62	101.15	114.42
30	B	606	CLA	CAA-CBA-CGA	-2.61	105.61	113.25
30	C	504	CLA	C3B-C4B-NB	-2.61	108.09	110.52
39	C	516	DGD	C1E-O6E-C5E	2.61	118.82	113.69
30	C	520	CLA	O2D-CGD-CBD	2.61	115.91	111.27
42	16	310	A86	C3-C4-C5	-2.61	118.12	123.47
30	w	102	CLA	C3B-C4B-NB	-2.61	108.09	110.52
30	17	305	CLA	C3B-C4B-NB	-2.61	108.09	110.52
39	C	517	DGD	O2D-C2D-C1D	-2.61	103.70	110.05
30	B	623	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
32	B	618	BCR	C3-C4-C5	-2.61	109.42	114.08
32	m	103	BCR	C24-C23-C22	-2.61	122.29	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	519	CLA	CHC-C4B-NB	2.61	127.02	124.26
32	c	520	BCR	C34-C9-C10	-2.61	119.27	122.92
36	w	101	LMG	C1-C2-C3	-2.61	104.57	110.00
30	19	301	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
42	17	311	A86	C40-C32-C31	-2.61	108.14	110.47
42	17	302	A86	C34-O4-C38	-2.61	113.04	117.90
30	15	304	CLA	CMB-C2B-C3B	2.61	132.90	126.59
30	19	303	CLA	C3B-C4B-NB	-2.61	108.10	110.52
40	D	404	PL9	C7-C8-C9	-2.61	122.45	126.79
30	b	612	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
30	16	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	H	102	DGD	C3G-C2G-C1G	-2.60	105.64	111.79
30	21	308	CLA	C3B-C4B-NB	-2.60	108.11	110.52
36	c	519	LMG	O2-C2-C1	-2.60	103.74	110.05
42	12	319	A86	C7-C6-C8	2.60	122.17	118.08
40	d	408	PL9	C31-C32-C33	-2.60	103.35	111.88
36	w	101	LMG	O3-C3-C2	-2.60	104.35	110.35
32	c	520	BCR	C28-C27-C26	-2.60	109.44	114.08
30	16	308	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	13	305	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	m	101	CLA	CHB-C4A-NA	2.59	128.10	124.51
42	11	314	A86	C7-C6-C8	2.59	122.16	118.08
30	17	303	CLA	CHC-C4B-NB	2.59	127.00	124.26
30	c	504	CLA	C2A-C1A-CHA	2.59	128.39	123.86
30	15	304	CLA	CHB-C4A-NA	2.59	128.10	124.51
42	14	301	A86	C7-C6-C8	2.59	122.16	118.08
36	M	102	LMG	O3-C3-C2	-2.59	104.36	110.35
30	17	301	CLA	CMA-C3A-C2A	-2.59	103.38	113.83
30	W	103	CLA	C3B-C4B-NB	-2.59	108.11	110.52
36	m	102	LMG	O3-C3-C2	-2.59	104.36	110.35
30	C	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
30	16	304	CLA	C3B-C4B-NB	-2.59	108.12	110.52
42	20	201	A86	C34-O4-C38	-2.59	113.08	117.90
30	18	310	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
30	18	308	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
30	B	613	CLA	C3B-C4B-NB	-2.58	108.12	110.52
30	C	509	CLA	O2D-CGD-CBD	2.58	115.86	111.27
32	C	518	BCR	C27-C26-C25	2.58	126.48	122.73
36	W	101	LMG	O3-C3-C2	-2.58	104.38	110.35
42	12	318	A86	C8-C6-C5	-2.58	114.98	118.94
30	17	309	CLA	C2A-C3A-C4A	-2.58	97.70	101.87
30	Z	102	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	617	BCR	C3-C4-C5	-2.58	109.47	114.08
30	b	622	CLA	CMD-C2D-C3D	2.58	133.54	127.61
40	d	405	PL9	C7-C8-C9	-2.58	122.50	126.79
30	12	314	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	B	604	CLA	CAA-CBA-CGA	-2.58	105.72	113.25
42	14	316	A86	C7-C6-C8	2.58	122.14	118.08
30	C	510	CLA	CHC-C4B-NB	2.58	126.98	124.26
30	c	508	CLA	CMB-C2B-C1B	-2.58	121.45	125.37
35	l	102	LHG	O8-C23-C24	2.58	119.99	111.91
42	15	314	A86	C7-C6-C8	2.57	122.13	118.08
30	c	504	CLA	CHB-C4A-NA	2.57	128.07	124.51
35	L	102	LHG	O8-C23-C24	2.57	119.98	111.91
32	B	617	BCR	C27-C26-C25	2.57	126.46	122.73
30	c	510	CLA	C3B-C4B-NB	-2.57	108.13	110.52
30	B	606	CLA	CHD-C1D-ND	-2.57	122.09	124.45
42	17	311	A86	O1-C15-C14	2.57	118.36	113.21
30	b	604	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
32	Y	101	BCR	C34-C9-C10	-2.57	119.33	122.92
32	b	616	BCR	C27-C26-C25	2.57	126.46	122.73
30	C	504	CLA	C2A-C1A-CHA	2.57	128.34	123.86
30	B	610	CLA	CAA-C2A-C3A	-2.56	105.75	112.78
30	18	303	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
42	16	310	A86	C34-O4-C38	-2.56	113.12	117.90
30	c	508	CLA	CHC-C4B-NB	2.56	126.97	124.26
30	b	604	CLA	C2A-C1A-CHA	2.56	128.34	123.86
32	B	617	BCR	C40-C30-C25	2.56	114.45	110.30
30	D	402	CLA	CHB-C1B-NB	2.56	126.97	124.26
36	W	101	LMG	C1-C2-C3	-2.56	104.66	110.00
36	W	101	LMG	C38-C37-C36	-2.56	101.43	114.42
30	c	509	CLA	O2D-CGD-CBD	2.56	115.81	111.27
30	c	509	CLA	C3B-C4B-NB	-2.56	108.14	110.52
41	v	201	HEM	C4A-CHB-C1B	-2.56	120.27	126.34
36	w	101	LMG	C38-C37-C36	-2.56	101.44	114.42
30	B	611	CLA	C3B-C4B-NB	-2.56	108.14	110.52
30	11	301	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
30	C	506	CLA	O2D-CGD-CBD	2.56	115.81	111.27
42	19	311	A86	O-C13-C11	-2.55	115.51	121.15
42	16	313	A86	C7-C6-C8	2.55	122.10	118.08
30	b	610	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
42	19	310	A86	C12-C11-C13	2.55	120.31	116.02
42	17	302	A86	C26-C25-C24	-2.55	115.26	123.22
42	16	310	A86	C4-C3-C2	-2.55	118.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	17	302	A86	C4-C3-C2	-2.55	118.25	123.47
30	11	309	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	B	624	BCR	C15-C14-C13	-2.55	123.67	127.31
30	c	511	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	C	510	CLA	C3B-C4B-NB	-2.55	108.15	110.52
30	b	611	CLA	C3B-C4B-NB	-2.55	108.15	110.52
32	b	623	BCR	C15-C14-C13	-2.55	123.67	127.31
30	11	304	CLA	O2D-CGD-CBD	2.55	115.80	111.27
37	B	625	LMU	O5B-C1B-C2B	2.55	115.74	110.35
30	d	401	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	20	203	CLA	CHB-C1B-NB	2.54	126.95	124.26
30	W	103	CLA	CHB-C1B-NB	2.54	126.95	124.26
30	B	604	CLA	C2A-C1A-CHA	2.54	128.31	123.86
30	C	508	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
30	12	305	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
32	a	408	BCR	C15-C14-C13	-2.54	123.68	127.31
30	11	303	CLA	C3B-C4B-NB	-2.54	108.16	110.52
41	V	201	HEM	C4A-CHB-C1B	-2.54	120.31	126.34
30	21	309	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
39	c	518	DGD	O6D-C5D-C6D	-2.54	101.53	106.67
30	C	509	CLA	C3B-C4B-NB	-2.54	108.16	110.52
30	d	402	CLA	CHB-C1B-NB	2.54	126.95	124.26
30	13	306	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	C	508	CLA	CHC-C4B-NB	2.54	126.94	124.26
40	d	408	PL9	C7-C3-C4	2.54	118.94	116.88
42	11	310	A86	C25-C24-C1	-2.54	119.29	126.42
30	14	302	CLA	C3B-C4B-NB	-2.54	108.16	110.52
42	17	316	A86	C7-C6-C8	2.54	122.07	118.08
30	B	615	CLA	CHB-C4A-NA	2.53	128.02	124.51
30	14	309	CLA	CMB-C2B-C1B	-2.53	121.51	125.37
32	F	101	BCR	C11-C10-C9	-2.53	123.69	127.31
30	13	308	CLA	C2A-C1A-CHA	2.53	128.29	123.86
30	D	401	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	11	305	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
32	f	101	BCR	C11-C10-C9	-2.53	123.70	127.31
30	21	306	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	d	407	CLA	O2D-CGD-CBD	2.53	115.76	111.27
30	D	406	CLA	O2D-CGD-CBD	2.53	115.76	111.27
30	C	520	CLA	C2A-C1A-CHA	2.53	128.28	123.86
30	d	406	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	c	503	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
30	13	302	CLA	O2D-CGD-O1D	-2.53	118.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	622	LHG	C11-C10-C9	-2.53	101.59	114.42
30	11	315	CLA	C3B-C4B-NB	-2.53	108.17	110.52
35	L	101	LHG	C20-C19-C18	-2.53	101.59	114.42
30	14	303	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
32	B	616	BCR	C15-C14-C13	-2.53	123.70	127.31
33	a	405	SQD	O7-S-C6	2.53	109.94	106.94
30	w	103	CLA	CHB-C4A-NA	2.53	128.00	124.51
39	C	517	DGD	O6D-C5D-C6D	-2.52	101.57	106.67
35	d	409	LHG	C20-C19-C18	-2.52	101.61	114.42
32	b	616	BCR	C15-C16-C17	-2.52	118.31	123.47
42	13	301	A86	C41-C32-C31	-2.52	108.21	110.47
42	13	311	A86	C25-C24-C1	-2.52	119.33	126.42
30	c	510	CLA	CHC-C4B-NB	2.52	126.93	124.26
30	C	503	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
42	13	311	A86	C7-C6-C8	2.52	122.05	118.08
30	12	311	CLA	C2A-C1A-CHA	2.52	128.27	123.86
32	f	101	BCR	C7-C8-C9	-2.52	122.42	126.23
36	M	102	LMG	O2-C2-C1	-2.52	103.92	110.05
40	D	407	PL9	C7-C3-C4	2.52	118.92	116.88
30	17	305	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
32	c	516	BCR	C29-C30-C25	2.52	114.36	110.48
30	12	307	CLA	C3B-C4B-NB	-2.52	108.18	110.52
42	14	301	A86	C3-C4-C5	-2.52	118.31	123.47
30	b	605	CLA	CHB-C1B-NB	2.52	126.92	124.26
42	15	310	A86	C25-C24-C1	-2.52	119.34	126.42
36	m	102	LMG	O2-C2-C1	-2.52	103.93	110.05
30	12	309	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
42	21	313	A86	O1-C15-C14	-2.52	108.16	113.21
32	B	617	BCR	C15-C16-C17	-2.52	118.32	123.47
30	12	308	CLA	O2D-CGD-CBD	2.52	115.74	111.27
30	12	312	CLA	C3B-C4B-NB	-2.52	108.18	110.52
30	14	307	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
30	C	511	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	20	208	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	20	207	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
30	19	301	CLA	C3B-C4B-NB	-2.51	108.18	110.52
32	A	409	BCR	C15-C14-C13	-2.51	123.72	127.31
32	m	103	BCR	C15-C14-C13	-2.51	123.72	127.31
31	D	403	PHO	C2D-C1D-ND	-2.51	107.79	109.53
35	A	408	LHG	C20-C19-C18	-2.51	101.66	114.42
30	19	303	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
35	b	621	LHG	C11-C10-C9	-2.51	101.67	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	616	BCR	C40-C30-C25	2.51	114.38	110.30
36	w	101	LMG	O1-C1-C2	-2.51	104.38	108.30
42	18	313	A86	C7-C6-C8	2.51	122.03	118.08
30	15	301	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
42	11	314	A86	C3-C4-C5	-2.51	118.33	123.47
30	16	308	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
42	15	314	A86	C3-C4-C5	-2.51	118.33	123.47
30	B	607	CLA	CMB-C2B-C3B	2.51	132.67	126.59
30	18	303	CLA	CHC-C4B-NB	2.51	126.91	124.26
42	12	304	A86	C41-C32-C31	-2.51	108.23	110.47
30	15	303	CLA	C3B-C4B-NB	-2.51	108.19	110.52
30	b	615	CLA	CHB-C4A-NA	2.51	127.98	124.51
42	14	313	A86	C20-C19-C18	-2.51	107.79	112.75
35	a	407	LHG	C20-C19-C18	-2.51	101.69	114.42
39	J	101	DGD	O3D-C3D-C4D	-2.51	104.55	110.35
42	11	316	A86	C41-C32-C31	-2.51	108.23	110.47
42	14	316	A86	C3-C4-C5	-2.51	118.34	123.47
42	17	312	A86	C20-C19-C18	-2.51	107.79	112.75
30	B	604	CLA	CHC-C4B-NB	2.51	126.91	124.26
42	17	316	A86	C3-C4-C5	-2.51	118.34	123.47
30	13	305	CLA	O2D-CGD-CBD	2.51	115.72	111.27
32	H	101	BCR	C37-C22-C21	-2.51	119.41	122.92
42	18	315	A86	C40-C32-C31	-2.51	108.23	110.47
30	b	612	CLA	CMB-C2B-C3B	2.50	132.66	126.59
42	14	312	A86	C25-C24-C1	-2.50	119.38	126.42
36	W	101	LMG	O1-C1-C2	-2.50	104.39	108.30
30	20	202	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
30	18	303	CLA	CHB-C1B-NB	2.50	126.91	124.26
39	j	101	DGD	O3D-C3D-C4D	-2.50	104.56	110.35
30	C	507	CLA	C3B-C4B-NB	-2.50	108.19	110.52
30	13	308	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
32	F	101	BCR	C7-C8-C9	-2.50	122.45	126.23
42	19	311	A86	C9-C10-C11	-2.50	119.25	126.61
30	17	305	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
30	11	307	CLA	C2A-C1A-CHA	2.50	128.23	123.86
30	14	309	CLA	C2A-C1A-CHA	2.50	128.23	123.86
42	12	316	A86	C20-C19-C18	-2.50	107.80	112.75
30	c	507	CLA	C3B-C4B-NB	-2.50	108.19	110.52
42	12	315	A86	C25-C24-C1	-2.50	119.39	126.42
36	D	408	LMG	O6-C1-O1	-2.50	104.05	109.97
30	W	103	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	c	503	CLA	C2A-C1A-CHA	2.50	128.23	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	307	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
42	13	314	A86	C40-C32-C31	-2.50	108.24	110.47
42	18	313	A86	C25-C24-C1	-2.50	119.40	126.42
30	b	607	CLA	CMB-C2B-C3B	2.50	132.64	126.59
30	c	506	CLA	O2D-CGD-CBD	2.50	115.70	111.27
42	16	313	A86	C3-C4-C5	-2.50	118.36	123.47
32	C	515	BCR	C29-C30-C25	2.50	114.32	110.48
30	12	311	CLA	CMB-C2B-C1B	-2.50	121.57	125.37
42	13	312	A86	C20-C19-C18	-2.49	107.81	112.75
42	16	310	A86	C10-C9-C8	-2.49	115.43	123.22
30	w	103	CLA	C3B-C4B-NB	-2.49	108.20	110.52
42	15	313	A86	C40-C32-C31	-2.49	108.24	110.47
30	19	301	CLA	CHB-C4A-NA	2.49	127.96	124.51
42	15	311	A86	C20-C19-C18	-2.49	107.82	112.75
30	18	310	CLA	C3B-C4B-NB	-2.49	108.20	110.52
42	14	312	A86	C7-C6-C8	2.49	122.00	118.08
42	12	318	A86	C40-C32-C31	-2.49	108.24	110.47
30	19	306	CLA	CHC-C4B-NB	2.49	126.90	124.26
42	15	311	A86	C25-C24-C1	-2.49	119.41	126.42
42	14	315	A86	C40-C32-C31	-2.49	108.24	110.47
42	11	311	A86	C25-C24-C1	-2.49	119.42	126.42
30	17	301	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
30	19	309	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
39	C	516	DGD	O3D-C3D-C4D	-2.49	104.59	110.35
30	c	513	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
36	d	410	LMG	O6-C1-O1	-2.49	104.08	109.97
36	b	618	LMG	O6-C1-O1	-2.49	104.08	109.97
30	b	604	CLA	CHC-C4B-NB	2.49	126.89	124.26
30	17	301	CLA	C3B-C4B-NB	-2.49	108.21	110.52
30	C	513	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
30	b	608	CLA	CHB-C1B-NB	2.49	126.89	124.26
30	12	303	CLA	C3B-C4B-NB	-2.49	108.21	110.52
30	20	203	CLA	CHC-C4B-NB	2.49	126.89	124.26
30	21	304	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
42	15	316	A86	C12-C11-C13	2.48	120.19	116.02
42	17	311	A86	C4-C3-C2	-2.48	118.39	123.47
30	12	308	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
42	21	313	A86	C4-C5-C6	-2.48	123.77	127.31
30	B	612	CLA	CMB-C2B-C3B	2.48	132.60	126.59
30	c	510	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
30	16	304	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
30	20	203	CLA	O2D-CGD-O1D	-2.48	118.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	310	A86	C7-C6-C8	2.48	121.99	118.08
30	15	301	CLA	CHC-C4B-NB	2.48	126.88	124.26
42	18	314	A86	C20-C19-C18	-2.48	107.84	112.75
31	D	403	PHO	O2D-CGD-O1D	-2.48	118.99	123.84
30	B	606	CLA	CHC-C1C-NC	2.48	127.97	124.20
30	11	302	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	13	303	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	20	207	CLA	C3B-C4B-NB	-2.48	108.22	110.52
42	12	319	A86	C3-C4-C5	-2.48	118.40	123.47
42	16	311	A86	C20-C19-C18	-2.48	107.84	112.75
42	21	313	A86	C20-C19-C18	-2.48	107.84	112.75
30	D	406	CLA	CHC-C4B-NB	2.48	126.88	124.26
30	16	302	CLA	C1-C2-C3	-2.48	121.76	126.04
30	b	604	CLA	C3C-C4C-NC	-2.48	107.79	110.57
30	b	606	CLA	CHD-C1D-ND	-2.48	122.18	124.45
42	16	311	A86	C25-C24-C1	-2.48	119.46	126.42
42	14	313	A86	C25-C24-C1	-2.48	119.46	126.42
36	Q	301	LMG	C9-C8-C7	-2.48	105.93	111.79
30	13	304	CLA	C3B-C4B-NB	-2.48	108.22	110.52
32	B	616	BCR	C27-C26-C25	2.48	126.33	122.73
30	B	608	CLA	CHB-C1B-NB	2.48	126.88	124.26
32	c	515	BCR	C7-C8-C9	-2.48	122.49	126.23
30	C	510	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
42	11	311	A86	C20-C19-C18	-2.48	107.85	112.75
42	20	201	A86	O1-C15-C14	2.48	118.18	113.21
30	18	312	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
31	A	403	PHO	CAA-CBA-CGA	-2.47	106.02	113.25
32	C	518	BCR	C15-C14-C13	-2.47	123.78	127.31
42	13	312	A86	C25-C24-C1	-2.47	119.46	126.42
42	20	213	A86	C7-C6-C8	2.47	121.98	118.08
30	11	304	CLA	CBA-CAA-C2A	-2.47	106.56	113.86
42	18	314	A86	C25-C24-C1	-2.47	119.47	126.42
30	14	304	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
30	14	306	CLA	CBA-CAA-C2A	-2.47	106.56	113.86
30	B	605	CLA	CHB-C1B-NB	2.47	126.88	124.26
42	15	315	A86	C41-C32-C31	-2.47	108.26	110.47
31	d	404	PHO	C2D-C1D-ND	-2.47	107.82	109.53
30	D	405	CLA	CMB-C2B-C3B	2.47	132.58	126.59
31	d	403	PHO	CAA-CBA-CGA	-2.47	106.03	113.25
42	11	310	A86	C7-C6-C8	2.47	121.97	118.08
42	12	315	A86	C7-C6-C8	2.47	121.97	118.08
30	18	304	CLA	C2A-C1A-CHA	2.47	128.18	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	405	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
30	d	407	CLA	CHB-C1B-NB	2.47	126.87	124.26
41	V	201	HEM	CAC-C3C-C2C	-2.47	120.47	128.60
30	D	405	CLA	CHB-C4A-NA	2.47	127.92	124.51
42	13	315	A86	C41-C32-C31	-2.47	108.26	110.47
30	A	404	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
30	w	103	CLA	CHB-C1B-NB	2.46	126.87	124.26
30	17	303	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
39	c	517	DGD	O3D-C3D-C4D	-2.46	104.65	110.35
42	12	316	A86	C25-C24-C1	-2.46	119.50	126.42
30	13	305	CLA	CBA-CAA-C2A	-2.46	106.59	113.86
30	20	205	CLA	CMB-C2B-C3B	2.46	132.55	126.59
36	B	619	LMG	O6-C1-O1	-2.46	104.14	109.97
30	C	503	CLA	C2A-C1A-CHA	2.46	128.16	123.86
35	L	102	LHG	C11-C10-C9	-2.46	101.93	114.42
42	20	210	A86	C26-C25-C24	-2.46	115.54	123.22
30	D	406	CLA	CHB-C1B-NB	2.46	126.86	124.26
30	12	306	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	15	309	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
39	J	101	DGD	O3E-C3E-C2E	-2.46	104.66	110.35
42	15	316	A86	C41-C32-C31	-2.46	108.27	110.47
30	16	309	CLA	CHC-C4B-NB	2.46	126.86	124.26
30	16	304	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
42	14	312	A86	C10-C9-C8	-2.46	115.55	123.22
30	c	514	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
30	20	208	CLA	CMB-C2B-C3B	2.46	132.54	126.59
42	11	313	A86	C40-C32-C31	-2.45	108.28	110.47
30	b	606	CLA	CHC-C1C-NC	2.45	127.93	124.20
41	v	201	HEM	CAC-C3C-C2C	-2.45	120.52	128.60
42	17	312	A86	C25-C24-C1	-2.45	119.52	126.42
42	21	312	A86	C40-C32-C31	-2.45	108.28	110.47
42	13	311	A86	C10-C9-C8	-2.45	115.56	123.22
35	l	102	LHG	C11-C10-C9	-2.45	101.98	114.42
30	17	303	CLA	C1-C2-C3	-2.45	121.80	126.04
30	13	305	CLA	C2D-C1D-ND	-2.45	108.30	110.10
42	12	315	A86	C10-C9-C8	-2.45	115.57	123.22
42	11	310	A86	C10-C9-C8	-2.45	115.57	123.22
32	m	103	BCR	C27-C26-C25	2.45	126.29	122.73
39	j	101	DGD	O3E-C3E-C2E	-2.45	104.68	110.35
30	b	605	CLA	C3B-C4B-NB	-2.45	108.24	110.52
42	21	314	A86	C7-C6-C8	2.45	121.94	118.08
30	C	514	CLA	CAA-C2A-C3A	-2.45	106.07	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	15	310	A86	C10-C9-C8	-2.45	115.58	123.22
42	20	212	A86	C9-C10-C11	-2.45	119.41	126.61
32	h	101	BCR	C37-C22-C21	-2.45	119.50	122.92
30	B	611	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
42	18	313	A86	C10-C9-C8	-2.45	115.58	123.22
42	13	315	A86	C12-C11-C13	2.45	120.13	116.02
42	17	311	A86	C17-C16-C15	2.45	111.66	109.16
32	Z	101	BCR	C7-C8-C9	-2.45	122.54	126.23
30	a	403	CLA	CAA-C2A-C3A	-2.44	106.08	112.78
32	c	521	BCR	C15-C14-C13	-2.44	123.82	127.31
30	20	205	CLA	CHB-C1B-C2B	-2.44	120.34	127.24
30	C	504	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
30	20	202	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
36	B	619	LMG	O3-C3-C2	-2.44	104.71	110.35
30	18	311	CLA	CHC-C4B-NB	2.44	126.84	124.26
33	b	620	SQD	O48-C23-O10	-2.44	117.44	123.59
33	A	406	SQD	O7-S-C6	2.44	109.84	106.94
42	17	314	A86	C40-C32-C31	-2.44	108.29	110.47
30	20	205	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	d	406	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
33	B	621	SQD	O48-C23-O10	-2.44	117.44	123.59
30	C	513	CLA	C3B-C4B-NB	-2.44	108.25	110.52
37	12	302	LMU	O5B-C1B-C2B	2.44	115.51	110.35
30	13	307	CLA	C2A-C1A-CHA	2.44	128.12	123.86
30	b	609	CLA	C2A-C1A-CHA	2.44	128.12	123.86
36	c	519	LMG	C9-C8-C7	-2.44	106.03	111.79
30	c	503	CLA	C1D-ND-C4D	2.44	108.06	106.33
42	19	312	A86	C41-C32-C31	-2.43	108.29	110.47
36	c	519	LMG	C40-C39-C38	-2.43	102.07	114.42
36	b	618	LMG	O3-C3-C2	-2.43	104.72	110.35
42	13	301	A86	C12-C11-C13	2.43	120.11	116.02
30	c	504	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
42	11	316	A86	C12-C11-C13	2.43	120.10	116.02
42	17	313	A86	C9-C10-C11	-2.43	119.47	126.61
42	14	314	A86	C9-C10-C11	-2.43	119.47	126.61
42	15	312	A86	C9-C10-C11	-2.43	119.47	126.61
30	d	406	CLA	CMB-C2B-C3B	2.43	132.47	126.59
30	C	502	CLA	CMB-C2B-C3B	2.43	132.47	126.59
30	14	305	CLA	C3B-C4B-NB	-2.43	108.26	110.52
42	19	310	A86	C34-O4-C38	-2.43	113.37	117.90
30	21	306	CLA	CBA-CAA-C2A	-2.43	106.70	113.86
42	18	302	A86	C12-C11-C13	2.43	120.10	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	505	CLA	CHD-C1D-ND	-2.43	122.22	124.45
40	d	405	PL9	C20-C19-C21	2.43	119.35	115.27
30	11	306	CLA	C2A-C1A-CHA	2.42	128.10	123.86
32	Y	101	BCR	C7-C8-C9	-2.42	122.57	126.23
30	14	308	CLA	C2A-C1A-CHA	2.42	128.10	123.86
42	15	315	A86	C12-C11-C13	2.42	120.09	116.02
35	A	408	LHG	C11-C10-C9	-2.42	102.12	114.42
36	B	620	LMG	O1-C1-C2	-2.42	104.52	108.30
30	B	615	CLA	CHA-C1A-NA	-2.42	120.85	126.40
30	D	401	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
30	14	309	CLA	CHA-C1A-NA	-2.42	120.85	126.40
30	13	308	CLA	CHA-C1A-NA	-2.42	120.85	126.40
31	d	404	PHO	O2D-CGD-O1D	-2.42	119.10	123.84
30	B	604	CLA	C3C-C4C-NC	-2.42	107.86	110.57
30	c	508	CLA	CHA-C1A-NA	-2.42	120.86	126.40
32	H	101	BCR	C11-C10-C9	-2.42	123.86	127.31
32	h	101	BCR	C11-C10-C9	-2.42	123.86	127.31
30	14	306	CLA	C2D-C1D-ND	-2.42	108.32	110.10
30	b	612	CLA	CMD-C2D-C1D	-2.42	120.45	124.71
42	13	313	A86	C9-C10-C11	-2.42	119.50	126.61
30	19	306	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	B	612	CLA	CMD-C2D-C1D	-2.42	120.45	124.71
30	B	605	CLA	C3C-C4C-NC	-2.42	107.86	110.57
30	b	615	CLA	CHA-C1A-NA	-2.42	120.86	126.40
30	19	304	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
36	Q	301	LMG	C40-C39-C38	-2.41	102.17	114.42
36	D	408	LMG	C6-C5-C4	-2.41	107.35	113.00
32	c	516	BCR	C7-C8-C9	-2.41	122.59	126.23
40	D	407	PL9	C36-C34-C33	-2.41	116.23	121.12
30	17	307	CLA	CHB-C1B-NB	2.41	126.81	124.26
30	18	310	CLA	CHB-C4A-NA	2.41	127.85	124.51
42	11	312	A86	C9-C10-C11	-2.41	119.51	126.61
42	21	312	A86	C35-C34-C33	2.41	114.09	109.88
30	c	502	CLA	CMB-C2B-C3B	2.41	132.43	126.59
42	17	312	A86	C40-C32-C31	-2.41	108.31	110.47
36	d	410	LMG	C6-C5-C4	-2.41	107.35	113.00
42	14	312	A86	C23-C16-C22	-2.41	103.81	107.37
41	F	102	HEM	CAC-C3C-C4C	-2.41	119.07	124.90
42	12	304	A86	C12-C11-C13	2.41	120.07	116.02
42	12	317	A86	C9-C10-C11	-2.41	119.52	126.61
30	16	309	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
33	a	405	SQD	C1-C2-C3	-2.41	104.98	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	407	LHG	C11-C10-C9	-2.41	102.19	114.42
39	c	518	DGD	O3E-C3E-C2E	-2.41	104.78	110.35
40	D	404	PL9	C20-C19-C21	2.41	119.32	115.27
30	C	505	CLA	CHD-C1D-ND	-2.41	122.24	124.45
42	21	313	A86	C34-O4-C38	-2.41	113.41	117.90
30	b	622	CLA	CHB-C1B-NB	2.40	126.80	124.26
32	H	101	BCR	C15-C14-C13	-2.40	123.88	127.31
36	Q	301	LMG	C38-C37-C36	-2.40	102.23	114.42
35	L	101	LHG	O8-C23-C24	2.40	119.45	111.91
30	12	310	CLA	C2A-C1A-CHA	2.40	128.06	123.86
30	16	302	CLA	C2A-C1A-CHA	2.40	128.06	123.86
30	16	306	CLA	C3B-C4B-NB	-2.40	108.29	110.52
42	21	312	A86	C7-C6-C8	2.40	121.86	118.08
39	c	518	DGD	C3D-C4D-C5D	-2.40	105.96	110.24
30	16	303	CLA	CHA-C1A-NA	-2.40	120.90	126.40
33	A	406	SQD	C1-C2-C3	-2.40	105.00	110.00
32	F	101	BCR	C35-C13-C14	-2.40	119.56	122.92
39	c	517	DGD	O6E-C5E-C6E	-2.40	100.47	106.44
30	20	205	CLA	C3A-C2A-C1A	2.40	104.93	101.34
30	B	609	CLA	C2A-C1A-CHA	2.40	128.05	123.86
39	C	517	DGD	O3E-C3E-C2E	-2.40	104.81	110.35
36	c	519	LMG	C38-C37-C36	-2.40	102.26	114.42
40	d	408	PL9	C36-C34-C33	-2.40	116.27	121.12
30	b	611	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
42	13	312	A86	C40-C32-C31	-2.40	108.33	110.47
41	f	102	HEM	CAC-C3C-C4C	-2.40	119.11	124.90
42	13	311	A86	C23-C16-C22	-2.40	103.84	107.37
30	b	604	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
35	d	409	LHG	O8-C23-C24	2.39	119.42	111.91
32	f	101	BCR	C35-C13-C14	-2.39	119.57	122.92
36	1	101	LMG	C1-C2-C3	-2.39	105.01	110.00
30	C	506	CLA	CMC-C2C-C1C	-2.39	121.39	125.04
30	20	207	CLA	C2A-C1A-CHA	2.39	128.04	123.86
42	16	312	A86	C9-C10-C11	-2.39	119.57	126.61
33	B	621	SQD	C4-C3-C2	2.39	115.00	110.82
42	15	310	A86	C23-C16-C22	-2.39	103.84	107.37
39	C	516	DGD	CDB-CCB-CBB	-2.39	102.28	114.42
30	B	602	CLA	CHD-C1D-ND	-2.39	122.26	124.45
36	d	410	LMG	O3-C3-C2	-2.39	104.82	110.35
42	17	311	A86	C12-C11-C13	2.39	120.04	116.02
30	15	301	CLA	C1-C2-C3	-2.39	121.91	126.04
30	15	307	CLA	CAA-C2A-C1A	2.39	119.80	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	18	313	A86	C23-C16-C22	-2.39	103.85	107.37
42	21	313	A86	C28-C27-C26	-2.39	119.58	122.92
42	19	310	A86	C10-C9-C8	-2.39	115.77	123.22
42	18	302	A86	C41-C32-C31	-2.39	108.33	110.47
36	D	408	LMG	C40-C39-C38	-2.39	102.30	114.42
42	12	315	A86	C23-C16-C22	-2.39	103.85	107.37
30	20	206	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
42	20	201	A86	C7-C6-C8	2.39	121.84	118.08
30	19	303	CLA	CHB-C1B-NB	2.39	126.78	124.26
30	c	510	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
36	D	408	LMG	O3-C3-C2	-2.38	104.84	110.35
30	15	307	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
30	b	612	CLA	CMD-C2D-C3D	2.38	133.09	127.61
30	12	311	CLA	CHA-C1A-NA	-2.38	120.94	126.40
30	A	402	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	18	306	CLA	C2A-C1A-CHA	2.38	128.02	123.86
30	b	611	CLA	CHB-C4A-NA	2.38	127.80	124.51
42	18	314	A86	C10-C9-C8	-2.38	115.79	123.22
32	h	101	BCR	C15-C14-C13	-2.38	123.91	127.31
30	20	208	CLA	C2A-C1A-CHA	2.38	128.02	123.86
30	18	305	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
39	C	517	DGD	C3D-C4D-C5D	-2.38	106.00	110.24
30	19	306	CLA	O2A-CGA-O1A	-2.38	117.37	123.30
30	11	307	CLA	CHA-C1A-NA	-2.38	120.95	126.40
33	b	620	SQD	C4-C3-C2	2.38	114.97	110.82
32	c	515	BCR	C33-C5-C6	-2.38	121.86	124.53
39	c	517	DGD	CDB-CCB-CBB	-2.38	102.36	114.42
30	17	304	CLA	CHA-C1A-NA	-2.38	120.95	126.40
32	c	520	BCR	C7-C8-C9	-2.38	122.64	126.23
30	c	506	CLA	CMC-C2C-C1C	-2.38	121.42	125.04
30	17	304	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
36	d	410	LMG	C40-C39-C38	-2.38	102.36	114.42
30	18	308	CLA	C3B-C4B-NB	-2.38	108.31	110.52
30	C	519	CLA	CHB-C1B-NB	2.38	126.77	124.26
35	A	408	LHG	C18-C17-C16	-2.37	102.37	114.42
33	b	620	SQD	C1-O5-C5	2.37	118.35	113.69
36	m	102	LMG	O6-C1-O1	-2.37	104.35	109.97
30	21	309	CLA	CHD-C1D-ND	-2.37	122.27	124.45
42	11	310	A86	C23-C16-C22	-2.37	103.87	107.37
30	B	615	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
42	17	302	A86	C9-C10-C11	-2.37	119.63	126.61
32	b	616	BCR	C24-C23-C22	-2.37	122.65	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	17	304	CLA	CAA-C2A-C1A	2.37	119.75	111.97
32	B	624	BCR	C33-C5-C6	-2.37	121.86	124.53
30	17	305	CLA	CHC-C4B-NB	2.37	126.77	124.26
42	13	312	A86	C10-C9-C8	-2.37	115.81	123.22
42	14	313	A86	C10-C9-C8	-2.37	115.81	123.22
42	16	311	A86	C40-C32-C31	-2.37	108.35	110.47
30	d	407	CLA	CHC-C4B-NB	2.37	126.77	124.26
30	11	301	CLA	CHC-C4B-NB	2.37	126.77	124.26
30	14	303	CLA	CHC-C4B-NB	2.37	126.77	124.26
42	17	312	A86	C10-C9-C8	-2.37	115.82	123.22
32	f	101	BCR	C16-C15-C14	-2.37	118.62	123.47
30	c	513	CLA	C3B-C4B-NB	-2.37	108.32	110.52
35	a	407	LHG	C18-C17-C16	-2.37	102.41	114.42
33	B	621	SQD	C1-O5-C5	2.37	118.33	113.69
36	b	619	LMG	O1-C1-C2	-2.37	104.61	108.30
32	B	618	BCR	C15-C16-C17	-2.37	118.62	123.47
30	B	604	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
30	B	623	CLA	CHB-C1B-NB	2.37	126.76	124.26
30	c	509	CLA	CMB-C2B-C3B	2.37	132.32	126.59
41	V	201	HEM	CAD-CBD-CGD	-2.37	108.51	113.60
32	F	101	BCR	C16-C15-C14	-2.37	118.63	123.47
30	18	309	CLA	CMB-C2B-C3B	2.36	132.31	126.59
30	12	308	CLA	CHB-C1B-C2B	-2.36	120.56	127.24
36	b	619	LMG	O2-C2-C1	-2.36	104.30	110.05
36	w	101	LMG	C40-C39-C38	-2.36	102.42	114.42
42	11	311	A86	C10-C9-C8	-2.36	115.84	123.22
30	W	102	CLA	CHB-C1B-NB	2.36	126.76	124.26
40	d	408	PL9	C42-C43-C44	-2.36	121.97	127.66
30	12	308	CLA	C2D-C1D-ND	-2.36	108.36	110.10
30	d	401	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
42	20	213	A86	C40-C32-C31	-2.36	108.36	110.47
30	C	509	CLA	CMB-C2B-C3B	2.36	132.31	126.59
30	19	309	CLA	CBC-CAC-C3C	2.36	118.94	112.43
42	21	314	A86	C40-C32-C31	-2.36	108.36	110.47
36	W	101	LMG	O2-C2-C1	-2.36	104.31	110.05
39	c	517	DGD	O5E-C6E-C5E	-2.36	103.19	111.29
30	15	308	CLA	CBA-CAA-C2A	-2.36	106.89	113.86
30	17	309	CLA	CHA-C1A-NA	-2.36	120.99	126.40
30	16	302	CLA	CHC-C4B-NB	2.36	126.76	124.26
30	12	305	CLA	CHC-C4B-NB	2.36	126.75	124.26
32	C	515	BCR	C7-C8-C9	-2.36	122.67	126.23
30	17	309	CLA	C3B-C4B-NB	-2.36	108.33	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	316	A86	C10-C9-C8	-2.36	115.86	123.22
30	c	503	CLA	C2D-C1D-ND	-2.36	108.37	110.10
42	15	311	A86	C40-C32-C31	-2.36	108.36	110.47
36	W	101	LMG	C40-C39-C38	-2.36	102.46	114.42
30	B	612	CLA	CMD-C2D-C3D	2.36	133.03	127.61
32	b	616	BCR	C30-C25-C26	-2.36	119.30	122.61
30	b	615	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
30	16	301	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	19	302	CLA	O2A-CGA-O1A	-2.35	117.43	123.30
39	C	516	DGD	O6E-C5E-C6E	-2.35	100.58	106.44
36	B	619	LMG	O1-C7-C8	-2.35	105.22	110.90
30	19	309	CLA	CAA-C2A-C1A	-2.35	104.26	111.97
42	11	316	A86	C9-C10-C11	-2.35	119.69	126.61
36	W	101	LMG	C6-C5-C4	-2.35	107.49	113.00
36	w	101	LMG	O2-C2-C1	-2.35	104.33	110.05
36	w	101	LMG	C6-C5-C4	-2.35	107.50	113.00
30	C	510	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
42	15	311	A86	C10-C9-C8	-2.35	115.88	123.22
30	19	307	CLA	C11-C12-C13	-2.35	108.32	115.92
30	b	605	CLA	C3C-C4C-NC	-2.35	107.94	110.57
30	11	304	CLA	CHB-C1B-C2B	-2.35	120.60	127.24
42	16	311	A86	C10-C9-C8	-2.35	115.89	123.22
30	c	507	CLA	O1D-CGD-CBD	2.35	129.29	124.48
30	16	308	CLA	CBB-CAB-C3B	-2.35	115.93	127.62
40	D	407	PL9	O1-C4-C3	-2.35	118.13	120.72
30	w	102	CLA	CHB-C1B-NB	2.35	126.74	124.26
30	b	614	CLA	C2A-C1A-CHA	2.35	127.96	123.86
30	17	306	CLA	C2A-C1A-CHA	2.35	127.96	123.86
42	12	316	A86	C40-C32-C31	-2.35	108.37	110.47
36	M	102	LMG	O6-C1-O1	-2.35	104.42	109.97
30	19	308	CLA	CMB-C2B-C3B	2.35	132.27	126.59
42	14	313	A86	C40-C32-C31	-2.34	108.37	110.47
30	D	401	CLA	CHC-C4B-NB	2.34	126.74	124.26
36	b	619	LMG	O7-C10-O9	-2.34	118.04	123.70
30	B	613	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
41	v	201	HEM	CAD-CBD-CGD	-2.34	108.56	113.60
30	11	301	CLA	CHB-C1B-NB	2.34	126.73	124.26
39	j	101	DGD	CAB-C9B-C8B	-2.34	102.54	114.42
30	21	305	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
32	b	617	BCR	C15-C16-C17	-2.34	118.68	123.47
42	12	304	A86	C9-C10-C11	-2.34	119.73	126.61
42	20	213	A86	C41-C32-C31	-2.34	108.38	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	605	CLA	C3B-C4B-NB	-2.34	108.34	110.52
30	d	401	CLA	CHC-C4B-NB	2.34	126.73	124.26
30	14	306	CLA	CHB-C1B-C2B	-2.34	120.64	127.24
36	B	620	LMG	O2-C2-C1	-2.34	104.37	110.05
30	C	520	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
36	B	620	LMG	O7-C10-O9	-2.34	118.06	123.70
36	B	619	LMG	C40-C39-C38	-2.34	102.57	114.42
42	13	315	A86	C9-C10-C11	-2.33	119.75	126.61
42	15	316	A86	C9-C10-C11	-2.33	119.75	126.61
42	13	301	A86	C9-C10-C11	-2.33	119.75	126.61
36	B	619	LMG	O1-C1-C2	-2.33	104.66	108.30
36	b	618	LMG	O1-C7-C8	-2.33	105.27	110.90
39	J	101	DGD	CAB-C9B-C8B	-2.33	102.58	114.42
30	m	101	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
32	B	617	BCR	C24-C23-C22	-2.33	122.71	126.23
30	M	101	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
30	b	611	CLA	C1-C2-C3	-2.33	122.01	126.04
36	b	618	LMG	C40-C39-C38	-2.33	102.59	114.42
30	c	509	CLA	CGD-CBD-CAD	-2.33	103.18	110.73
30	c	505	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
30	12	313	CLA	CHA-C1A-NA	-2.33	121.06	126.40
30	13	305	CLA	CHB-C1B-C2B	-2.33	120.65	127.24
41	V	201	HEM	CHD-C4C-C3C	2.33	129.24	125.26
42	15	315	A86	C9-C10-C11	-2.33	119.76	126.61
30	11	304	CLA	C2D-C1D-ND	-2.33	108.39	110.10
30	14	303	CLA	CHB-C1B-NB	2.33	126.72	124.26
30	B	603	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
30	C	508	CLA	CHA-C1A-NA	-2.33	121.07	126.40
30	11	308	CLA	CHA-C1A-NA	-2.33	121.07	126.40
30	b	613	CLA	C4-C3-C5	2.33	119.19	115.27
30	b	602	CLA	CHD-C1D-ND	-2.33	122.32	124.45
30	W	103	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
30	B	614	CLA	C2A-C1A-CHA	2.33	127.92	123.86
30	20	204	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
42	16	310	A86	C7-C6-C8	2.32	121.74	118.08
30	b	613	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
42	18	314	A86	C40-C32-C31	-2.32	108.39	110.47
30	B	611	CLA	CHB-C4A-NA	2.32	127.72	124.51
30	c	511	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	b	601	CLA	CHB-C1B-NB	2.32	126.71	124.26
36	12	301	LMG	C1-C2-C3	-2.32	105.16	110.00
30	z	101	CLA	CHB-C1B-NB	2.32	126.71	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	505	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
30	16	305	CLA	C2A-C1A-CHA	2.32	127.91	123.86
30	c	511	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
32	c	515	BCR	C27-C26-C25	2.32	126.10	122.73
39	c	517	DGD	O2D-C2D-C1D	-2.32	104.42	110.05
30	B	611	CLA	C3C-C4C-NC	-2.32	107.97	110.57
30	20	209	CLA	C2A-C1A-CHA	2.32	127.91	123.86
32	h	101	BCR	C27-C26-C25	2.32	126.09	122.73
39	C	516	DGD	O2D-C2D-C1D	-2.32	104.42	110.05
30	C	510	CLA	CMB-C2B-C3B	2.32	132.20	126.59
30	21	301	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
36	b	618	LMG	O1-C1-C2	-2.32	104.69	108.30
30	B	611	CLA	C7-C6-C5	-2.32	107.07	113.36
30	b	611	CLA	C3C-C4C-NC	-2.32	107.97	110.57
30	14	310	CLA	CHA-C1A-NA	-2.32	121.10	126.40
32	Z	101	BCR	C33-C5-C6	-2.31	121.93	124.53
30	13	309	CLA	CHA-C1A-NA	-2.31	121.10	126.40
30	C	509	CLA	CGD-CBD-CAD	-2.31	103.24	110.73
30	c	504	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
40	D	407	PL9	C11-C9-C8	-2.31	116.44	121.12
40	D	407	PL9	C42-C43-C44	-2.31	122.09	127.66
30	B	611	CLA	C1-C2-C3	-2.31	122.05	126.04
41	v	201	HEM	CHD-C4C-C3C	2.31	129.21	125.26
31	d	404	PHO	C1C-C2C-C3C	-2.31	106.69	108.61
36	Q	301	LMG	O3-C3-C2	-2.31	105.01	110.35
40	d	408	PL9	C11-C9-C8	-2.31	116.44	121.12
30	b	603	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
33	L	103	SQD	O8-S-C6	2.31	109.42	105.74
39	C	516	DGD	O5E-C6E-C5E	-2.31	103.38	111.29
30	c	507	CLA	CHC-C4B-NB	2.31	126.70	124.26
30	13	302	CLA	CHC-C4B-NB	2.31	126.70	124.26
36	D	408	LMG	C38-C37-C36	-2.31	102.72	114.42
30	b	611	CLA	C7-C6-C5	-2.31	107.10	113.36
32	Z	101	BCR	C27-C26-C25	2.31	126.08	122.73
32	F	101	BCR	C15-C16-C17	-2.31	118.75	123.47
36	c	519	LMG	O3-C3-C2	-2.31	105.02	110.35
30	18	301	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
30	B	613	CLA	C2A-C1A-CHA	2.30	127.89	123.86
30	a	402	CLA	CHB-C4A-NA	2.30	127.70	124.51
30	C	503	CLA	C1D-ND-C4D	2.30	107.97	106.33
30	C	511	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
42	18	302	A86	C9-C10-C11	-2.30	119.84	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	M	101	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	15	303	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	19	308	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
42	21	314	A86	C41-C32-C31	-2.30	108.41	110.47
30	11	303	CLA	CHC-C4B-NB	2.30	126.69	124.26
30	b	607	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
30	21	305	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	C	504	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	C	503	CLA	C2D-C1D-ND	-2.30	108.41	110.10
42	11	311	A86	C40-C32-C31	-2.30	108.42	110.47
30	b	606	CLA	C3C-C4C-NC	-2.30	108.00	110.57
36	d	410	LMG	C38-C37-C36	-2.30	102.77	114.42
35	d	409	LHG	C18-C17-C16	-2.30	102.77	114.42
42	17	316	A86	C-C1-C24	2.30	121.69	118.08
40	d	408	PL9	O1-C4-C3	-2.30	118.19	120.72
30	c	512	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	20	209	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
30	C	511	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
32	f	101	BCR	C15-C16-C17	-2.29	118.78	123.47
40	D	404	PL9	C36-C34-C33	-2.29	116.48	121.12
30	B	602	CLA	C3C-C4C-NC	-2.29	108.00	110.57
30	z	101	CLA	C2A-C1A-CHA	2.29	127.87	123.86
30	16	309	CLA	C2D-C1D-ND	-2.29	108.41	110.10
39	H	102	DGD	CBB-CAB-C9B	-2.29	102.79	114.42
32	b	623	BCR	C33-C5-C6	-2.29	121.95	124.53
42	12	304	A86	C35-C34-C33	2.29	113.87	109.88
35	L	101	LHG	C18-C17-C16	-2.29	102.79	114.42
30	B	607	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
31	A	403	PHO	CBA-CAA-C2A	-2.29	107.12	113.81
30	14	307	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
32	B	617	BCR	C30-C25-C26	-2.29	119.39	122.61
30	C	507	CLA	O1D-CGD-CBD	2.29	129.17	124.48
30	B	601	CLA	C2A-C1A-CHA	2.29	127.86	123.86
30	19	304	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
30	B	606	CLA	C3C-C4C-NC	-2.29	108.00	110.57
30	b	606	CLA	CHB-C1B-NB	2.29	126.68	124.26
42	21	312	A86	C10-C9-C8	-2.29	116.08	123.22
39	h	102	DGD	CBB-CAB-C9B	-2.29	102.81	114.42
30	B	603	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
30	A	404	CLA	CHC-C4B-NB	2.29	126.68	124.26
30	15	308	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
30	b	622	CLA	C1-C2-C3	-2.29	122.09	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	304	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
30	11	306	CLA	C3B-C4B-NB	-2.28	108.40	110.52
30	w	103	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
42	21	310	A86	C7-C6-C8	2.28	121.67	118.08
36	B	620	LMG	C6-C5-C4	-2.28	107.66	113.00
30	B	613	CLA	C4-C3-C5	2.28	119.11	115.27
30	13	304	CLA	CHC-C4B-NB	2.28	126.67	124.26
36	b	619	LMG	C6-C5-C4	-2.28	107.66	113.00
30	20	205	CLA	C2A-C1A-CHA	2.28	127.84	123.86
35	l	102	LHG	C18-C17-C16	-2.28	102.86	114.42
42	12	317	A86	C7-C6-C8	2.28	121.67	118.08
30	C	507	CLA	CHC-C4B-NB	2.28	126.67	124.26
30	15	308	CLA	CHC-C4B-NB	2.28	126.67	124.26
42	11	314	A86	C-C1-C24	2.28	121.66	118.08
30	c	503	CLA	CHA-C1A-NA	-2.28	121.19	126.40
30	B	606	CLA	CHB-C1B-NB	2.28	126.67	124.26
42	15	315	A86	C35-C34-C33	2.28	113.85	109.88
30	C	512	CLA	CHB-C1B-NB	2.27	126.67	124.26
30	Z	102	CLA	CHB-C1B-NB	2.27	126.67	124.26
30	19	309	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
30	12	305	CLA	CHB-C1B-NB	2.27	126.66	124.26
30	c	507	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
30	13	306	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
35	L	102	LHG	C18-C17-C16	-2.27	102.89	114.42
42	16	313	A86	C-C1-C24	2.27	121.66	118.08
32	h	101	BCR	C24-C23-C22	-2.27	122.80	126.23
30	c	510	CLA	CMB-C2B-C3B	2.27	132.08	126.59
30	b	613	CLA	C2A-C1A-CHA	2.27	127.83	123.86
30	C	504	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
30	b	603	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
30	C	505	CLA	C3B-C4B-NB	-2.27	108.41	110.52
31	d	403	PHO	CBA-CAA-C2A	-2.27	107.19	113.81
30	19	304	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
30	b	602	CLA	C3C-C4C-NC	-2.26	108.03	110.57
30	B	615	CLA	C2A-C1A-CHA	2.26	127.82	123.86
30	B	607	CLA	C3B-C4B-NB	-2.26	108.42	110.52
30	c	504	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
30	C	507	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
30	B	601	CLA	CHB-C1B-NB	2.26	126.65	124.26
30	B	603	CLA	CHC-C4B-NB	2.26	126.65	124.26
42	15	316	A86	C35-C34-C33	2.26	113.82	109.88
32	a	404	BCR	C35-C13-C14	-2.26	119.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	513	CLA	CHB-C1B-NB	2.26	126.65	124.26
42	13	313	A86	C7-C6-C8	2.26	121.64	118.08
30	b	601	CLA	C2A-C1A-CHA	2.26	127.81	123.86
30	c	508	CLA	C2D-C1D-ND	-2.26	108.44	110.10
30	19	301	CLA	CHD-C1D-ND	-2.26	122.38	124.45
42	12	319	A86	C-C1-C24	2.26	121.63	118.08
30	21	305	CLA	CMB-C2B-C3B	2.26	132.05	126.59
30	C	519	CLA	C2A-C1A-CHA	2.26	127.81	123.86
30	18	301	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
40	d	405	PL9	C36-C34-C33	-2.26	116.55	121.12
42	17	311	A86	C34-O4-C38	-2.26	113.69	117.90
31	D	403	PHO	C1C-C2C-C3C	-2.26	106.73	108.61
30	18	304	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
36	b	618	LMG	C38-C37-C36	-2.25	102.98	114.42
42	16	312	A86	C7-C6-C8	2.25	121.63	118.08
33	l	101	SQD	O8-S-C6	2.25	109.33	105.74
30	C	510	CLA	CHB-C1B-NB	2.25	126.64	124.26
42	14	301	A86	C-C1-C24	2.25	121.62	118.08
30	14	309	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
30	C	503	CLA	CHA-C1A-NA	-2.25	121.24	126.40
30	c	510	CLA	C16-C15-C13	-2.25	108.64	115.92
35	b	621	LHG	C18-C17-C16	-2.25	103.00	114.42
42	11	316	A86	C35-C34-C33	2.25	113.80	109.88
37	B	625	LMU	C1B-O5B-C5B	2.25	118.11	113.69
36	12	301	LMG	O2-C2-C3	-2.25	105.15	110.35
42	15	314	A86	C-C1-C24	2.25	121.62	118.08
30	16	305	CLA	C2D-C1D-ND	-2.25	108.45	110.10
39	C	517	DGD	O6E-C1E-O5D	-2.25	104.65	109.97
30	13	302	CLA	CHB-C1B-NB	2.25	126.64	124.26
40	D	404	PL9	C37-C38-C39	-2.25	122.25	127.66
30	m	101	CLA	CHB-C1B-NB	2.25	126.63	124.26
30	b	604	CLA	CHA-C1A-NA	-2.25	121.26	126.40
30	b	622	CLA	CHA-C1A-NA	-2.24	121.26	126.40
30	W	102	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
42	13	301	A86	C35-C34-C33	2.24	113.79	109.88
30	21	308	CLA	C2A-C1A-CHA	2.24	127.78	123.86
30	C	510	CLA	C16-C15-C13	-2.24	108.67	115.92
30	15	306	CLA	O2D-CGD-CBD	2.24	115.25	111.27
42	14	316	A86	C-C1-C24	2.24	121.61	118.08
30	17	305	CLA	O2A-C1-C2	-2.24	102.74	108.64
35	B	622	LHG	C18-C17-C16	-2.24	103.05	114.42
30	21	309	CLA	C3B-C4B-NB	-2.24	108.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	623	CLA	CMD-C2D-C1D	-2.24	120.77	124.71
30	b	615	CLA	C2A-C1A-CHA	2.24	127.78	123.86
32	A	405	BCR	C35-C13-C14	-2.24	119.79	122.92
42	18	302	A86	C35-C34-C33	2.24	113.78	109.88
30	d	406	CLA	C3B-C4B-NB	-2.24	108.44	110.52
30	11	307	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
30	b	602	CLA	O2D-CGD-CBD	2.24	115.25	111.27
32	c	515	BCR	C15-C14-C13	-2.24	124.12	127.31
42	21	310	A86	O1-C15-C14	-2.24	108.72	113.21
39	J	101	DGD	C3D-C4D-C5D	-2.24	106.25	110.24
30	b	609	CLA	O1D-CGD-CBD	2.24	129.06	124.48
30	w	102	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
42	17	313	A86	C7-C6-C8	2.24	121.60	118.08
30	b	607	CLA	C3B-C4B-NB	-2.24	108.44	110.52
31	D	403	PHO	C1-C2-C3	-2.24	122.18	126.04
30	a	403	CLA	CHC-C4B-NB	2.23	126.62	124.26
32	b	623	BCR	C27-C26-C25	2.23	125.97	122.73
30	21	309	CLA	O2A-CGA-O1A	-2.23	117.73	123.30
30	B	623	CLA	CMD-C2D-C3D	2.23	132.75	127.61
30	C	505	CLA	CHC-C1C-NC	2.23	127.59	124.20
36	B	619	LMG	C38-C37-C36	-2.23	103.10	114.42
30	20	202	CLA	C1-C2-C3	-2.23	122.18	126.04
30	c	510	CLA	CHB-C1B-NB	2.23	126.62	124.26
42	21	312	A86	C19-C18-C17	-2.23	106.47	110.77
42	21	310	A86	C19-C18-C17	-2.23	106.47	110.77
30	15	308	CLA	C3B-C4B-NB	-2.23	108.45	110.52
32	m	103	BCR	C33-C5-C6	-2.23	122.02	124.53
30	13	308	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
30	20	204	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
30	C	503	CLA	CHC-C1C-NC	2.23	127.58	124.20
42	21	311	A86	C7-C6-C8	2.23	121.59	118.08
30	19	307	CLA	C2D-C1D-ND	-2.23	108.46	110.10
30	b	602	CLA	C3B-C4B-NB	-2.23	108.45	110.52
30	B	602	CLA	O2D-CGD-CBD	2.23	115.23	111.27
30	B	608	CLA	O2D-CGD-CBD	2.23	115.23	111.27
40	d	405	PL9	C37-C38-C39	-2.23	122.30	127.66
30	19	307	CLA	CHC-C4B-NB	2.23	126.61	124.26
39	C	517	DGD	C3G-C2G-C1G	-2.23	106.52	111.79
30	14	305	CLA	CHC-C4B-NB	2.23	126.61	124.26
42	19	311	A86	C26-C25-C24	-2.23	116.27	123.22
32	F	101	BCR	C27-C26-C25	2.23	125.96	122.73
42	15	312	A86	C7-C6-C8	2.23	121.58	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	302	LMU	C1B-O5B-C5B	2.23	118.06	113.69
32	b	617	BCR	C11-C10-C9	-2.22	124.14	127.31
30	21	306	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
30	B	605	CLA	C2D-C1D-ND	-2.22	108.47	110.10
30	b	606	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
39	C	517	DGD	CAB-C9B-C8B	-2.22	103.14	114.42
30	c	503	CLA	CHC-C4B-NB	2.22	126.61	124.26
30	18	309	CLA	CAA-C2A-C1A	2.22	119.26	111.97
30	13	309	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
30	12	307	CLA	CHC-C4B-NB	2.22	126.61	124.26
32	H	101	BCR	C24-C23-C22	-2.22	122.88	126.23
36	B	620	LMG	C38-C37-C36	-2.22	103.15	114.42
42	13	315	A86	C35-C34-C33	2.22	113.75	109.88
30	21	305	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
30	a	402	CLA	CMB-C2B-C3B	2.22	131.96	126.59
30	11	305	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
42	11	312	A86	C7-C6-C8	2.22	121.57	118.08
33	L	103	SQD	C44-O6-C1	2.22	118.07	113.74
39	c	518	DGD	O6E-C1E-O5D	-2.22	104.72	109.97
30	19	301	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
42	20	211	A86	C7-C6-C8	2.22	121.57	118.08
30	17	304	CLA	CHC-C4B-NB	2.22	126.60	124.26
42	20	201	A86	C7-C6-C5	-2.22	119.82	122.92
32	H	101	BCR	C27-C26-C25	2.22	125.95	122.73
39	C	517	DGD	O5D-C6D-C5D	-2.22	104.95	109.05
30	19	309	CLA	O2A-CGA-O1A	-2.22	117.78	123.30
30	c	513	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
30	B	609	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
30	B	609	CLA	O1D-CGD-CBD	2.21	129.01	124.48
30	17	307	CLA	CHC-C4B-NB	2.21	126.60	124.26
30	c	506	CLA	C3B-C4B-NB	-2.21	108.46	110.52
30	b	609	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
30	c	505	CLA	CHC-C1C-NC	2.21	127.56	124.20
30	20	202	CLA	CHB-C1B-NB	2.21	126.60	124.26
36	b	619	LMG	C38-C37-C36	-2.21	103.19	114.42
32	c	520	BCR	C29-C30-C25	2.21	113.89	110.48
30	12	309	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
32	B	618	BCR	C11-C10-C9	-2.21	124.15	127.31
30	17	308	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
42	21	311	A86	O1-C15-C14	-2.21	108.78	113.21
30	W	102	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
42	14	314	A86	C7-C6-C8	2.21	121.56	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	404	PHO	C1-C2-C3	-2.21	122.22	126.04
30	15	306	CLA	CHD-C1D-ND	-2.21	122.43	124.45
33	A	406	SQD	O48-C23-O10	-2.21	118.02	123.59
30	D	405	CLA	C3B-C4B-NB	-2.21	108.47	110.52
30	11	302	CLA	CHA-C1A-NA	-2.21	121.35	126.40
30	15	303	CLA	CHD-C1D-ND	-2.21	122.43	124.45
30	15	307	CLA	CMB-C2B-C3B	2.21	131.93	126.59
30	B	611	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
30	18	305	CLA	CHD-C1D-ND	-2.20	122.43	124.45
30	13	307	CLA	C3B-C4B-NB	-2.20	108.47	110.52
30	12	306	CLA	CHA-C1A-NA	-2.20	121.35	126.40
30	14	310	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
42	16	310	A86	C8-C6-C5	-2.20	115.56	118.94
30	B	604	CLA	CHA-C1A-NA	-2.20	121.35	126.40
40	d	408	PL9	C36-C37-C38	-2.20	104.64	111.88
30	B	606	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
30	d	401	CLA	O2D-CGD-CBD	2.20	115.18	111.27
30	b	608	CLA	O2D-CGD-CBD	2.20	115.18	111.27
30	17	307	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	11	308	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	18	306	CLA	C3A-C2A-C1A	2.20	104.63	101.34
42	16	310	A86	C9-C10-C11	-2.20	120.14	126.61
30	C	513	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
30	16	305	CLA	O2A-CGA-O1A	-2.20	117.82	123.30
30	18	301	CLA	CAC-C3C-C4C	2.20	127.66	124.81
30	17	307	CLA	CMC-C2C-C3C	2.20	132.08	126.12
39	c	518	DGD	CAB-C9B-C8B	-2.20	103.27	114.42
30	19	304	CLA	C3A-C2A-C1A	2.20	104.63	101.34
30	C	502	CLA	C7-C6-C5	-2.20	107.39	113.36
39	c	518	DGD	O5D-C6D-C5D	-2.20	104.98	109.05
30	19	302	CLA	O1A-CGA-CBA	2.20	130.14	123.08
41	V	201	HEM	CHC-C1C-NC	2.20	126.81	124.44
39	j	101	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
30	19	304	CLA	CHA-C1A-NA	-2.20	121.37	126.40
30	14	304	CLA	CHA-C1A-NA	-2.19	121.37	126.40
30	B	623	CLA	C1-C2-C3	-2.19	122.25	126.04
41	f	102	HEM	C1C-CHC-C4B	-2.19	121.32	126.06
30	w	102	CLA	C2D-C1D-ND	-2.19	108.49	110.10
33	a	405	SQD	O48-C23-O10	-2.19	118.06	123.59
30	C	505	CLA	CHB-C1B-NB	2.19	126.58	124.26
32	B	618	BCR	C16-C15-C14	-2.19	118.98	123.47
30	A	402	CLA	CMB-C2B-C3B	2.19	131.90	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	F	102	HEM	C1C-CHC-C4B	-2.19	121.33	126.06
32	b	617	BCR	C27-C26-C25	2.19	125.91	122.73
30	c	502	CLA	C7-C6-C5	-2.19	107.41	113.36
30	D	405	CLA	CAC-C3C-C4C	2.19	127.65	124.81
30	18	305	CLA	C3B-C4B-NB	-2.19	108.48	110.52
30	b	603	CLA	CHC-C4B-NB	2.19	126.57	124.26
42	19	312	A86	C12-C11-C13	2.19	119.70	116.02
30	12	313	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
30	16	308	CLA	CHA-C1A-NA	-2.19	121.39	126.40
30	d	406	CLA	CAC-C3C-C4C	2.19	127.65	124.81
30	w	102	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
42	12	304	A86	C28-C27-C26	-2.19	119.86	122.92
32	b	623	BCR	C38-C26-C27	-2.19	109.41	113.62
30	13	306	CLA	CHB-C1B-NB	2.19	126.57	124.26
32	B	618	BCR	C15-C14-C13	-2.19	124.19	127.31
32	f	101	BCR	C27-C26-C25	2.19	125.91	122.73
39	c	518	DGD	C3G-C2G-C1G	-2.19	106.62	111.79
30	17	306	CLA	C3A-C2A-C1A	2.19	104.61	101.34
30	21	304	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
39	j	101	DGD	C3D-C4D-C5D	-2.19	106.34	110.24
30	B	609	CLA	C3B-C4B-NB	-2.18	108.49	110.52
30	18	312	CLA	O2A-CGA-O1A	-2.18	117.85	123.30
32	H	101	BCR	C40-C30-C25	2.18	113.84	110.30
30	15	302	CLA	O2D-CGD-CBD	2.18	115.15	111.27
30	C	508	CLA	CHB-C1B-NB	2.18	126.57	124.26
42	20	211	A86	O1-C15-C14	-2.18	108.83	113.21
39	J	101	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
36	M	102	LMG	C1-C2-C3	-2.18	105.45	110.00
40	D	407	PL9	C50-C49-C48	-2.18	116.34	122.65
30	19	305	CLA	CHB-C1B-NB	2.18	126.57	124.26
32	c	521	BCR	C20-C21-C22	-2.18	124.20	127.31
35	b	621	LHG	C20-C19-C18	-2.18	103.36	114.42
30	C	508	CLA	C2D-C1D-ND	-2.18	108.50	110.10
36	b	619	LMG	C40-C39-C38	-2.18	103.37	114.42
30	17	304	CLA	CMB-C2B-C3B	2.18	131.86	126.59
30	18	309	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
30	14	304	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
40	D	407	PL9	C36-C37-C38	-2.18	104.73	111.88
30	16	304	CLA	CHC-C4B-NB	2.18	126.56	124.26
30	16	308	CLA	CHC-C4B-NB	2.18	126.56	124.26
35	A	408	LHG	C5-O7-C7	-2.18	112.44	117.79
32	b	617	BCR	C15-C14-C13	-2.17	124.21	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
30	12	306	CLA	CHC-C4B-NB	2.17	126.56	124.26
30	B	606	CLA	C6-C7-C8	-2.17	108.89	115.92
30	b	605	CLA	C2D-C1D-ND	-2.17	108.50	110.10
42	15	315	A86	C28-C27-C26	-2.17	119.88	122.92
35	B	622	LHG	C20-C19-C18	-2.17	103.39	114.42
30	c	505	CLA	CHB-C1B-NB	2.17	126.56	124.26
32	Y	101	BCR	C29-C30-C25	2.17	113.83	110.48
30	21	302	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
30	14	305	CLA	O2A-C1-C2	-2.17	102.92	108.64
30	c	503	CLA	CHC-C1C-NC	2.17	127.50	124.20
30	16	302	CLA	O2D-CGD-CBD	2.17	115.13	111.27
32	h	101	BCR	C40-C30-C25	2.17	113.82	110.30
33	l	101	SQD	C44-O6-C1	2.17	117.98	113.74
30	c	508	CLA	CMB-C2B-C3B	2.17	131.85	126.59
30	20	202	CLA	CMB-C2B-C3B	2.17	131.85	126.59
30	15	309	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
30	C	512	CLA	CHA-C4D-ND	2.17	137.04	132.50
30	13	303	CLA	CHA-C1A-NA	-2.17	121.42	126.40
32	C	518	BCR	C20-C21-C22	-2.17	124.21	127.31
39	c	518	DGD	O5E-C6E-C5E	-2.17	103.84	111.29
42	13	301	A86	C28-C27-C26	-2.17	119.88	122.92
30	16	301	CLA	CHC-C4B-NB	2.17	126.55	124.26
30	b	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
39	C	517	DGD	O5E-C6E-C5E	-2.17	103.85	111.29
30	20	205	CLA	C2B-C1B-NB	2.17	111.69	110.23
30	19	302	CLA	CHB-C1B-NB	2.17	126.55	124.26
42	20	212	A86	C-C1-C2	-2.17	119.89	122.92
42	17	311	A86	C7-C6-C8	2.17	121.49	118.08
40	D	404	PL9	O2-C1-C6	2.17	124.34	120.59
30	18	311	CLA	O2A-CGA-O1A	-2.17	117.90	123.30
32	B	616	BCR	C33-C5-C6	-2.17	122.09	124.53
30	c	512	CLA	CHA-C4D-ND	2.17	137.03	132.50
40	d	405	PL9	O2-C1-C6	2.17	124.34	120.59
30	12	311	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
32	b	617	BCR	C16-C15-C14	-2.17	119.04	123.47
30	19	302	CLA	C2A-C1A-CHA	2.17	127.65	123.86
40	d	408	PL9	C50-C49-C48	-2.17	116.39	122.65
32	Z	101	BCR	C15-C14-C13	-2.17	124.22	127.31
30	17	307	CLA	CMC-C2C-C1C	-2.17	121.74	125.04
36	c	519	LMG	C3-C4-C5	-2.17	106.38	110.24
30	D	401	CLA	CAA-C2A-C3A	-2.17	106.85	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	18	307	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
33	b	620	SQD	O48-C23-C24	2.17	118.70	111.91
30	C	514	CLA	C2A-C1A-CHA	2.17	127.64	123.86
30	b	603	CLA	O1D-CGD-CBD	2.17	128.91	124.48
30	d	401	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
42	17	314	A86	C-C1-C24	2.16	121.49	118.08
36	B	620	LMG	C40-C39-C38	-2.16	103.44	114.42
32	B	624	BCR	C38-C26-C27	-2.16	109.46	113.62
30	18	301	CLA	C3C-C4C-NC	-2.16	108.14	110.57
42	11	316	A86	C28-C27-C26	-2.16	119.89	122.92
30	c	508	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
30	12	310	CLA	C3B-C4B-NB	-2.16	108.51	110.52
30	c	513	CLA	CHB-C1B-NB	2.16	126.55	124.26
30	18	306	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
36	m	102	LMG	C1-C2-C3	-2.16	105.49	110.00
42	18	302	A86	C28-C27-C26	-2.16	119.89	122.92
36	Q	301	LMG	C3-C4-C5	-2.16	106.38	110.24
30	D	401	CLA	O2D-CGD-CBD	2.16	115.11	111.27
30	12	306	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
39	H	102	DGD	C5B-C4B-C3B	-2.16	103.46	114.42
39	h	102	DGD	C5B-C4B-C3B	-2.16	103.46	114.42
42	18	315	A86	C-C1-C24	2.16	121.48	118.08
30	c	511	CLA	C2A-C1A-CHA	2.16	127.64	123.86
35	a	407	LHG	C5-O7-C7	-2.16	112.47	117.79
30	11	302	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
30	c	512	CLA	CHA-C1A-NA	-2.16	121.45	126.40
32	B	624	BCR	C27-C26-C25	2.16	125.86	122.73
30	C	508	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
30	18	309	CLA	CHA-C1A-NA	-2.16	121.45	126.40
33	B	621	SQD	O48-C23-C24	2.16	118.68	111.91
30	13	303	CLA	CHC-C4B-NB	2.16	126.54	124.26
30	15	303	CLA	CHB-C1B-NB	2.16	126.54	124.26
30	17	309	CLA	CAA-CBA-CGA	-2.16	106.78	112.51
30	b	606	CLA	C6-C7-C8	-2.16	108.95	115.92
30	15	301	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
30	c	505	CLA	C3B-C4B-NB	-2.15	108.52	110.52
30	B	607	CLA	CHC-C4B-NB	2.15	126.54	124.26
30	19	303	CLA	C3A-C2A-C1A	2.15	104.57	101.34
30	C	508	CLA	CMB-C2B-C3B	2.15	131.81	126.59
36	M	102	LMG	C9-C8-C7	-2.15	106.69	111.79
32	a	408	BCR	C27-C26-C25	2.15	125.86	122.73
30	B	613	CLA	CAA-C2A-C3A	-2.15	106.89	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	101	BCR	C24-C23-C22	-2.15	122.98	126.23
30	17	301	CLA	CHB-C4A-NA	2.15	127.49	124.51
42	14	314	A86	C-C1-C24	2.15	121.47	118.08
42	11	313	A86	C-C1-C24	2.15	121.46	118.08
30	A	402	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
36	m	102	LMG	C9-C8-C7	-2.15	106.71	111.79
30	18	310	CLA	C2A-C1A-CHA	2.15	127.61	123.86
30	b	613	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
30	14	308	CLA	C3B-C4B-NB	-2.15	108.52	110.52
41	f	102	HEM	CAA-C2A-C1A	2.15	129.11	124.89
30	20	206	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
30	C	520	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
32	c	515	BCR	C16-C15-C14	-2.14	119.08	123.47
30	18	311	CLA	O2D-CGD-CBD	2.14	115.08	111.27
30	21	307	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
42	21	313	A86	C41-C32-C31	-2.14	108.55	110.47
36	M	102	LMG	O1-C7-C8	-2.14	105.73	110.90
42	13	314	A86	C-C1-C24	2.14	121.45	118.08
30	B	603	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
42	13	315	A86	C28-C27-C26	-2.14	119.92	122.92
30	a	402	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	b	607	CLA	CHC-C4B-NB	2.14	126.52	124.26
30	A	404	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
39	j	101	DGD	O6E-C1E-O5D	-2.14	104.90	109.97
39	C	517	DGD	C8B-C7B-C6B	-2.14	103.56	114.42
30	C	506	CLA	C3B-C4B-NB	-2.14	108.53	110.52
42	12	318	A86	C-C1-C24	2.14	121.44	118.08
42	14	315	A86	C-C1-C24	2.14	121.44	118.08
30	B	602	CLA	C3B-C4B-NB	-2.14	108.53	110.52
30	11	305	CLA	C2A-C1A-CHA	2.14	127.59	123.86
30	B	604	CLA	C1D-ND-C4D	2.14	107.85	106.33
30	b	609	CLA	C3B-C4B-NB	-2.14	108.53	110.52
30	14	307	CLA	CHB-C1B-NB	2.13	126.52	124.26
30	19	308	CLA	CHC-C4B-NB	2.13	126.52	124.26
30	18	310	CLA	C2D-C1D-ND	-2.13	108.53	110.10
30	C	512	CLA	CHA-C1A-NA	-2.13	121.51	126.40
30	b	602	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
36	m	102	LMG	O1-C7-C8	-2.13	105.75	110.90
30	b	603	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
30	b	603	CLA	C4-C3-C5	2.13	118.86	115.27
30	14	308	CLA	CHB-C1B-NB	2.13	126.52	124.26
32	Z	101	BCR	C16-C15-C14	-2.13	119.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	V	201	HEM	CAA-CBA-CGA	-2.13	109.01	113.60
42	19	312	A86	C4-C3-C2	-2.13	119.11	123.47
30	c	508	CLA	CHB-C1B-NB	2.13	126.51	124.26
30	Z	102	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
30	B	603	CLA	C4-C3-C5	2.13	118.86	115.27
30	W	102	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
36	c	519	LMG	C1-C2-C3	-2.13	105.56	110.00
30	17	301	CLA	C1-C2-C3	-2.13	122.36	126.04
36	m	102	LMG	C1-O6-C5	-2.13	109.51	113.69
30	21	309	CLA	CAA-CBA-CGA	-2.13	106.85	112.51
42	12	318	A86	C34-O4-C38	-2.13	113.93	117.90
30	W	102	CLA	C2D-C1D-ND	-2.13	108.53	110.10
30	b	615	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
30	Z	102	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
32	B	618	BCR	C40-C30-C25	2.13	113.75	110.30
36	M	102	LMG	C1-O6-C5	-2.13	109.51	113.69
30	B	623	CLA	CHA-C1A-NA	-2.13	121.53	126.40
30	16	307	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
41	v	201	HEM	CHC-C1C-NC	2.13	126.74	124.44
30	b	611	CLA	CHD-C1D-ND	-2.13	122.50	124.45
36	b	618	LMG	O2-C2-C1	-2.12	104.89	110.05
32	B	618	BCR	C27-C26-C25	2.12	125.81	122.73
42	11	313	A86	C34-O4-C38	-2.12	113.94	117.90
30	13	307	CLA	CHB-C1B-NB	2.12	126.50	124.26
42	15	313	A86	C-C1-C24	2.12	121.42	118.08
30	C	503	CLA	CHC-C4B-NB	2.12	126.50	124.26
30	16	303	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
30	c	502	CLA	C11-C12-C13	-2.12	109.06	115.92
32	c	516	BCR	C30-C25-C26	-2.12	119.63	122.61
32	c	520	BCR	C16-C17-C18	-2.12	124.28	127.31
30	16	302	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
42	15	312	A86	C-C1-C24	2.12	121.42	118.08
42	20	212	A86	C12-C11-C13	2.12	119.58	116.02
30	21	307	CLA	CHB-C1B-NB	2.12	126.50	124.26
40	d	405	PL9	O2-C1-C2	-2.12	116.93	121.78
41	v	201	HEM	CAA-CBA-CGA	-2.12	109.05	113.60
30	a	403	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
30	C	506	CLA	CMC-C2C-C3C	2.12	131.87	126.12
35	L	102	LHG	C27-C26-C25	-2.12	103.68	114.42
30	21	302	CLA	CHA-C1A-NA	-2.12	121.55	126.40
30	C	520	CLA	C3A-C2A-C1A	2.12	104.51	101.34
30	C	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	17	307	CLA	CHC-C1C-NC	2.12	127.41	124.20
40	d	408	PL9	C27-C28-C29	-2.12	122.56	127.66
30	11	305	CLA	CHB-C1B-NB	2.12	126.50	124.26
32	A	409	BCR	C27-C26-C25	2.12	125.80	122.73
30	C	508	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	c	518	DGD	C8B-C7B-C6B	-2.11	103.69	114.42
30	17	307	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
32	F	101	BCR	C24-C23-C22	-2.11	123.04	126.23
30	19	307	CLA	CHB-C1B-NB	2.11	126.50	124.26
30	14	307	CLA	C2A-C1A-CHA	2.11	127.56	123.86
30	16	301	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
42	17	315	A86	C23-C16-C22	-2.11	104.25	107.37
30	B	615	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
42	17	314	A86	C34-O4-C38	-2.11	113.96	117.90
42	15	313	A86	C34-O4-C38	-2.11	113.96	117.90
42	18	315	A86	C34-O4-C38	-2.11	113.96	117.90
32	c	520	BCR	C15-C16-C17	-2.11	119.15	123.47
30	11	306	CLA	CHB-C1B-NB	2.11	126.49	124.26
30	18	312	CLA	CHB-C1B-NB	2.11	126.49	124.26
30	16	307	CLA	CHD-C1D-ND	-2.11	122.51	124.45
30	b	604	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
41	F	102	HEM	CAA-C2A-C1A	2.11	129.04	124.89
32	b	616	BCR	C38-C26-C27	-2.11	109.56	113.62
30	17	306	CLA	CHC-C4B-NB	2.11	126.49	124.26
42	12	317	A86	C-C1-C24	2.11	121.40	118.08
30	C	511	CLA	C2A-C1A-CHA	2.11	127.55	123.86
42	14	315	A86	C34-O4-C38	-2.11	113.97	117.90
30	b	601	CLA	CHC-C4B-NB	2.11	126.49	124.26
30	15	308	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	B	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
30	D	402	CLA	CHD-C1D-ND	-2.11	122.52	124.45
30	B	623	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
30	c	508	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
42	11	316	A86	C8-C6-C5	2.11	122.17	118.94
30	21	308	CLA	CHC-C4B-NB	2.11	126.49	124.26
30	14	305	CLA	CAA-C2A-C1A	2.11	118.88	111.97
30	12	309	CLA	C2A-C1A-CHA	2.11	127.54	123.86
32	B	617	BCR	C38-C26-C27	-2.11	109.57	113.62
32	Y	101	BCR	C15-C16-C17	-2.10	119.16	123.47
30	B	614	CLA	C3A-C2A-C1A	2.10	104.49	101.34
30	16	305	CLA	C3A-C2A-C1A	2.10	104.49	101.34
30	c	503	CLA	C3C-C4C-NC	-2.10	108.21	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	304	A86	C8-C6-C5	2.10	122.17	118.94
30	13	308	CLA	CHC-C4B-NB	2.10	126.48	124.26
30	17	308	CLA	C2A-C1A-CHA	2.10	127.54	123.86
42	15	316	A86	C28-C27-C26	-2.10	119.98	122.92
30	C	511	CLA	C1-C2-C3	-2.10	122.41	126.04
30	11	302	CLA	CHC-C4B-NB	2.10	126.48	124.26
30	12	309	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	B	602	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
30	c	505	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
32	Y	101	BCR	C16-C17-C18	-2.10	124.31	127.31
35	l	102	LHG	C27-C26-C25	-2.10	103.75	114.42
30	b	606	CLA	C2D-C1D-ND	-2.10	108.56	110.10
42	13	314	A86	C34-O4-C38	-2.10	113.98	117.90
30	c	511	CLA	C1-C2-C3	-2.10	122.41	126.04
30	18	303	CLA	C1-C2-C3	-2.10	122.41	126.04
30	c	514	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	b	614	CLA	C3A-C2A-C1A	2.10	104.48	101.34
30	17	308	CLA	CHA-C1A-NA	-2.10	121.59	126.40
42	21	310	A86	C-C1-C2	-2.10	119.98	122.92
30	D	405	CLA	CHC-C4B-NB	2.10	126.48	124.26
30	18	307	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	17	307	CLA	C3B-C4B-NB	-2.10	108.57	110.52
30	B	611	CLA	CHD-C1D-ND	-2.10	122.53	124.45
30	c	503	CLA	CHB-C1B-NB	2.10	126.48	124.26
42	13	313	A86	C-C1-C24	2.10	121.38	118.08
42	17	313	A86	C-C1-C24	2.10	121.38	118.08
30	16	308	CLA	O1A-CGA-CBA	2.10	129.82	123.08
30	18	301	CLA	C2A-C1A-CHA	2.10	127.53	123.86
39	j	101	DGD	C7B-C6B-C5B	-2.10	103.77	114.42
30	C	502	CLA	C11-C12-C13	-2.10	109.14	115.92
30	21	302	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
36	B	619	LMG	O2-C2-C1	-2.10	104.95	110.05
40	D	404	PL9	O2-C1-C2	-2.10	116.97	121.78
30	B	604	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
42	13	301	A86	C8-C6-C5	2.10	122.16	118.94
32	b	617	BCR	C40-C30-C25	2.10	113.70	110.30
30	B	603	CLA	O1D-CGD-CBD	2.10	128.78	124.48
30	b	608	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
30	C	511	CLA	CHA-C4D-ND	2.10	136.88	132.50
30	b	614	CLA	CHC-C4B-NB	2.10	126.48	124.26
30	15	309	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	C	506	CLA	O2A-CGA-O1A	-2.10	118.30	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	404	BCR	C7-C8-C9	-2.10	123.07	126.23
30	13	304	CLA	CAA-C2A-C1A	2.10	118.84	111.97
30	C	504	CLA	CHC-C4B-NB	2.10	126.47	124.26
30	12	307	CLA	CAA-C2A-C1A	2.09	118.84	111.97
42	11	312	A86	C-C1-C24	2.09	121.38	118.08
30	18	311	CLA	CHA-C1A-NA	-2.09	121.60	126.40
36	1	101	LMG	O2-C2-C3	-2.09	105.51	110.35
30	15	301	CLA	CMC-C2C-C1C	2.09	128.23	125.04
30	c	511	CLA	CHA-C4D-ND	2.09	136.88	132.50
30	B	606	CLA	C2D-C1D-ND	-2.09	108.56	110.10
39	J	101	DGD	C7B-C6B-C5B	-2.09	103.81	114.42
30	12	312	CLA	C2A-C1A-CHA	2.09	127.52	123.86
30	16	309	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
30	17	305	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	18	301	CLA	CHB-C1B-NB	2.09	126.47	124.26
40	d	405	PL9	C22-C23-C24	-2.09	122.63	127.66
30	c	503	CLA	C3B-C4B-NB	-2.09	108.58	110.52
30	11	304	CLA	C3B-C4B-NB	-2.09	108.58	110.52
30	14	309	CLA	CMB-C2B-C3B	2.09	131.65	126.59
30	19	304	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
32	C	515	BCR	C30-C25-C26	-2.09	119.67	122.61
30	18	308	CLA	C2A-C1A-CHA	2.09	127.51	123.86
37	B	625	LMU	C2'-C3'-C4'	2.09	114.45	109.68
40	d	405	PL9	O1-C4-C3	-2.09	118.42	120.72
30	C	507	CLA	CHA-C1A-NA	-2.09	121.61	126.40
30	15	303	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
30	c	506	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	c	507	CLA	CHA-C1A-NA	-2.09	121.61	126.40
30	C	503	CLA	C3C-C4C-NC	-2.09	108.23	110.57
30	15	304	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
30	11	307	CLA	CMB-C2B-C3B	2.09	131.64	126.59
42	15	316	A86	C8-C6-C5	2.09	122.14	118.94
30	21	304	CLA	CMB-C2B-C3B	2.09	131.64	126.59
40	D	407	PL9	C27-C28-C29	-2.09	122.64	127.66
42	20	213	A86	C34-O4-C38	-2.09	114.01	117.90
30	19	308	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
30	13	306	CLA	C2A-C1A-CHA	2.09	127.51	123.86
30	12	310	CLA	CHB-C1B-NB	2.09	126.47	124.26
36	Q	301	LMG	C1-C2-C3	-2.09	105.65	110.00
42	19	312	A86	C28-C27-C26	-2.09	120.00	122.92
40	D	404	PL9	C36-C37-C38	-2.08	105.03	111.88
30	b	615	CLA	CHB-C1B-C2B	-2.08	121.35	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	306	CLA	C2A-C1A-CHA	2.08	127.50	123.86
42	19	311	A86	C7-C6-C5	-2.08	120.00	122.92
30	19	302	CLA	C2D-C1D-ND	-2.08	108.57	110.10
30	18	308	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
30	21	303	CLA	C2A-C1A-CHA	2.08	127.50	123.86
30	B	614	CLA	CHC-C4B-NB	2.08	126.46	124.26
30	B	615	CLA	CHB-C1B-C2B	-2.08	121.36	127.24
30	11	303	CLA	CAA-C2A-C1A	2.08	118.80	111.97
42	16	312	A86	C-C1-C24	2.08	121.36	118.08
39	J	101	DGD	O6E-C1E-O5D	-2.08	105.04	109.97
30	20	206	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	c	506	CLA	CMC-C2C-C3C	2.08	131.77	126.12
30	20	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
32	b	616	BCR	C16-C15-C14	-2.08	119.21	123.47
30	13	302	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
30	C	512	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
30	20	207	CLA	CAA-C2A-C1A	2.08	118.79	111.97
30	20	207	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
30	16	302	CLA	C3A-C2A-C1A	2.08	104.45	101.34
30	20	209	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	c	504	CLA	CHC-C4B-NB	2.08	126.45	124.26
32	B	617	BCR	C16-C15-C14	-2.08	119.22	123.47
30	20	204	CLA	C2A-C1A-CHA	2.08	127.49	123.86
30	17	310	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	b	622	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
42	21	314	A86	C34-O4-C38	-2.07	114.03	117.90
40	D	404	PL9	C22-C23-C24	-2.07	122.67	127.66
42	18	302	A86	C8-C6-C5	2.07	122.12	118.94
30	14	305	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	12	303	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	20	203	CLA	C2A-C1A-CHA	2.07	127.48	123.86
42	13	315	A86	C8-C6-C5	2.07	122.12	118.94
30	17	306	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
30	a	402	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
30	12	305	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
30	14	302	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	21	306	CLA	C2A-C1A-CHA	2.07	127.48	123.86
35	b	621	LHG	C27-C26-C25	-2.07	103.92	114.42
31	d	403	PHO	CMA-C3A-C4A	-2.07	109.84	114.38
30	11	301	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
35	d	409	LHG	C5-O7-C7	-2.07	112.70	117.79
42	15	315	A86	C8-C6-C5	2.07	122.12	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	21	304	CLA	CHB-C4A-NA	2.07	127.37	124.51
31	A	403	PHO	CMA-C3A-C4A	-2.07	109.85	114.38
42	17	316	A86	C19-C18-C17	-2.07	106.78	110.77
30	14	303	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
40	D	407	PL9	C46-C47-C48	-2.07	105.08	111.88
30	A	402	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
30	B	601	CLA	CHC-C4B-NB	2.07	126.45	124.26
30	15	305	CLA	CHB-C1B-NB	2.07	126.45	124.26
30	16	302	CLA	CHD-C1D-ND	-2.07	122.55	124.45
35	L	101	LHG	C5-O7-C7	-2.07	112.70	117.79
30	19	309	CLA	CMB-C2B-C3B	2.07	131.59	126.59
30	B	612	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	Z	102	CLA	CHC-C4B-NB	2.07	126.44	124.26
30	20	208	CLA	CHA-C1A-NA	-2.07	121.67	126.40
30	B	612	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
30	W	103	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
30	C	502	CLA	C1-C2-C3	-2.06	122.47	126.04
30	b	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
30	B	605	CLA	C1-C2-C3	-2.06	122.47	126.04
30	c	512	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
30	13	309	CLA	C3B-C4B-NB	-2.06	108.60	110.52
32	A	405	BCR	C7-C8-C9	-2.06	123.12	126.23
32	C	515	BCR	C24-C23-C22	-2.06	123.12	126.23
42	21	313	A86	C19-C18-C17	-2.06	106.79	110.77
30	20	209	CLA	CMB-C2B-C3B	2.06	131.58	126.59
30	A	402	CLA	C3B-C4B-NB	-2.06	108.60	110.52
30	B	613	CLA	CHB-C1B-NB	2.06	126.44	124.26
33	L	103	SQD	O48-C23-O10	-2.06	118.39	123.59
30	C	520	CLA	CMB-C2B-C3B	2.06	131.58	126.59
30	B	606	CLA	C3B-C4B-NB	-2.06	108.60	110.52
30	d	402	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	20	205	CLA	C2D-C1D-ND	-2.06	108.59	110.10
30	w	102	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
30	13	308	CLA	CMB-C2B-C3B	2.06	131.58	126.59
30	12	308	CLA	C3B-C4B-NB	-2.06	108.61	110.52
35	B	622	LHG	C27-C26-C25	-2.06	103.97	114.42
30	17	303	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
40	d	405	PL9	C36-C37-C38	-2.06	105.12	111.88
30	15	307	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
30	17	305	CLA	CHB-C1B-NB	2.06	126.44	124.26
42	20	212	A86	C35-C34-C33	2.06	113.47	109.88
33	l	101	SQD	O48-C23-O10	-2.06	118.40	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	615	CLA	O2D-CGD-CBD	2.06	114.92	111.27
30	21	303	CLA	CHB-C1B-NB	2.06	126.43	124.26
30	c	502	CLA	C1-C2-C3	-2.06	122.49	126.04
30	21	305	CLA	C2A-C1A-CHA	2.06	127.45	123.86
30	c	512	CLA	C7-C6-C5	-2.05	107.78	113.36
32	B	624	BCR	C15-C16-C17	-2.05	119.27	123.47
30	b	612	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
30	C	513	CLA	C2A-C1A-CHA	2.05	127.45	123.86
30	b	612	CLA	C2A-C1A-CHA	2.05	127.45	123.86
30	17	307	CLA	C2A-C1A-CHA	2.05	127.45	123.86
30	b	602	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
30	16	301	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	15	301	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
30	12	307	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	d	406	CLA	CHC-C4B-NB	2.05	126.43	124.26
30	15	304	CLA	C2A-C1A-CHA	2.05	127.44	123.86
31	A	403	PHO	C1C-C2C-C3C	-2.05	106.91	108.61
30	12	311	CLA	CMB-C2B-C3B	2.05	131.55	126.59
39	C	516	DGD	C4E-C3E-C2E	-2.05	107.25	110.82
30	Z	102	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
36	12	301	LMG	O6-C1-O1	-2.05	105.13	109.97
39	C	516	DGD	CBB-CAB-C9B	-2.05	104.04	114.42
30	11	315	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	19	304	CLA	O1A-CGA-CBA	2.04	129.65	123.08
30	C	503	CLA	CHB-C1B-NB	2.04	126.42	124.26
30	15	303	CLA	C3A-C2A-C1A	2.04	104.39	101.34
30	15	306	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
30	c	507	CLA	CHB-C4A-NA	2.04	127.33	124.51
30	b	604	CLA	C1D-ND-C4D	2.04	107.78	106.33
30	B	602	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
39	c	517	DGD	C4E-C3E-C2E	-2.04	107.26	110.82
42	14	316	A86	C19-C18-C17	-2.04	106.83	110.77
30	d	401	CLA	CMB-C2B-C3B	2.04	131.53	126.59
30	B	604	CLA	CHB-C1B-NB	2.04	126.42	124.26
30	15	304	CLA	CHA-C4D-ND	2.04	136.76	132.50
30	13	305	CLA	C3B-C4B-NB	-2.04	108.62	110.52
30	16	303	CLA	C2D-C1D-ND	-2.04	108.60	110.10
42	21	313	A86	C-C1-C24	2.04	121.29	118.08
30	B	615	CLA	O2D-CGD-CBD	2.04	114.89	111.27
30	16	304	CLA	CHB-C1B-NB	2.04	126.41	124.26
42	17	315	A86	C9-C10-C11	-2.04	120.62	126.61
42	17	311	A86	C26-C25-C24	-2.04	116.86	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	408	BCR	C24-C23-C22	-2.04	123.16	126.23
30	12	313	CLA	C3B-C4B-NB	-2.04	108.63	110.52
30	20	203	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
39	C	516	DGD	O3E-C3E-C2E	-2.04	105.64	110.35
30	c	513	CLA	C2A-C1A-CHA	2.04	127.42	123.86
30	c	502	CLA	C3B-C4B-NB	-2.04	108.63	110.52
40	D	404	PL9	C31-C32-C33	-2.04	105.19	111.88
40	D	404	PL9	O1-C4-C3	-2.03	118.48	120.72
30	C	512	CLA	C7-C6-C5	-2.03	107.83	113.36
30	19	305	CLA	O1A-CGA-CBA	2.03	129.62	123.08
32	b	617	BCR	C1-C6-C5	-2.03	119.75	122.61
30	19	301	CLA	CHB-C1B-NB	2.03	126.41	124.26
39	c	517	DGD	CBB-CAB-C9B	-2.03	104.10	114.42
30	B	603	CLA	C3B-C4B-NB	-2.03	108.63	110.52
30	14	306	CLA	C3B-C4B-NB	-2.03	108.63	110.52
42	17	302	A86	C-C1-C24	2.03	121.28	118.08
42	20	201	A86	C23-C16-C17	-2.03	105.45	108.98
42	17	311	A86	C3-C4-C5	-2.03	119.31	123.47
30	d	401	CLA	C3A-C2A-C1A	2.03	104.38	101.34
32	F	101	BCR	C40-C30-C25	2.03	113.59	110.30
42	15	314	A86	C19-C18-C17	-2.03	106.85	110.77
39	J	101	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
30	14	308	CLA	CHA-C1A-NA	-2.03	121.75	126.40
42	20	210	A86	C34-O4-C38	-2.03	114.11	117.90
42	15	314	A86	C8-C6-C5	-2.03	115.83	118.94
36	b	618	LMG	C6-C5-C4	-2.03	108.25	113.00
39	j	101	DGD	C5B-C4B-C3B	-2.03	104.12	114.42
42	14	301	A86	C19-C18-C17	-2.03	106.86	110.77
39	c	517	DGD	O3E-C3E-C2E	-2.03	105.66	110.35
42	20	210	A86	C4-C3-C2	-2.03	119.32	123.47
30	19	308	CLA	CHB-C1B-NB	2.03	126.40	124.26
39	H	102	DGD	O6E-C1E-O5D	-2.03	105.17	109.97
40	d	408	PL9	C20-C19-C21	2.03	118.68	115.27
30	13	304	CLA	C2A-C1A-CHA	2.03	127.40	123.86
42	19	310	A86	C7-C6-C8	2.03	121.27	118.08
40	d	408	PL9	C46-C47-C48	-2.03	105.22	111.88
40	d	405	PL9	C31-C32-C33	-2.03	105.22	111.88
32	c	520	BCR	C37-C22-C21	-2.03	120.08	122.92
30	18	307	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
30	w	103	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
42	17	302	A86	C35-C34-C33	2.03	113.41	109.88
30	16	306	CLA	O2A-CGA-O1A	-2.03	118.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	11	314	A86	C19-C18-C17	-2.03	106.86	110.77
30	15	304	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
30	d	406	CLA	C1-C2-C3	-2.02	122.54	126.04
39	c	517	DGD	C7A-C6A-C5A	-2.02	104.15	114.42
30	12	310	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
32	C	515	BCR	C21-C20-C19	-2.02	116.90	123.22
30	18	306	CLA	C3B-C4B-NB	-2.02	108.64	110.52
42	11	312	A86	C7-C6-C5	-2.02	120.09	122.92
32	m	103	BCR	C16-C15-C14	-2.02	119.33	123.47
41	V	201	HEM	CHD-C1D-ND	2.02	126.62	124.42
41	V	201	HEM	CAD-C3D-C2D	-2.02	124.11	127.88
30	21	302	CLA	CHC-C4B-NB	2.02	126.40	124.26
30	19	304	CLA	C3B-C4B-NB	-2.02	108.64	110.52
30	20	206	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
30	18	301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	b	603	CLA	CHC-C1C-NC	2.02	127.27	124.20
30	D	401	CLA	CMB-C2B-C3B	2.02	131.48	126.59
30	20	207	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	c	512	CLA	O2D-CGD-CBD	2.02	114.86	111.27
42	12	319	A86	C19-C18-C17	-2.02	106.87	110.77
40	D	407	PL9	C20-C19-C21	2.02	118.67	115.27
30	A	402	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
30	B	603	CLA	CHB-C1B-NB	2.02	126.39	124.26
30	14	309	CLA	CHC-C4B-NB	2.02	126.39	124.26
30	B	603	CLA	C2D-C1D-ND	-2.02	108.62	110.10
30	c	514	CLA	C3B-C4B-NB	-2.02	108.64	110.52
30	17	301	CLA	C7-C6-C5	-2.02	107.88	113.36
30	18	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
42	11	314	A86	C8-C6-C5	-2.02	115.85	118.94
30	20	204	CLA	CHB-C1B-NB	2.02	126.39	124.26
30	17	305	CLA	C2A-C1A-CHA	2.02	127.38	123.86
39	C	516	DGD	C7A-C6A-C5A	-2.02	104.19	114.42
30	B	601	CLA	C3A-C2A-C1A	2.02	104.36	101.34
30	18	309	CLA	C1-C2-C3	-2.02	122.56	126.04
30	C	502	CLA	CHD-C1D-ND	-2.02	122.60	124.45
30	C	514	CLA	O1D-CGD-CBD	2.02	128.61	124.48
30	20	204	CLA	O1D-CGD-CBD	2.02	128.61	124.48
30	b	602	CLA	C4-C3-C5	2.01	118.66	115.27
32	H	101	BCR	C20-C21-C22	-2.01	124.44	127.31
32	h	101	BCR	C20-C21-C22	-2.01	124.44	127.31
32	b	623	BCR	C15-C16-C17	-2.01	119.35	123.47
30	D	401	CLA	C3A-C2A-C1A	2.01	104.36	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	502	CLA	C3C-C4C-NC	-2.01	108.31	110.57
30	C	504	CLA	C3A-C2A-C1A	2.01	104.35	101.34
30	21	305	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
30	14	311	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
42	15	312	A86	C7-C6-C5	-2.01	120.10	122.92
42	20	210	A86	C28-C27-C26	-2.01	120.10	122.92
30	16	302	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
42	14	301	A86	C8-C6-C5	-2.01	115.85	118.94
32	h	101	BCR	C33-C5-C6	-2.01	122.27	124.53
39	h	102	DGD	O6E-C1E-O5D	-2.01	105.21	109.97
30	b	605	CLA	C1-C2-C3	-2.01	122.56	126.04
30	c	512	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
30	17	305	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
30	17	307	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
39	c	518	DGD	C7B-C6B-C5B	-2.01	104.22	114.42
30	C	503	CLA	C3B-C4B-NB	-2.01	108.65	110.52
30	11	308	CLA	C3B-C4B-NB	-2.01	108.65	110.52
30	B	613	CLA	O1D-CGD-CBD	2.01	128.60	124.48
31	d	403	PHO	C1C-C2C-C3C	-2.01	106.94	108.61
32	B	616	BCR	C16-C15-C14	-2.01	119.36	123.47
30	15	307	CLA	CHA-C1A-NA	-2.01	121.80	126.40
30	15	303	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
36	c	519	LMG	C22-C21-C20	-2.01	104.23	114.42
30	b	603	CLA	C2D-C1D-ND	-2.01	108.62	110.10
32	c	516	BCR	C16-C15-C14	-2.01	119.36	123.47
30	D	405	CLA	C11-C12-C13	-2.01	109.43	115.92
36	12	301	LMG	O7-C10-O9	-2.01	118.85	123.70
30	20	208	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
30	b	603	CLA	CHB-C1B-NB	2.01	126.38	124.26
32	f	101	BCR	C40-C30-C25	2.01	113.55	110.30
30	19	301	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
30	c	509	CLA	C16-C15-C13	-2.01	109.44	115.92
30	d	406	CLA	C11-C12-C13	-2.01	109.44	115.92
30	c	504	CLA	C3A-C2A-C1A	2.01	104.34	101.34
30	C	509	CLA	C16-C15-C13	-2.01	109.44	115.92
32	c	516	BCR	C21-C20-C19	-2.01	116.96	123.22
35	A	408	LHG	C27-C26-C25	-2.01	104.25	114.42
39	C	517	DGD	C5B-C4B-C3B	-2.01	104.25	114.42
35	a	407	LHG	C27-C26-C25	-2.01	104.25	114.42
39	C	517	DGD	C7B-C6B-C5B	-2.01	104.25	114.42
36	Q	301	LMG	C22-C21-C20	-2.00	104.25	114.42
30	17	308	CLA	CHC-C4B-NB	2.00	126.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	502	CLA	CHD-C1D-ND	-2.00	122.61	124.45
30	B	604	CLA	CHA-C4D-ND	2.00	136.69	132.50
30	15	302	CLA	CHA-C1A-NA	-2.00	121.81	126.40
32	B	618	BCR	C1-C6-C5	-2.00	119.79	122.61
30	C	506	CLA	CHC-C1C-NC	2.00	127.24	124.20
30	b	606	CLA	C3B-C4B-NB	-2.00	108.66	110.52
30	15	304	CLA	CHC-C4B-NB	2.00	126.38	124.26
42	16	313	A86	C8-C6-C5	-2.00	115.87	118.94
30	16	302	CLA	C2B-C1B-NB	-2.00	108.89	110.23
42	12	304	A86	C23-C16-C17	-2.00	105.50	108.98
30	13	310	CLA	CHB-C1B-NB	2.00	126.38	124.26
39	c	518	DGD	C5B-C4B-C3B	-2.00	104.26	114.42
36	1	101	LMG	O7-C10-O9	-2.00	118.86	123.70
32	A	409	BCR	C24-C23-C22	-2.00	123.21	126.23
30	A	404	CLA	O2D-CGD-CBD	2.00	114.82	111.27
30	a	402	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
40	D	404	PL9	C27-C28-C29	-2.00	122.84	127.66

There are no chirality outliers.

All (3923) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	A	404	CLA	C2B-C3B-CAB-CBB
30	A	404	CLA	C4B-C3B-CAB-CBB
30	B	601	CLA	C1A-C2A-CAA-CBA
30	B	601	CLA	C2B-C3B-CAB-CBB
30	B	601	CLA	C4B-C3B-CAB-CBB
30	B	601	CLA	CHA-CBD-CGD-O1D
30	B	601	CLA	CHA-CBD-CGD-O2D
30	B	601	CLA	CAD-CBD-CGD-O1D
30	B	602	CLA	C2-C3-C5-C6
30	B	602	CLA	C4-C3-C5-C6
30	B	603	CLA	CAD-CBD-CGD-O1D
30	B	603	CLA	CAD-CBD-CGD-O2D
30	B	603	CLA	C4-C3-C5-C6
30	B	604	CLA	CHA-CBD-CGD-O1D
30	B	604	CLA	CHA-CBD-CGD-O2D
30	B	605	CLA	C2B-C3B-CAB-CBB
30	B	605	CLA	C4B-C3B-CAB-CBB
30	B	605	CLA	C2-C3-C5-C6
30	B	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	B	608	CLA	CHA-CBD-CGD-O1D
30	B	608	CLA	CHA-CBD-CGD-O2D
30	B	610	CLA	CHA-CBD-CGD-O2D
30	B	611	CLA	CHA-CBD-CGD-O1D
30	B	611	CLA	CHA-CBD-CGD-O2D
30	B	611	CLA	CBD-CGD-O2D-CED
30	B	612	CLA	C1A-C2A-CAA-CBA
30	B	612	CLA	C3A-C2A-CAA-CBA
30	B	613	CLA	C2-C3-C5-C6
30	B	613	CLA	C4-C3-C5-C6
30	B	614	CLA	CHA-CBD-CGD-O1D
30	B	614	CLA	CHA-CBD-CGD-O2D
30	B	615	CLA	CHA-CBD-CGD-O2D
30	C	502	CLA	C1A-C2A-CAA-CBA
30	C	503	CLA	C2B-C3B-CAB-CBB
30	C	503	CLA	C4B-C3B-CAB-CBB
30	C	504	CLA	C2B-C3B-CAB-CBB
30	C	504	CLA	C4B-C3B-CAB-CBB
30	C	504	CLA	CBD-CGD-O2D-CED
30	C	505	CLA	CHA-CBD-CGD-O1D
30	C	505	CLA	CHA-CBD-CGD-O2D
30	C	506	CLA	CHA-CBD-CGD-O1D
30	C	506	CLA	CHA-CBD-CGD-O2D
30	C	510	CLA	CBD-CGD-O2D-CED
30	C	510	CLA	C6-C7-C8-C9
30	C	512	CLA	CHA-CBD-CGD-O1D
30	C	514	CLA	CBD-CGD-O2D-CED
30	C	519	CLA	C2B-C3B-CAB-CBB
30	C	519	CLA	C4B-C3B-CAB-CBB
30	D	401	CLA	C2B-C3B-CAB-CBB
30	D	401	CLA	C4B-C3B-CAB-CBB
30	D	401	CLA	CHA-CBD-CGD-O1D
30	D	401	CLA	CHA-CBD-CGD-O2D
30	D	402	CLA	C2B-C3B-CAB-CBB
30	D	402	CLA	C4B-C3B-CAB-CBB
30	D	402	CLA	CHA-CBD-CGD-O1D
30	D	402	CLA	CHA-CBD-CGD-O2D
30	D	405	CLA	C1A-C2A-CAA-CBA
30	M	101	CLA	CHA-CBD-CGD-O1D
30	M	101	CLA	CHA-CBD-CGD-O2D
30	M	101	CLA	CAD-CBD-CGD-O1D
30	M	101	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	M	101	CLA	C2-C3-C5-C6
30	M	101	CLA	C4-C3-C5-C6
30	Z	102	CLA	C2B-C3B-CAB-CBB
30	Z	102	CLA	C4B-C3B-CAB-CBB
30	W	102	CLA	C1A-C2A-CAA-CBA
30	a	402	CLA	CBD-CGD-O2D-CED
30	a	403	CLA	C2B-C3B-CAB-CBB
30	a	403	CLA	C4B-C3B-CAB-CBB
30	b	601	CLA	C1A-C2A-CAA-CBA
30	b	601	CLA	C2B-C3B-CAB-CBB
30	b	601	CLA	C4B-C3B-CAB-CBB
30	b	601	CLA	CHA-CBD-CGD-O1D
30	b	601	CLA	CHA-CBD-CGD-O2D
30	b	601	CLA	CAD-CBD-CGD-O1D
30	b	602	CLA	C2-C3-C5-C6
30	b	602	CLA	C4-C3-C5-C6
30	b	603	CLA	CAD-CBD-CGD-O1D
30	b	603	CLA	CAD-CBD-CGD-O2D
30	b	603	CLA	C4-C3-C5-C6
30	b	604	CLA	CHA-CBD-CGD-O1D
30	b	604	CLA	CHA-CBD-CGD-O2D
30	b	605	CLA	C2B-C3B-CAB-CBB
30	b	605	CLA	C4B-C3B-CAB-CBB
30	b	605	CLA	C2-C3-C5-C6
30	b	605	CLA	C4-C3-C5-C6
30	b	608	CLA	CHA-CBD-CGD-O1D
30	b	608	CLA	CHA-CBD-CGD-O2D
30	b	610	CLA	CHA-CBD-CGD-O2D
30	b	611	CLA	CHA-CBD-CGD-O1D
30	b	611	CLA	CHA-CBD-CGD-O2D
30	b	611	CLA	CBD-CGD-O2D-CED
30	b	612	CLA	C1A-C2A-CAA-CBA
30	b	612	CLA	C3A-C2A-CAA-CBA
30	b	613	CLA	C2-C3-C5-C6
30	b	613	CLA	C4-C3-C5-C6
30	b	614	CLA	CHA-CBD-CGD-O1D
30	b	614	CLA	CHA-CBD-CGD-O2D
30	b	615	CLA	CHA-CBD-CGD-O2D
30	c	502	CLA	C1A-C2A-CAA-CBA
30	c	503	CLA	C2B-C3B-CAB-CBB
30	c	503	CLA	C4B-C3B-CAB-CBB
30	c	504	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	c	504	CLA	C4B-C3B-CAB-CBB
30	c	504	CLA	CBD-CGD-O2D-CED
30	c	505	CLA	CHA-CBD-CGD-O1D
30	c	505	CLA	CHA-CBD-CGD-O2D
30	c	506	CLA	CHA-CBD-CGD-O1D
30	c	506	CLA	CHA-CBD-CGD-O2D
30	c	510	CLA	CBD-CGD-O2D-CED
30	c	510	CLA	C6-C7-C8-C9
30	c	512	CLA	CHA-CBD-CGD-O1D
30	c	513	CLA	C1A-C2A-CAA-CBA
30	c	514	CLA	CBD-CGD-O2D-CED
30	d	401	CLA	C2B-C3B-CAB-CBB
30	d	401	CLA	C4B-C3B-CAB-CBB
30	d	401	CLA	CHA-CBD-CGD-O1D
30	d	401	CLA	CHA-CBD-CGD-O2D
30	d	402	CLA	C2B-C3B-CAB-CBB
30	d	402	CLA	C4B-C3B-CAB-CBB
30	d	402	CLA	CHA-CBD-CGD-O1D
30	d	402	CLA	CHA-CBD-CGD-O2D
30	d	406	CLA	C1A-C2A-CAA-CBA
30	m	101	CLA	CHA-CBD-CGD-O1D
30	m	101	CLA	CHA-CBD-CGD-O2D
30	m	101	CLA	CAD-CBD-CGD-O1D
30	m	101	CLA	CAD-CBD-CGD-O2D
30	m	101	CLA	C2-C3-C5-C6
30	m	101	CLA	C4-C3-C5-C6
30	z	101	CLA	C2B-C3B-CAB-CBB
30	z	101	CLA	C4B-C3B-CAB-CBB
30	w	102	CLA	C1A-C2A-CAA-CBA
30	11	301	CLA	C3A-C2A-CAA-CBA
30	11	303	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	CHA-CBD-CGD-O1D
30	11	304	CLA	CHA-CBD-CGD-O2D
30	11	305	CLA	C1A-C2A-CAA-CBA
30	11	305	CLA	C3A-C2A-CAA-CBA
30	11	305	CLA	CHA-CBD-CGD-O1D
30	11	308	CLA	C1A-C2A-CAA-CBA
30	11	309	CLA	C1A-C2A-CAA-CBA
30	11	309	CLA	C4B-C3B-CAB-CBB
30	11	315	CLA	CHA-CBD-CGD-O1D
30	11	315	CLA	CHA-CBD-CGD-O2D
30	12	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	12	303	CLA	CHA-CBD-CGD-O2D
30	12	305	CLA	C3A-C2A-CAA-CBA
30	12	307	CLA	C1A-C2A-CAA-CBA
30	12	308	CLA	CHA-CBD-CGD-O1D
30	12	308	CLA	CHA-CBD-CGD-O2D
30	12	309	CLA	C1A-C2A-CAA-CBA
30	12	309	CLA	C3A-C2A-CAA-CBA
30	12	309	CLA	CHA-CBD-CGD-O1D
30	12	312	CLA	CHA-CBD-CGD-O1D
30	12	312	CLA	CHA-CBD-CGD-O2D
30	12	313	CLA	C1A-C2A-CAA-CBA
30	12	314	CLA	C1A-C2A-CAA-CBA
30	12	314	CLA	C4B-C3B-CAB-CBB
30	13	302	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C1A-C2A-CAA-CBA
30	13	305	CLA	CHA-CBD-CGD-O1D
30	13	305	CLA	CHA-CBD-CGD-O2D
30	13	306	CLA	C1A-C2A-CAA-CBA
30	13	306	CLA	C3A-C2A-CAA-CBA
30	13	306	CLA	CHA-CBD-CGD-O1D
30	13	309	CLA	C1A-C2A-CAA-CBA
30	13	310	CLA	C1A-C2A-CAA-CBA
30	13	310	CLA	C4B-C3B-CAB-CBB
30	14	302	CLA	CHA-CBD-CGD-O1D
30	14	302	CLA	CHA-CBD-CGD-O2D
30	14	303	CLA	C3A-C2A-CAA-CBA
30	14	305	CLA	C1A-C2A-CAA-CBA
30	14	306	CLA	CHA-CBD-CGD-O1D
30	14	306	CLA	CHA-CBD-CGD-O2D
30	14	307	CLA	C1A-C2A-CAA-CBA
30	14	307	CLA	C3A-C2A-CAA-CBA
30	14	307	CLA	CHA-CBD-CGD-O1D
30	14	310	CLA	C1A-C2A-CAA-CBA
30	14	311	CLA	C1A-C2A-CAA-CBA
30	14	311	CLA	C4B-C3B-CAB-CBB
30	15	301	CLA	C1A-C2A-CAA-CBA
30	15	301	CLA	C3A-C2A-CAA-CBA
30	15	302	CLA	C1A-C2A-CAA-CBA
30	15	302	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	C1A-C2A-CAA-CBA
30	15	303	CLA	CHA-CBD-CGD-O1D
30	15	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	15	306	CLA	C2B-C3B-CAB-CBB
30	15	306	CLA	C4B-C3B-CAB-CBB
30	15	307	CLA	C1A-C2A-CAA-CBA
30	15	307	CLA	C3A-C2A-CAA-CBA
30	15	309	CLA	C2B-C3B-CAB-CBB
30	15	309	CLA	C4B-C3B-CAB-CBB
30	16	301	CLA	C2B-C3B-CAB-CBB
30	16	301	CLA	C4B-C3B-CAB-CBB
30	16	302	CLA	C2B-C3B-CAB-CBB
30	16	302	CLA	C4B-C3B-CAB-CBB
30	16	302	CLA	CBD-CGD-O2D-CED
30	16	303	CLA	C1A-C2A-CAA-CBA
30	16	303	CLA	CBD-CGD-O2D-CED
30	16	304	CLA	C1A-C2A-CAA-CBA
30	16	304	CLA	CHA-CBD-CGD-O1D
30	16	304	CLA	CHA-CBD-CGD-O2D
30	16	304	CLA	CAD-CBD-CGD-O1D
30	16	306	CLA	C4B-C3B-CAB-CBB
30	16	307	CLA	C1A-C2A-CAA-CBA
30	16	307	CLA	C3A-C2A-CAA-CBA
30	16	308	CLA	C1A-C2A-CAA-CBA
30	16	308	CLA	C3A-C2A-CAA-CBA
30	16	308	CLA	C2B-C3B-CAB-CBB
30	16	308	CLA	C4B-C3B-CAB-CBB
30	16	309	CLA	C1A-C2A-CAA-CBA
30	16	309	CLA	C2B-C3B-CAB-CBB
30	16	309	CLA	C4B-C3B-CAB-CBB
30	17	301	CLA	CHA-CBD-CGD-O1D
30	17	301	CLA	CHA-CBD-CGD-O2D
30	17	303	CLA	C1A-C2A-CAA-CBA
30	17	303	CLA	C3A-C2A-CAA-CBA
30	17	303	CLA	C2B-C3B-CAB-CBB
30	17	303	CLA	C4B-C3B-CAB-CBB
30	17	303	CLA	CHA-CBD-CGD-O1D
30	17	303	CLA	CHA-CBD-CGD-O2D
30	17	304	CLA	C1A-C2A-CAA-CBA
30	17	304	CLA	CBD-CGD-O2D-CED
30	17	305	CLA	C1A-C2A-CAA-CBA
30	17	305	CLA	CHA-CBD-CGD-O1D
30	17	305	CLA	CHA-CBD-CGD-O2D
30	17	306	CLA	CBD-CGD-O2D-CED
30	17	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	17	307	CLA	C4B-C3B-CAB-CBB
30	17	308	CLA	C1A-C2A-CAA-CBA
30	17	308	CLA	C3A-C2A-CAA-CBA
30	17	308	CLA	C2B-C3B-CAB-CBB
30	17	308	CLA	C4B-C3B-CAB-CBB
30	17	309	CLA	CHA-CBD-CGD-O2D
30	17	310	CLA	C1A-C2A-CAA-CBA
30	17	310	CLA	C4B-C3B-CAB-CBB
30	18	301	CLA	C2B-C3B-CAB-CBB
30	18	301	CLA	C4B-C3B-CAB-CBB
30	18	301	CLA	CHA-CBD-CGD-O1D
30	18	301	CLA	CHA-CBD-CGD-O2D
30	18	303	CLA	C1A-C2A-CAA-CBA
30	18	303	CLA	C3A-C2A-CAA-CBA
30	18	304	CLA	CBD-CGD-O2D-CED
30	18	305	CLA	C1A-C2A-CAA-CBA
30	18	305	CLA	C4B-C3B-CAB-CBB
30	18	305	CLA	CHA-CBD-CGD-O1D
30	18	305	CLA	CHA-CBD-CGD-O2D
30	18	308	CLA	C4B-C3B-CAB-CBB
30	18	309	CLA	C3A-C2A-CAA-CBA
30	18	310	CLA	C2B-C3B-CAB-CBB
30	18	310	CLA	C4B-C3B-CAB-CBB
30	18	311	CLA	C2B-C3B-CAB-CBB
30	18	311	CLA	C4B-C3B-CAB-CBB
30	18	311	CLA	CHA-CBD-CGD-O1D
30	18	311	CLA	CHA-CBD-CGD-O2D
30	18	312	CLA	C2B-C3B-CAB-CBB
30	18	312	CLA	C4B-C3B-CAB-CBB
30	19	301	CLA	C1A-C2A-CAA-CBA
30	19	301	CLA	C3A-C2A-CAA-CBA
30	19	302	CLA	CBD-CGD-O2D-CED
30	19	304	CLA	C4B-C3B-CAB-CBB
30	19	305	CLA	C1A-C2A-CAA-CBA
30	19	305	CLA	C3A-C2A-CAA-CBA
30	19	309	CLA	C1A-C2A-CAA-CBA
30	19	309	CLA	C3A-C2A-CAA-CBA
30	20	202	CLA	C1A-C2A-CAA-CBA
30	20	202	CLA	C3A-C2A-CAA-CBA
30	20	202	CLA	CHA-CBD-CGD-O1D
30	20	202	CLA	CHA-CBD-CGD-O2D
30	20	203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	20	203	CLA	C4B-C3B-CAB-CBB
30	20	204	CLA	C1A-C2A-CAA-CBA
30	20	206	CLA	C4B-C3B-CAB-CBB
30	20	207	CLA	C1A-C2A-CAA-CBA
30	20	208	CLA	C1A-C2A-CAA-CBA
30	20	209	CLA	C1A-C2A-CAA-CBA
30	20	209	CLA	C3A-C2A-CAA-CBA
30	20	209	CLA	C2B-C3B-CAB-CBB
30	20	209	CLA	C4B-C3B-CAB-CBB
30	21	301	CLA	C1A-C2A-CAA-CBA
30	21	302	CLA	C1A-C2A-CAA-CBA
30	21	302	CLA	CBD-CGD-O2D-CED
30	21	303	CLA	C1A-C2A-CAA-CBA
30	21	303	CLA	C2B-C3B-CAB-CBB
30	21	303	CLA	C4B-C3B-CAB-CBB
30	21	306	CLA	C1A-C2A-CAA-CBA
30	21	306	CLA	C3A-C2A-CAA-CBA
30	21	306	CLA	C2B-C3B-CAB-CBB
30	21	306	CLA	C4B-C3B-CAB-CBB
30	21	307	CLA	C4B-C3B-CAB-CBB
32	A	405	BCR	C7-C8-C9-C10
32	A	405	BCR	C35-C13-C14-C15
32	A	405	BCR	C14-C15-C16-C17
32	A	405	BCR	C16-C17-C18-C19
32	A	405	BCR	C16-C17-C18-C36
32	A	405	BCR	C18-C19-C20-C21
32	A	409	BCR	C6-C7-C8-C9
32	A	409	BCR	C7-C8-C9-C10
32	A	409	BCR	C7-C8-C9-C34
32	B	616	BCR	C23-C24-C25-C30
32	B	617	BCR	C1-C6-C7-C8
32	B	617	BCR	C7-C8-C9-C10
32	B	617	BCR	C20-C21-C22-C37
32	B	618	BCR	C1-C6-C7-C8
32	B	618	BCR	C7-C8-C9-C10
32	B	624	BCR	C6-C7-C8-C9
32	B	624	BCR	C7-C8-C9-C10
32	B	624	BCR	C10-C11-C12-C13
32	B	624	BCR	C11-C12-C13-C35
32	B	624	BCR	C16-C17-C18-C36
32	B	624	BCR	C20-C21-C22-C23
32	B	624	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
32	C	515	BCR	C1-C6-C7-C8
32	C	515	BCR	C22-C23-C24-C25
32	C	518	BCR	C1-C6-C7-C8
32	C	518	BCR	C21-C22-C23-C24
32	F	101	BCR	C7-C8-C9-C10
32	F	101	BCR	C11-C10-C9-C34
32	F	101	BCR	C35-C13-C14-C15
32	F	101	BCR	C16-C17-C18-C36
32	F	101	BCR	C21-C22-C23-C24
32	F	101	BCR	C37-C22-C23-C24
32	F	101	BCR	C22-C23-C24-C25
32	H	101	BCR	C1-C6-C7-C8
32	H	101	BCR	C20-C21-C22-C37
32	H	101	BCR	C37-C22-C23-C24
32	Y	101	BCR	C7-C8-C9-C34
32	Y	101	BCR	C11-C12-C13-C35
32	Y	101	BCR	C17-C18-C19-C20
32	Y	101	BCR	C18-C19-C20-C21
32	Y	101	BCR	C21-C22-C23-C24
32	Z	101	BCR	C11-C12-C13-C14
32	Z	101	BCR	C11-C12-C13-C35
32	Z	101	BCR	C16-C17-C18-C36
32	Z	101	BCR	C21-C22-C23-C24
32	Z	101	BCR	C23-C24-C25-C30
32	a	404	BCR	C7-C8-C9-C10
32	a	404	BCR	C35-C13-C14-C15
32	a	404	BCR	C14-C15-C16-C17
32	a	404	BCR	C16-C17-C18-C19
32	a	404	BCR	C16-C17-C18-C36
32	a	404	BCR	C18-C19-C20-C21
32	a	408	BCR	C6-C7-C8-C9
32	a	408	BCR	C7-C8-C9-C10
32	a	408	BCR	C7-C8-C9-C34
32	b	616	BCR	C1-C6-C7-C8
32	b	616	BCR	C7-C8-C9-C10
32	b	616	BCR	C20-C21-C22-C37
32	b	617	BCR	C1-C6-C7-C8
32	b	617	BCR	C7-C8-C9-C10
32	b	623	BCR	C6-C7-C8-C9
32	b	623	BCR	C7-C8-C9-C10
32	b	623	BCR	C10-C11-C12-C13
32	b	623	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
32	b	623	BCR	C16-C17-C18-C36
32	b	623	BCR	C20-C21-C22-C23
32	b	623	BCR	C20-C21-C22-C37
32	c	515	BCR	C11-C12-C13-C14
32	c	515	BCR	C11-C12-C13-C35
32	c	515	BCR	C16-C17-C18-C36
32	c	515	BCR	C21-C22-C23-C24
32	c	515	BCR	C23-C24-C25-C30
32	c	516	BCR	C1-C6-C7-C8
32	c	516	BCR	C22-C23-C24-C25
32	c	520	BCR	C7-C8-C9-C34
32	c	520	BCR	C11-C12-C13-C35
32	c	520	BCR	C17-C18-C19-C20
32	c	520	BCR	C18-C19-C20-C21
32	c	520	BCR	C21-C22-C23-C24
32	c	521	BCR	C1-C6-C7-C8
32	c	521	BCR	C21-C22-C23-C24
32	f	101	BCR	C7-C8-C9-C10
32	f	101	BCR	C11-C10-C9-C34
32	f	101	BCR	C35-C13-C14-C15
32	f	101	BCR	C16-C17-C18-C36
32	f	101	BCR	C21-C22-C23-C24
32	f	101	BCR	C37-C22-C23-C24
32	f	101	BCR	C22-C23-C24-C25
32	h	101	BCR	C1-C6-C7-C8
32	h	101	BCR	C20-C21-C22-C37
32	h	101	BCR	C37-C22-C23-C24
32	m	103	BCR	C23-C24-C25-C30
33	A	406	SQD	C5-C6-S-O7
33	B	621	SQD	C2-C1-O6-C44
33	L	103	SQD	O5-C1-O6-C44
33	L	103	SQD	C8-C7-O47-C45
33	L	103	SQD	O5-C5-C6-S
33	a	405	SQD	C5-C6-S-O7
33	b	620	SQD	C2-C1-O6-C44
33	l	101	SQD	O5-C1-O6-C44
33	l	101	SQD	C8-C7-O47-C45
33	l	101	SQD	O5-C5-C6-S
35	A	408	LHG	C3-O3-P-O5
35	A	408	LHG	C4-O6-P-O3
35	B	622	LHG	C3-O3-P-O4
35	B	622	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
35	L	101	LHG	O1-C1-C2-C3
35	L	101	LHG	C3-O3-P-O4
35	L	101	LHG	C3-O3-P-O6
35	L	102	LHG	C4-O6-P-O5
35	a	407	LHG	C3-O3-P-O5
35	a	407	LHG	C4-O6-P-O3
35	b	621	LHG	C3-O3-P-O4
35	b	621	LHG	C4-O6-P-O4
35	d	409	LHG	O1-C1-C2-C3
35	d	409	LHG	C3-O3-P-O4
35	d	409	LHG	C3-O3-P-O6
35	l	102	LHG	C4-O6-P-O5
36	M	102	LMG	O9-C10-O7-C8
36	W	101	LMG	O6-C1-O1-C7
36	W	101	LMG	O1-C7-C8-O7
36	1	101	LMG	O6-C1-O1-C7
36	m	102	LMG	O9-C10-O7-C8
36	w	101	LMG	O6-C1-O1-C7
36	w	101	LMG	O1-C7-C8-O7
36	12	301	LMG	O6-C1-O1-C7
37	12	302	LMU	C2-C1-O1'-C1'
40	D	404	PL9	C7-C8-C9-C11
40	D	404	PL9	C24-C26-C27-C28
40	D	404	PL9	C37-C38-C39-C40
40	D	404	PL9	C44-C46-C47-C48
40	D	407	PL9	C12-C13-C14-C16
40	D	407	PL9	C42-C43-C44-C45
40	d	405	PL9	C7-C8-C9-C11
40	d	405	PL9	C24-C26-C27-C28
40	d	405	PL9	C37-C38-C39-C40
40	d	405	PL9	C44-C46-C47-C48
40	d	408	PL9	C12-C13-C14-C16
40	d	408	PL9	C42-C43-C44-C45
42	11	310	A86	C39-C38-O4-C34
42	11	310	A86	C5-C6-C8-C9
42	11	310	A86	C7-C6-C8-C9
42	11	312	A86	C26-C27-C29-C30
42	11	312	A86	C28-C27-C29-C30
42	11	312	A86	C35-C34-O4-C38
42	11	313	A86	C2-C1-C24-C25
42	11	313	A86	C12-C11-C13-O
42	11	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
42	11	314	A86	C39-C38-O4-C34
42	11	314	A86	O5-C38-O4-C34
42	11	316	A86	C11-C13-C14-C15
42	11	316	A86	C13-C14-C15-C16
42	11	316	A86	C39-C38-O4-C34
42	11	316	A86	O5-C38-O4-C34
42	12	304	A86	C11-C13-C14-C15
42	12	304	A86	C13-C14-C15-C16
42	12	304	A86	C39-C38-O4-C34
42	12	304	A86	O5-C38-O4-C34
42	12	315	A86	C39-C38-O4-C34
42	12	315	A86	C5-C6-C8-C9
42	12	315	A86	C7-C6-C8-C9
42	12	317	A86	C26-C27-C29-C30
42	12	317	A86	C28-C27-C29-C30
42	12	317	A86	C35-C34-O4-C38
42	12	318	A86	C2-C1-C24-C25
42	12	318	A86	C12-C11-C13-O
42	12	319	A86	C24-C25-C26-C27
42	12	319	A86	C39-C38-O4-C34
42	12	319	A86	O5-C38-O4-C34
42	13	301	A86	C11-C13-C14-C15
42	13	301	A86	C13-C14-C15-C16
42	13	301	A86	C39-C38-O4-C34
42	13	301	A86	O5-C38-O4-C34
42	13	311	A86	C39-C38-O4-C34
42	13	311	A86	C5-C6-C8-C9
42	13	311	A86	C7-C6-C8-C9
42	13	313	A86	C26-C27-C29-C30
42	13	313	A86	C28-C27-C29-C30
42	13	313	A86	C35-C34-O4-C38
42	13	314	A86	C2-C1-C24-C25
42	13	314	A86	C12-C11-C13-O
42	13	315	A86	C11-C13-C14-C15
42	13	315	A86	C13-C14-C15-C16
42	13	315	A86	C39-C38-O4-C34
42	13	315	A86	O5-C38-O4-C34
42	14	301	A86	C24-C25-C26-C27
42	14	301	A86	C39-C38-O4-C34
42	14	301	A86	O5-C38-O4-C34
42	14	312	A86	C39-C38-O4-C34
42	14	312	A86	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
42	14	312	A86	C7-C6-C8-C9
42	14	314	A86	C26-C27-C29-C30
42	14	314	A86	C28-C27-C29-C30
42	14	314	A86	C35-C34-O4-C38
42	14	315	A86	C2-C1-C24-C25
42	14	315	A86	C12-C11-C13-O
42	14	316	A86	C24-C25-C26-C27
42	14	316	A86	C39-C38-O4-C34
42	14	316	A86	O5-C38-O4-C34
42	15	310	A86	C39-C38-O4-C34
42	15	310	A86	C5-C6-C8-C9
42	15	310	A86	C7-C6-C8-C9
42	15	312	A86	C26-C27-C29-C30
42	15	312	A86	C28-C27-C29-C30
42	15	312	A86	C35-C34-O4-C38
42	15	313	A86	C2-C1-C24-C25
42	15	313	A86	C12-C11-C13-O
42	15	314	A86	C24-C25-C26-C27
42	15	314	A86	C39-C38-O4-C34
42	15	314	A86	O5-C38-O4-C34
42	15	315	A86	C11-C13-C14-C15
42	15	315	A86	C13-C14-C15-C16
42	15	315	A86	C39-C38-O4-C34
42	15	315	A86	O5-C38-O4-C34
42	15	316	A86	C11-C13-C14-C15
42	15	316	A86	C13-C14-C15-C16
42	15	316	A86	C39-C38-O4-C34
42	15	316	A86	O5-C38-O4-C34
42	16	310	A86	C13-C14-C15-C16
42	16	310	A86	C26-C27-C29-C30
42	16	310	A86	C28-C27-C29-C30
42	16	312	A86	C26-C27-C29-C30
42	16	312	A86	C28-C27-C29-C30
42	16	312	A86	C35-C34-O4-C38
42	16	313	A86	C24-C25-C26-C27
42	16	313	A86	C39-C38-O4-C34
42	16	313	A86	O5-C38-O4-C34
42	17	302	A86	C-C1-C24-C25
42	17	302	A86	C2-C1-C24-C25
42	17	302	A86	C10-C11-C13-O
42	17	302	A86	C12-C11-C13-O
42	17	302	A86	C11-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
42	17	302	A86	C1-C2-C3-C4
42	17	302	A86	C39-C38-O4-C34
42	17	302	A86	O5-C38-O4-C34
42	17	311	A86	C28-C27-C29-C30
42	17	311	A86	C39-C38-O4-C34
42	17	311	A86	O5-C38-O4-C34
42	17	311	A86	C5-C6-C8-C9
42	17	311	A86	C7-C6-C8-C9
42	17	313	A86	C26-C27-C29-C30
42	17	313	A86	C28-C27-C29-C30
42	17	313	A86	C35-C34-O4-C38
42	17	314	A86	C2-C1-C24-C25
42	17	314	A86	C12-C11-C13-O
42	17	315	A86	C13-C14-C15-C16
42	17	315	A86	C1-C2-C3-C4
42	17	315	A86	C39-C38-O4-C34
42	17	316	A86	C24-C25-C26-C27
42	17	316	A86	C39-C38-O4-C34
42	17	316	A86	O5-C38-O4-C34
42	18	302	A86	C11-C13-C14-C15
42	18	302	A86	C13-C14-C15-C16
42	18	302	A86	C39-C38-O4-C34
42	18	302	A86	O5-C38-O4-C34
42	18	313	A86	C39-C38-O4-C34
42	18	313	A86	C5-C6-C8-C9
42	18	313	A86	C7-C6-C8-C9
42	18	315	A86	C2-C1-C24-C25
42	18	315	A86	C12-C11-C13-O
42	19	310	A86	C13-C14-C15-C16
42	19	310	A86	C1-C2-C3-C4
42	19	310	A86	O5-C38-O4-C34
42	19	310	A86	C5-C6-C8-C9
42	19	310	A86	C7-C6-C8-C9
42	19	311	A86	C12-C11-C13-C14
42	19	311	A86	O-C13-C14-C15
42	19	311	A86	C11-C13-C14-C15
42	19	311	A86	C13-C14-C15-C16
42	19	311	A86	C13-C14-C15-C20
42	19	311	A86	C33-C34-O4-C38
42	19	312	A86	C11-C10-C9-C8
42	19	312	A86	C26-C27-C29-C30
42	19	312	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
42	19	312	A86	C5-C6-C8-C9
42	19	312	A86	C7-C6-C8-C9
42	20	201	A86	C1-C2-C3-C4
42	20	210	A86	C-C1-C24-C25
42	20	210	A86	C2-C1-C24-C25
42	20	210	A86	C13-C14-C15-C16
42	20	210	A86	C26-C27-C29-C30
42	20	210	A86	C28-C27-C29-C30
42	20	210	A86	C39-C38-O4-C34
42	20	210	A86	C3-C4-C5-C6
42	20	210	A86	C5-C6-C8-C9
42	20	211	A86	C13-C14-C15-C16
42	20	212	A86	C11-C13-C14-C15
42	20	212	A86	C13-C14-C15-O1
42	20	212	A86	C35-C34-O4-C38
42	20	213	A86	C2-C1-C24-C25
42	20	213	A86	C13-C14-C15-O1
42	20	213	A86	C1-C2-C3-C4
42	20	213	A86	C39-C38-O4-C34
42	20	213	A86	O5-C38-O4-C34
42	20	213	A86	C5-C6-C8-C9
42	20	213	A86	C7-C6-C8-C9
42	21	310	A86	C24-C25-C26-C27
42	21	310	A86	C39-C38-O4-C34
42	21	310	A86	O5-C38-O4-C34
42	21	311	A86	C13-C14-C15-C16
42	21	312	A86	C35-C34-O4-C38
42	21	312	A86	C5-C6-C8-C9
42	21	312	A86	C7-C6-C8-C9
42	21	313	A86	C13-C14-C15-C16
42	21	313	A86	C24-C25-C26-C27
42	21	313	A86	C26-C27-C29-C30
42	21	313	A86	C28-C27-C29-C30
42	21	313	A86	C39-C38-O4-C34
42	21	313	A86	C5-C6-C8-C9
42	21	313	A86	C7-C6-C8-C9
42	21	314	A86	C2-C1-C24-C25
42	21	314	A86	C13-C14-C15-O1
42	21	314	A86	C1-C2-C3-C4
42	21	314	A86	C39-C38-O4-C34
42	21	314	A86	O5-C38-O4-C34
42	21	314	A86	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
42	21	314	A86	C7-C6-C8-C9
42	11	311	A86	C39-C38-O4-C34
42	11	312	A86	C39-C38-O4-C34
42	12	316	A86	C39-C38-O4-C34
42	12	317	A86	C39-C38-O4-C34
42	13	312	A86	C39-C38-O4-C34
42	13	313	A86	C39-C38-O4-C34
42	14	313	A86	C39-C38-O4-C34
42	14	314	A86	C39-C38-O4-C34
42	15	311	A86	C39-C38-O4-C34
42	15	312	A86	C39-C38-O4-C34
42	16	311	A86	C39-C38-O4-C34
42	16	312	A86	C39-C38-O4-C34
42	17	312	A86	C39-C38-O4-C34
42	17	313	A86	C39-C38-O4-C34
42	17	315	A86	O5-C38-O4-C34
42	18	314	A86	C39-C38-O4-C34
42	19	310	A86	C39-C38-O4-C34
42	20	201	A86	C39-C38-O4-C34
30	16	302	CLA	O1D-CGD-O2D-CED
30	16	303	CLA	O1D-CGD-O2D-CED
30	18	304	CLA	O1D-CGD-O2D-CED
30	19	302	CLA	O1D-CGD-O2D-CED
30	19	304	CLA	O1D-CGD-O2D-CED
30	20	208	CLA	O1D-CGD-O2D-CED
42	11	310	A86	O5-C38-O4-C34
42	12	315	A86	O5-C38-O4-C34
42	13	311	A86	O5-C38-O4-C34
42	14	312	A86	O5-C38-O4-C34
42	15	310	A86	O5-C38-O4-C34
42	16	310	A86	C39-C38-O4-C34
42	18	313	A86	O5-C38-O4-C34
42	20	210	A86	O5-C38-O4-C34
42	21	313	A86	O5-C38-O4-C34
30	A	402	CLA	O1D-CGD-O2D-CED
30	C	510	CLA	O1D-CGD-O2D-CED
30	a	402	CLA	O1D-CGD-O2D-CED
30	c	510	CLA	O1D-CGD-O2D-CED
30	11	304	CLA	O1D-CGD-O2D-CED
30	11	305	CLA	O1D-CGD-O2D-CED
30	12	308	CLA	O1D-CGD-O2D-CED
30	12	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	13	305	CLA	O1D-CGD-O2D-CED
30	13	306	CLA	O1D-CGD-O2D-CED
30	14	306	CLA	O1D-CGD-O2D-CED
30	14	307	CLA	O1D-CGD-O2D-CED
30	15	302	CLA	O1D-CGD-O2D-CED
30	15	303	CLA	O1D-CGD-O2D-CED
30	17	304	CLA	O1D-CGD-O2D-CED
30	17	309	CLA	O1D-CGD-O2D-CED
30	18	305	CLA	O1D-CGD-O2D-CED
30	18	306	CLA	O1D-CGD-O2D-CED
30	18	311	CLA	O1D-CGD-O2D-CED
30	20	204	CLA	O1D-CGD-O2D-CED
30	B	603	CLA	CBD-CGD-O2D-CED
30	B	604	CLA	CBD-CGD-O2D-CED
30	C	508	CLA	CBD-CGD-O2D-CED
30	C	520	CLA	CBD-CGD-O2D-CED
30	W	103	CLA	CBD-CGD-O2D-CED
30	b	603	CLA	CBD-CGD-O2D-CED
30	b	604	CLA	CBD-CGD-O2D-CED
30	c	508	CLA	CBD-CGD-O2D-CED
30	w	103	CLA	CBD-CGD-O2D-CED
30	11	301	CLA	CBD-CGD-O2D-CED
30	11	304	CLA	CBD-CGD-O2D-CED
30	11	305	CLA	CBD-CGD-O2D-CED
30	12	305	CLA	CBD-CGD-O2D-CED
30	12	308	CLA	CBD-CGD-O2D-CED
30	12	309	CLA	CBD-CGD-O2D-CED
30	13	302	CLA	CBD-CGD-O2D-CED
30	13	305	CLA	CBD-CGD-O2D-CED
30	13	306	CLA	CBD-CGD-O2D-CED
30	14	303	CLA	CBD-CGD-O2D-CED
30	14	306	CLA	CBD-CGD-O2D-CED
30	14	307	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	CBD-CGD-O2D-CED
30	15	304	CLA	CBD-CGD-O2D-CED
30	15	306	CLA	CBD-CGD-O2D-CED
30	15	307	CLA	CBD-CGD-O2D-CED
30	16	305	CLA	CBD-CGD-O2D-CED
30	16	306	CLA	CBD-CGD-O2D-CED
30	17	303	CLA	CBD-CGD-O2D-CED
30	17	309	CLA	CBD-CGD-O2D-CED
30	18	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	18	306	CLA	CBD-CGD-O2D-CED
30	18	311	CLA	CBD-CGD-O2D-CED
30	19	301	CLA	CBD-CGD-O2D-CED
30	19	304	CLA	CBD-CGD-O2D-CED
30	20	204	CLA	CBD-CGD-O2D-CED
30	20	205	CLA	CBD-CGD-O2D-CED
30	20	208	CLA	CBD-CGD-O2D-CED
30	21	301	CLA	CBD-CGD-O2D-CED
30	21	304	CLA	CBD-CGD-O2D-CED
30	21	307	CLA	CBD-CGD-O2D-CED
30	15	307	CLA	O1A-CGA-O2A-C1
30	21	301	CLA	O1A-CGA-O2A-C1
30	15	304	CLA	O1D-CGD-O2D-CED
30	19	301	CLA	O1D-CGD-O2D-CED
30	B	611	CLA	O1D-CGD-O2D-CED
30	C	504	CLA	O1D-CGD-O2D-CED
30	C	514	CLA	O1D-CGD-O2D-CED
30	W	103	CLA	O1D-CGD-O2D-CED
30	b	611	CLA	O1D-CGD-O2D-CED
30	c	504	CLA	O1D-CGD-O2D-CED
30	c	514	CLA	O1D-CGD-O2D-CED
30	w	103	CLA	O1D-CGD-O2D-CED
30	17	303	CLA	O1D-CGD-O2D-CED
30	21	302	CLA	O1D-CGD-O2D-CED
30	21	304	CLA	O1D-CGD-O2D-CED
30	21	301	CLA	CBA-CGA-O2A-C1
40	D	404	PL9	C47-C48-C49-C50
40	D	404	PL9	C47-C48-C49-C51
40	d	405	PL9	C47-C48-C49-C50
40	d	405	PL9	C47-C48-C49-C51
30	B	602	CLA	CBD-CGD-O2D-CED
30	B	609	CLA	CBD-CGD-O2D-CED
30	B	614	CLA	CBD-CGD-O2D-CED
30	C	507	CLA	CBD-CGD-O2D-CED
30	b	602	CLA	CBD-CGD-O2D-CED
30	b	609	CLA	CBD-CGD-O2D-CED
30	b	614	CLA	CBD-CGD-O2D-CED
30	c	507	CLA	CBD-CGD-O2D-CED
30	11	303	CLA	CBD-CGD-O2D-CED
30	11	309	CLA	CBD-CGD-O2D-CED
30	12	307	CLA	CBD-CGD-O2D-CED
30	12	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	13	304	CLA	CBD-CGD-O2D-CED
30	13	310	CLA	CBD-CGD-O2D-CED
30	14	305	CLA	CBD-CGD-O2D-CED
30	14	311	CLA	CBD-CGD-O2D-CED
30	15	301	CLA	CBD-CGD-O2D-CED
30	15	309	CLA	CBD-CGD-O2D-CED
30	16	301	CLA	CBD-CGD-O2D-CED
30	16	308	CLA	CBD-CGD-O2D-CED
30	17	310	CLA	CBD-CGD-O2D-CED
30	18	308	CLA	CBD-CGD-O2D-CED
30	18	312	CLA	CBD-CGD-O2D-CED
30	19	305	CLA	CBD-CGD-O2D-CED
30	21	308	CLA	CBD-CGD-O2D-CED
42	20	201	A86	O5-C38-O4-C34
30	B	615	CLA	O1A-CGA-O2A-C1
30	b	615	CLA	O1A-CGA-O2A-C1
30	15	301	CLA	O1A-CGA-O2A-C1
30	15	303	CLA	O1A-CGA-O2A-C1
30	17	305	CLA	O1A-CGA-O2A-C1
30	17	308	CLA	O1A-CGA-O2A-C1
30	18	303	CLA	O1A-CGA-O2A-C1
30	18	309	CLA	O1A-CGA-O2A-C1
30	20	204	CLA	O1A-CGA-O2A-C1
30	21	306	CLA	O1A-CGA-O2A-C1
30	17	306	CLA	O1D-CGD-O2D-CED
42	11	312	A86	O5-C38-O4-C34
42	12	317	A86	O5-C38-O4-C34
42	13	313	A86	O5-C38-O4-C34
42	14	314	A86	O5-C38-O4-C34
42	15	312	A86	O5-C38-O4-C34
42	16	312	A86	O5-C38-O4-C34
42	17	313	A86	O5-C38-O4-C34
30	B	607	CLA	CBD-CGD-O2D-CED
30	C	502	CLA	CBD-CGD-O2D-CED
30	Z	102	CLA	CBD-CGD-O2D-CED
30	b	607	CLA	CBD-CGD-O2D-CED
30	c	502	CLA	CBD-CGD-O2D-CED
30	17	305	CLA	CBD-CGD-O2D-CED
30	21	301	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	O49-C7-O47-C45
33	l	101	SQD	O49-C7-O47-C45
30	B	607	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	C	513	CLA	C3-C5-C6-C7
30	M	101	CLA	C3-C5-C6-C7
30	b	607	CLA	C3-C5-C6-C7
30	c	513	CLA	C3-C5-C6-C7
30	m	101	CLA	C3-C5-C6-C7
30	17	303	CLA	C3-C5-C6-C7
30	19	301	CLA	C3-C5-C6-C7
30	20	204	CLA	C3-C5-C6-C7
30	B	615	CLA	CBA-CGA-O2A-C1
30	C	519	CLA	CBA-CGA-O2A-C1
30	b	615	CLA	CBA-CGA-O2A-C1
30	z	101	CLA	CBA-CGA-O2A-C1
30	15	301	CLA	CBA-CGA-O2A-C1
30	15	303	CLA	CBA-CGA-O2A-C1
30	15	307	CLA	CBA-CGA-O2A-C1
30	17	308	CLA	CBA-CGA-O2A-C1
30	18	303	CLA	CBA-CGA-O2A-C1
30	18	309	CLA	CBA-CGA-O2A-C1
30	20	204	CLA	CBA-CGA-O2A-C1
30	21	306	CLA	CBA-CGA-O2A-C1
42	11	313	A86	C39-C38-O4-C34
42	12	318	A86	C39-C38-O4-C34
42	13	314	A86	C39-C38-O4-C34
42	14	315	A86	C39-C38-O4-C34
42	15	313	A86	C39-C38-O4-C34
42	17	314	A86	C39-C38-O4-C34
42	18	315	A86	C39-C38-O4-C34
36	M	102	LMG	C11-C10-O7-C8
36	m	102	LMG	C11-C10-O7-C8
30	C	508	CLA	O1D-CGD-O2D-CED
30	c	508	CLA	O1D-CGD-O2D-CED
30	16	305	CLA	O1D-CGD-O2D-CED
30	20	205	CLA	O1D-CGD-O2D-CED
30	19	307	CLA	CBD-CGD-O2D-CED
30	20	209	CLA	CBD-CGD-O2D-CED
30	C	502	CLA	C4-C3-C5-C6
30	c	502	CLA	C4-C3-C5-C6
30	C	512	CLA	CBD-CGD-O2D-CED
30	c	512	CLA	CBD-CGD-O2D-CED
30	A	402	CLA	C2A-CAA-CBA-CGA
30	B	601	CLA	C2A-CAA-CBA-CGA
30	B	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	B	610	CLA	C2A-CAA-CBA-CGA
30	C	503	CLA	C2A-CAA-CBA-CGA
30	C	513	CLA	C2A-CAA-CBA-CGA
30	C	520	CLA	C2A-CAA-CBA-CGA
30	W	103	CLA	C2A-CAA-CBA-CGA
30	a	402	CLA	C2A-CAA-CBA-CGA
30	b	601	CLA	C2A-CAA-CBA-CGA
30	b	606	CLA	C2A-CAA-CBA-CGA
30	b	610	CLA	C2A-CAA-CBA-CGA
30	c	503	CLA	C2A-CAA-CBA-CGA
30	c	513	CLA	C2A-CAA-CBA-CGA
30	w	103	CLA	C2A-CAA-CBA-CGA
30	11	301	CLA	C2A-CAA-CBA-CGA
30	11	307	CLA	C2A-CAA-CBA-CGA
30	12	305	CLA	C2A-CAA-CBA-CGA
30	12	311	CLA	C2A-CAA-CBA-CGA
30	13	302	CLA	C2A-CAA-CBA-CGA
30	13	308	CLA	C2A-CAA-CBA-CGA
30	14	303	CLA	C2A-CAA-CBA-CGA
30	14	309	CLA	C2A-CAA-CBA-CGA
30	15	301	CLA	C2A-CAA-CBA-CGA
30	15	304	CLA	C2A-CAA-CBA-CGA
30	15	306	CLA	C2A-CAA-CBA-CGA
30	16	302	CLA	C2A-CAA-CBA-CGA
30	16	305	CLA	C2A-CAA-CBA-CGA
30	16	306	CLA	C2A-CAA-CBA-CGA
30	16	308	CLA	C2A-CAA-CBA-CGA
30	17	304	CLA	C2A-CAA-CBA-CGA
30	18	306	CLA	C2A-CAA-CBA-CGA
30	20	205	CLA	C2A-CAA-CBA-CGA
30	21	304	CLA	C2A-CAA-CBA-CGA
30	21	308	CLA	C2A-CAA-CBA-CGA
30	C	505	CLA	C3-C5-C6-C7
30	c	505	CLA	C3-C5-C6-C7
31	A	403	PHO	C3-C5-C6-C7
31	d	403	PHO	C3-C5-C6-C7
30	C	508	CLA	CBA-CGA-O2A-C1
30	c	508	CLA	CBA-CGA-O2A-C1
30	16	304	CLA	CBA-CGA-O2A-C1
30	17	305	CLA	CBA-CGA-O2A-C1
36	W	101	LMG	O6-C5-C6-O5
36	w	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
42	11	311	A86	O5-C38-O4-C34
42	12	316	A86	O5-C38-O4-C34
42	13	312	A86	O5-C38-O4-C34
42	14	313	A86	O5-C38-O4-C34
42	15	311	A86	O5-C38-O4-C34
42	16	311	A86	O5-C38-O4-C34
42	17	312	A86	O5-C38-O4-C34
42	18	314	A86	O5-C38-O4-C34
39	H	102	DGD	C4D-C5D-C6D-O5D
39	h	102	DGD	C4D-C5D-C6D-O5D
42	21	311	A86	C39-C38-O4-C34
30	11	301	CLA	O1D-CGD-O2D-CED
30	12	305	CLA	O1D-CGD-O2D-CED
30	13	302	CLA	O1D-CGD-O2D-CED
30	14	303	CLA	O1D-CGD-O2D-CED
40	D	404	PL9	C37-C38-C39-C41
40	D	407	PL9	C7-C8-C9-C11
40	D	407	PL9	C42-C43-C44-C46
40	d	405	PL9	C37-C38-C39-C41
40	d	408	PL9	C7-C8-C9-C11
40	d	408	PL9	C42-C43-C44-C46
30	C	519	CLA	O1A-CGA-O2A-C1
30	z	101	CLA	O1A-CGA-O2A-C1
30	11	301	CLA	O1A-CGA-O2A-C1
30	12	305	CLA	O1A-CGA-O2A-C1
30	13	302	CLA	O1A-CGA-O2A-C1
30	14	303	CLA	O1A-CGA-O2A-C1
30	16	304	CLA	O1A-CGA-O2A-C1
42	16	310	A86	O5-C38-O4-C34
42	20	211	A86	C39-C38-O4-C34
30	15	306	CLA	O1D-CGD-O2D-CED
30	15	307	CLA	O1D-CGD-O2D-CED
42	11	311	A86	C24-C25-C26-C27
42	12	316	A86	C24-C25-C26-C27
42	13	312	A86	C24-C25-C26-C27
42	14	313	A86	C24-C25-C26-C27
42	15	311	A86	C24-C25-C26-C27
42	16	311	A86	C24-C25-C26-C27
42	17	311	A86	C1-C2-C3-C4
42	17	311	A86	C3-C4-C5-C6
42	17	312	A86	C24-C25-C26-C27
42	18	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
42	19	310	A86	C24-C25-C26-C27
42	19	310	A86	C3-C4-C5-C6
42	20	201	A86	C3-C4-C5-C6
42	20	211	A86	C3-C4-C5-C6
42	20	212	A86	C24-C25-C26-C27
42	21	310	A86	C1-C2-C3-C4
42	21	311	A86	C3-C4-C5-C6
42	21	312	A86	C1-C2-C3-C4
30	B	610	CLA	CBD-CGD-O2D-CED
30	B	623	CLA	CBD-CGD-O2D-CED
30	M	101	CLA	CBD-CGD-O2D-CED
30	b	610	CLA	CBD-CGD-O2D-CED
30	b	622	CLA	CBD-CGD-O2D-CED
30	m	101	CLA	CBD-CGD-O2D-CED
30	15	305	CLA	CBD-CGD-O2D-CED
30	16	307	CLA	CBD-CGD-O2D-CED
30	17	301	CLA	CBD-CGD-O2D-CED
30	18	310	CLA	CBD-CGD-O2D-CED
30	20	207	CLA	CBD-CGD-O2D-CED
30	B	603	CLA	O1D-CGD-O2D-CED
30	b	603	CLA	O1D-CGD-O2D-CED
30	C	512	CLA	CBA-CGA-O2A-C1
30	C	513	CLA	CBA-CGA-O2A-C1
30	c	512	CLA	CBA-CGA-O2A-C1
30	c	513	CLA	CBA-CGA-O2A-C1
30	11	301	CLA	CBA-CGA-O2A-C1
30	12	305	CLA	CBA-CGA-O2A-C1
30	13	302	CLA	CBA-CGA-O2A-C1
30	14	303	CLA	CBA-CGA-O2A-C1
30	16	306	CLA	O1D-CGD-O2D-CED
30	21	307	CLA	O1D-CGD-O2D-CED
31	A	403	PHO	C10-C11-C12-C13
31	d	403	PHO	C10-C11-C12-C13
30	B	604	CLA	O1D-CGD-O2D-CED
30	b	604	CLA	O1D-CGD-O2D-CED
30	C	503	CLA	CBD-CGD-O2D-CED
30	19	306	CLA	CBD-CGD-O2D-CED
30	19	309	CLA	CBD-CGD-O2D-CED
36	B	619	LMG	O6-C5-C6-O5
36	b	618	LMG	O6-C5-C6-O5
36	W	101	LMG	C4-C5-C6-O5
36	w	101	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	c	503	CLA	CBD-CGD-O2D-CED
30	B	623	CLA	C3-C5-C6-C7
30	D	401	CLA	C3-C5-C6-C7
30	b	622	CLA	C3-C5-C6-C7
30	d	401	CLA	C3-C5-C6-C7
30	C	508	CLA	O1A-CGA-O2A-C1
30	C	513	CLA	O1A-CGA-O2A-C1
30	c	508	CLA	O1A-CGA-O2A-C1
37	B	625	LMU	O5B-C5B-C6B-O6B
37	12	302	LMU	O5B-C5B-C6B-O6B
30	17	308	CLA	C4-C3-C5-C6
30	B	603	CLA	C2-C3-C5-C6
30	b	603	CLA	C2-C3-C5-C6
30	17	308	CLA	C2-C3-C5-C6
30	17	306	CLA	C2A-CAA-CBA-CGA
30	20	202	CLA	C2A-CAA-CBA-CGA
36	12	301	LMG	O6-C5-C6-O5
30	c	513	CLA	O1A-CGA-O2A-C1
40	D	404	PL9	C19-C21-C22-C23
40	d	405	PL9	C19-C21-C22-C23
30	A	402	CLA	CBA-CGA-O2A-C1
30	C	511	CLA	CBA-CGA-O2A-C1
30	c	511	CLA	CBA-CGA-O2A-C1
30	18	305	CLA	CBA-CGA-O2A-C1
30	19	301	CLA	CBA-CGA-O2A-C1
33	b	620	SQD	C24-C23-O48-C46
39	H	102	DGD	O6E-C5E-C6E-O5E
39	h	102	DGD	O6E-C5E-C6E-O5E
30	C	507	CLA	O1D-CGD-O2D-CED
30	C	520	CLA	O1D-CGD-O2D-CED
30	b	602	CLA	O1D-CGD-O2D-CED
30	c	507	CLA	O1D-CGD-O2D-CED
30	C	512	CLA	O1A-CGA-O2A-C1
30	c	512	CLA	O1A-CGA-O2A-C1
30	18	305	CLA	O1A-CGA-O2A-C1
30	B	602	CLA	O1D-CGD-O2D-CED
30	15	301	CLA	O1D-CGD-O2D-CED
30	15	309	CLA	O1D-CGD-O2D-CED
30	16	301	CLA	O1D-CGD-O2D-CED
30	17	310	CLA	O1D-CGD-O2D-CED
30	18	312	CLA	O1D-CGD-O2D-CED
30	19	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	21	308	CLA	O1D-CGD-O2D-CED
30	B	614	CLA	O1D-CGD-O2D-CED
30	19	301	CLA	O1A-CGA-O2A-C1
30	B	602	CLA	C3-C5-C6-C7
30	b	602	CLA	C3-C5-C6-C7
30	15	303	CLA	C3-C5-C6-C7
30	16	302	CLA	C3-C5-C6-C7
30	b	614	CLA	O1D-CGD-O2D-CED
30	C	505	CLA	CBA-CGA-O2A-C1
30	C	506	CLA	CBA-CGA-O2A-C1
30	a	402	CLA	CBA-CGA-O2A-C1
30	c	505	CLA	CBA-CGA-O2A-C1
30	c	506	CLA	CBA-CGA-O2A-C1
30	20	202	CLA	CBA-CGA-O2A-C1
33	B	621	SQD	C24-C23-O48-C46
30	11	306	CLA	CBD-CGD-O2D-CED
30	12	310	CLA	CBD-CGD-O2D-CED
30	13	307	CLA	CBD-CGD-O2D-CED
30	14	308	CLA	CBD-CGD-O2D-CED
32	B	624	BCR	C15-C16-C17-C18
32	b	623	BCR	C15-C16-C17-C18
42	11	310	A86	C24-C25-C26-C27
42	11	312	A86	C24-C25-C26-C27
42	12	315	A86	C24-C25-C26-C27
42	12	317	A86	C24-C25-C26-C27
42	13	311	A86	C24-C25-C26-C27
42	13	313	A86	C24-C25-C26-C27
42	14	312	A86	C24-C25-C26-C27
42	14	314	A86	C24-C25-C26-C27
42	15	310	A86	C24-C25-C26-C27
42	15	312	A86	C24-C25-C26-C27
42	16	312	A86	C24-C25-C26-C27
42	17	313	A86	C24-C25-C26-C27
42	18	313	A86	C24-C25-C26-C27
42	19	311	A86	C1-C2-C3-C4
42	19	312	A86	C24-C25-C26-C27
42	20	201	A86	C24-C25-C26-C27
42	20	210	A86	C24-C25-C26-C27
42	20	211	A86	C1-C2-C3-C4
42	20	213	A86	C24-C25-C26-C27
42	21	311	A86	C1-C2-C3-C4
42	21	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	B	610	CLA	C15-C16-C17-C18
30	b	610	CLA	C15-C16-C17-C18
30	b	622	CLA	C5-C6-C7-C8
30	11	307	CLA	C8-C10-C11-C12
30	12	311	CLA	C8-C10-C11-C12
30	13	308	CLA	C8-C10-C11-C12
30	14	309	CLA	C8-C10-C11-C12
30	B	601	CLA	C8-C10-C11-C12
30	B	611	CLA	C10-C11-C12-C13
30	B	623	CLA	C5-C6-C7-C8
30	M	101	CLA	C13-C15-C16-C17
30	W	103	CLA	C13-C15-C16-C17
30	b	601	CLA	C8-C10-C11-C12
30	b	611	CLA	C10-C11-C12-C13
30	m	101	CLA	C13-C15-C16-C17
30	w	103	CLA	C13-C15-C16-C17
30	C	511	CLA	O1A-CGA-O2A-C1
30	c	511	CLA	O1A-CGA-O2A-C1
36	B	619	LMG	C4-C5-C6-O5
36	b	618	LMG	C4-C5-C6-O5
30	C	502	CLA	C2-C3-C5-C6
30	c	502	CLA	C2-C3-C5-C6
30	B	601	CLA	C11-C10-C8-C9
30	B	604	CLA	C11-C10-C8-C9
30	B	610	CLA	C11-C12-C13-C14
30	C	506	CLA	C11-C12-C13-C14
30	C	511	CLA	C11-C12-C13-C14
30	C	519	CLA	C11-C12-C13-C14
30	M	101	CLA	C6-C7-C8-C9
30	b	601	CLA	C11-C10-C8-C9
30	b	604	CLA	C11-C10-C8-C9
30	b	610	CLA	C11-C12-C13-C14
30	c	506	CLA	C11-C12-C13-C14
30	c	511	CLA	C11-C12-C13-C14
30	m	101	CLA	C6-C7-C8-C9
30	z	101	CLA	C11-C12-C13-C14
30	16	302	CLA	C6-C7-C8-C9
30	19	307	CLA	C11-C10-C8-C9
31	A	403	PHO	C11-C10-C8-C9
31	D	403	PHO	C6-C7-C8-C9
31	d	403	PHO	C11-C10-C8-C9
31	d	404	PHO	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	609	CLA	O1D-CGD-O2D-CED
30	b	609	CLA	O1D-CGD-O2D-CED
32	B	624	BCR	C7-C8-C9-C34
32	B	624	BCR	C37-C22-C23-C24
32	C	515	BCR	C11-C12-C13-C35
32	C	515	BCR	C37-C22-C23-C24
32	C	518	BCR	C37-C22-C23-C24
32	F	101	BCR	C7-C8-C9-C34
32	Y	101	BCR	C37-C22-C23-C24
32	Z	101	BCR	C37-C22-C23-C24
32	b	623	BCR	C7-C8-C9-C34
32	b	623	BCR	C37-C22-C23-C24
32	c	515	BCR	C37-C22-C23-C24
32	c	516	BCR	C11-C12-C13-C35
32	c	516	BCR	C37-C22-C23-C24
32	c	520	BCR	C37-C22-C23-C24
32	c	521	BCR	C37-C22-C23-C24
32	f	101	BCR	C7-C8-C9-C34
42	11	313	A86	C-C1-C24-C25
42	12	318	A86	C-C1-C24-C25
42	13	314	A86	C-C1-C24-C25
42	14	315	A86	C-C1-C24-C25
42	15	313	A86	C-C1-C24-C25
42	17	302	A86	C7-C6-C8-C9
42	17	314	A86	C-C1-C24-C25
42	18	315	A86	C-C1-C24-C25
42	20	201	A86	C7-C6-C8-C9
42	20	210	A86	C7-C6-C8-C9
42	21	313	A86	C-C1-C24-C25
42	17	302	A86	C5-C6-C8-C9
42	20	201	A86	C5-C6-C8-C9
42	21	313	A86	C2-C1-C24-C25
36	1	101	LMG	O6-C5-C6-O5
35	L	101	LHG	C8-C7-O7-C5
35	d	409	LHG	C8-C7-O7-C5
36	12	301	LMG	C4-C5-C6-O5
39	H	102	DGD	C4E-C5E-C6E-O5E
39	h	102	DGD	C4E-C5E-C6E-O5E
30	C	506	CLA	O1A-CGA-O2A-C1
30	c	506	CLA	O1A-CGA-O2A-C1
30	B	608	CLA	C15-C16-C17-C18
30	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	b	608	CLA	C15-C16-C17-C18
30	b	615	CLA	C8-C10-C11-C12
30	z	101	CLA	C8-C10-C11-C12
30	16	304	CLA	C10-C11-C12-C13
30	16	304	CLA	C15-C16-C17-C18
36	Q	301	LMG	O6-C5-C6-O5
36	c	519	LMG	O6-C5-C6-O5
30	11	303	CLA	O1D-CGD-O2D-CED
30	12	307	CLA	O1D-CGD-O2D-CED
30	17	305	CLA	C3-C5-C6-C7
30	17	308	CLA	C3-C5-C6-C7
30	11	307	CLA	CBA-CGA-O2A-C1
30	12	311	CLA	CBA-CGA-O2A-C1
30	13	308	CLA	CBA-CGA-O2A-C1
30	B	615	CLA	C13-C15-C16-C17
30	C	519	CLA	C8-C10-C11-C12
30	b	615	CLA	C13-C15-C16-C17
30	b	622	CLA	C13-C15-C16-C17
30	17	303	CLA	C15-C16-C17-C18
30	17	308	CLA	C5-C6-C7-C8
31	A	403	PHO	C15-C16-C17-C18
31	d	403	PHO	C15-C16-C17-C18
36	1	101	LMG	C10-C11-C12-C13
30	13	304	CLA	O1D-CGD-O2D-CED
30	14	305	CLA	O1D-CGD-O2D-CED
30	C	513	CLA	CBD-CGD-O2D-CED
30	B	604	CLA	C8-C10-C11-C12
30	B	606	CLA	C10-C11-C12-C13
30	B	613	CLA	C10-C11-C12-C13
30	B	623	CLA	C13-C15-C16-C17
30	C	508	CLA	C8-C10-C11-C12
30	C	509	CLA	C8-C10-C11-C12
30	C	514	CLA	C8-C10-C11-C12
30	C	520	CLA	C5-C6-C7-C8
30	C	520	CLA	C10-C11-C12-C13
30	D	402	CLA	C15-C16-C17-C18
30	W	102	CLA	C10-C11-C12-C13
30	W	103	CLA	C10-C11-C12-C13
30	b	604	CLA	C8-C10-C11-C12
30	b	606	CLA	C10-C11-C12-C13
30	b	613	CLA	C10-C11-C12-C13
30	c	508	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	c	509	CLA	C8-C10-C11-C12
30	c	514	CLA	C8-C10-C11-C12
30	d	402	CLA	C15-C16-C17-C18
30	w	102	CLA	C10-C11-C12-C13
30	w	103	CLA	C10-C11-C12-C13
30	15	307	CLA	C8-C10-C11-C12
30	16	308	CLA	O1D-CGD-O2D-CED
40	D	407	PL9	C7-C8-C9-C10
40	d	408	PL9	C7-C8-C9-C10
35	B	622	LHG	C23-C24-C25-C26
35	L	101	LHG	C7-C8-C9-C10
35	b	621	LHG	C23-C24-C25-C26
35	d	409	LHG	C7-C8-C9-C10
36	12	301	LMG	C10-C11-C12-C13
30	c	513	CLA	CBD-CGD-O2D-CED
30	A	404	CLA	C8-C10-C11-C12
30	B	601	CLA	C5-C6-C7-C8
30	C	511	CLA	C8-C10-C11-C12
30	a	403	CLA	C8-C10-C11-C12
30	b	601	CLA	C5-C6-C7-C8
30	c	511	CLA	C8-C10-C11-C12
30	17	308	CLA	C10-C11-C12-C13
30	14	309	CLA	CBA-CGA-O2A-C1
41	F	102	HEM	C1A-C2A-CAA-CBA
41	f	102	HEM	C1A-C2A-CAA-CBA
30	C	513	CLA	C8-C10-C11-C12
30	12	314	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	C28-C29-C30-C31
36	b	618	LMG	C28-C29-C30-C31
30	C	504	CLA	C5-C6-C7-C8
30	C	505	CLA	C15-C16-C17-C18
30	c	504	CLA	C5-C6-C7-C8
30	c	505	CLA	C15-C16-C17-C18
30	c	513	CLA	C8-C10-C11-C12
30	C	502	CLA	O1D-CGD-O2D-CED
30	B	615	CLA	C6-C7-C8-C10
30	C	504	CLA	C6-C7-C8-C10
30	C	505	CLA	C6-C7-C8-C10
30	Z	102	CLA	C12-C13-C15-C16
30	W	103	CLA	C12-C13-C15-C16
30	b	615	CLA	C6-C7-C8-C10
30	c	504	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	c	505	CLA	C6-C7-C8-C10
30	w	103	CLA	C12-C13-C15-C16
30	11	307	CLA	C6-C7-C8-C10
30	12	311	CLA	C6-C7-C8-C10
30	13	308	CLA	C6-C7-C8-C10
30	14	309	CLA	C6-C7-C8-C10
30	C	505	CLA	O1A-CGA-O2A-C1
30	c	505	CLA	O1A-CGA-O2A-C1
42	11	313	A86	C24-C25-C26-C27
42	11	316	A86	C11-C10-C9-C8
42	12	304	A86	C11-C10-C9-C8
42	12	318	A86	C24-C25-C26-C27
42	13	301	A86	C11-C10-C9-C8
42	13	314	A86	C24-C25-C26-C27
42	13	315	A86	C11-C10-C9-C8
42	14	315	A86	C24-C25-C26-C27
42	15	313	A86	C24-C25-C26-C27
42	15	315	A86	C11-C10-C9-C8
42	15	316	A86	C11-C10-C9-C8
42	16	310	A86	C1-C2-C3-C4
42	16	310	A86	C24-C25-C26-C27
42	17	311	A86	C11-C10-C9-C8
42	17	314	A86	C24-C25-C26-C27
42	17	315	A86	C3-C4-C5-C6
42	18	302	A86	C11-C10-C9-C8
42	18	315	A86	C24-C25-C26-C27
42	20	210	A86	C11-C10-C9-C8
42	21	310	A86	C3-C4-C5-C6
42	21	312	A86	C24-C25-C26-C27
30	11	306	CLA	C2A-CAA-CBA-CGA
30	12	310	CLA	C2A-CAA-CBA-CGA
30	13	307	CLA	C2A-CAA-CBA-CGA
30	14	308	CLA	C2A-CAA-CBA-CGA
30	18	308	CLA	C2A-CAA-CBA-CGA
30	Z	102	CLA	O1D-CGD-O2D-CED
30	c	502	CLA	O1D-CGD-O2D-CED
30	11	309	CLA	O1D-CGD-O2D-CED
30	13	310	CLA	O1D-CGD-O2D-CED
30	14	311	CLA	O1D-CGD-O2D-CED
30	B	602	CLA	C5-C6-C7-C8
30	16	302	CLA	C10-C11-C12-C13
30	17	308	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	19	301	CLA	C15-C16-C17-C18
30	20	209	CLA	C5-C6-C7-C8
30	20	202	CLA	O1A-CGA-O2A-C1
30	W	102	CLA	CBD-CGD-O2D-CED
33	B	621	SQD	O5-C1-O6-C44
33	b	620	SQD	O5-C1-O6-C44
39	C	517	DGD	O6E-C1E-O5D-C6D
39	c	518	DGD	O6E-C1E-O5D-C6D
30	b	602	CLA	C5-C6-C7-C8
30	18	308	CLA	O1D-CGD-O2D-CED
40	D	404	PL9	C9-C11-C12-C13
40	D	404	PL9	C29-C31-C32-C33
40	D	404	PL9	C34-C36-C37-C38
40	D	404	PL9	C39-C41-C42-C43
40	d	405	PL9	C9-C11-C12-C13
40	d	405	PL9	C29-C31-C32-C33
40	d	405	PL9	C34-C36-C37-C38
40	d	405	PL9	C39-C41-C42-C43
32	B	617	BCR	C10-C11-C12-C13
32	F	101	BCR	C10-C11-C12-C13
32	Z	101	BCR	C10-C11-C12-C13
32	b	616	BCR	C10-C11-C12-C13
32	c	515	BCR	C10-C11-C12-C13
32	f	101	BCR	C10-C11-C12-C13
37	B	625	LMU	C4B-C5B-C6B-O6B
30	B	612	CLA	C10-C11-C12-C13
30	C	505	CLA	C8-C10-C11-C12
30	C	508	CLA	C10-C11-C12-C13
30	D	402	CLA	C10-C11-C12-C13
30	M	101	CLA	C8-C10-C11-C12
30	Z	102	CLA	C10-C11-C12-C13
30	b	612	CLA	C10-C11-C12-C13
30	c	505	CLA	C8-C10-C11-C12
30	c	508	CLA	C10-C11-C12-C13
30	d	402	CLA	C10-C11-C12-C13
30	m	101	CLA	C8-C10-C11-C12
30	18	309	CLA	C5-C6-C7-C8
30	w	102	CLA	CBD-CGD-O2D-CED
30	20	209	CLA	O1D-CGD-O2D-CED
30	A	402	CLA	O1A-CGA-O2A-C1
30	a	402	CLA	O1A-CGA-O2A-C1
30	11	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	12	311	CLA	O1A-CGA-O2A-C1
30	13	308	CLA	O1A-CGA-O2A-C1
37	12	302	LMU	C4B-C5B-C6B-O6B
30	17	305	CLA	O1D-CGD-O2D-CED
30	C	505	CLA	C13-C15-C16-C17
30	C	507	CLA	C10-C11-C12-C13
30	C	507	CLA	C15-C16-C17-C18
30	C	508	CLA	C15-C16-C17-C18
30	W	102	CLA	C8-C10-C11-C12
30	c	504	CLA	C10-C11-C12-C13
30	c	507	CLA	C10-C11-C12-C13
30	c	507	CLA	C15-C16-C17-C18
30	c	508	CLA	C15-C16-C17-C18
30	w	102	CLA	C8-C10-C11-C12
30	18	310	CLA	C15-C16-C17-C18
42	13	314	A86	O5-C38-O4-C34
30	b	607	CLA	O1D-CGD-O2D-CED
30	14	309	CLA	O1A-CGA-O2A-C1
36	W	101	LMG	C11-C10-O7-C8
36	w	101	LMG	C11-C10-O7-C8
30	B	607	CLA	O1D-CGD-O2D-CED
30	B	602	CLA	C15-C16-C17-C18
30	B	608	CLA	C8-C10-C11-C12
30	B	613	CLA	C5-C6-C7-C8
30	C	504	CLA	C10-C11-C12-C13
30	C	510	CLA	C13-C15-C16-C17
30	C	519	CLA	C13-C15-C16-C17
30	b	602	CLA	C15-C16-C17-C18
30	b	608	CLA	C8-C10-C11-C12
30	b	613	CLA	C5-C6-C7-C8
30	c	505	CLA	C13-C15-C16-C17
30	c	510	CLA	C13-C15-C16-C17
30	z	101	CLA	C13-C15-C16-C17
30	16	301	CLA	C8-C10-C11-C12
30	16	301	CLA	C13-C15-C16-C17
35	B	622	LHG	C4-O6-P-O3
35	L	101	LHG	C4-O6-P-O3
35	L	102	LHG	C3-O3-P-O6
35	b	621	LHG	C4-O6-P-O3
35	d	409	LHG	C4-O6-P-O3
35	l	102	LHG	C3-O3-P-O6
42	11	313	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
42	12	318	A86	O5-C38-O4-C34
42	14	315	A86	O5-C38-O4-C34
42	15	313	A86	O5-C38-O4-C34
42	17	314	A86	O5-C38-O4-C34
42	18	315	A86	O5-C38-O4-C34
30	B	607	CLA	CBA-CGA-O2A-C1
30	D	406	CLA	CBA-CGA-O2A-C1
30	b	607	CLA	CBA-CGA-O2A-C1
30	d	407	CLA	CBA-CGA-O2A-C1
36	W	101	LMG	C29-C28-O8-C9
36	w	101	LMG	C29-C28-O8-C9
39	J	101	DGD	C2A-C1A-O1G-C1G
39	j	101	DGD	C2A-C1A-O1G-C1G
36	1	101	LMG	C4-C5-C6-O5
39	H	102	DGD	C1B-C2B-C3B-C4B
30	19	307	CLA	O1D-CGD-O2D-CED
35	A	408	LHG	O9-C7-O7-C5
35	a	407	LHG	O9-C7-O7-C5
30	D	406	CLA	C4-C3-C5-C6
30	d	407	CLA	C4-C3-C5-C6
30	D	401	CLA	C13-C15-C16-C17
30	D	405	CLA	C15-C16-C17-C18
30	d	401	CLA	C13-C15-C16-C17
30	d	406	CLA	C15-C16-C17-C18
30	18	301	CLA	CBD-CGD-O2D-CED
42	12	304	A86	C35-C34-O4-C38
42	15	315	A86	C35-C34-O4-C38
30	C	502	CLA	C2A-CAA-CBA-CGA
30	c	502	CLA	C2A-CAA-CBA-CGA
30	19	304	CLA	C2A-CAA-CBA-CGA
30	b	611	CLA	C16-C17-C18-C19
30	18	310	CLA	C16-C17-C18-C20
30	B	615	CLA	C3-C5-C6-C7
30	b	615	CLA	C3-C5-C6-C7
30	W	103	CLA	CBA-CGA-O2A-C1
30	w	103	CLA	CBA-CGA-O2A-C1
36	B	620	LMG	C29-C28-O8-C9
36	b	619	LMG	C29-C28-O8-C9
36	B	620	LMG	C10-C11-C12-C13
36	b	619	LMG	C10-C11-C12-C13
42	16	310	A86	C3-C4-C5-C6
42	17	302	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
42	17	311	A86	C24-C25-C26-C27
42	11	316	A86	C35-C34-O4-C38
42	13	301	A86	C35-C34-O4-C38
42	13	315	A86	C35-C34-O4-C38
42	15	316	A86	C35-C34-O4-C38
42	18	302	A86	C35-C34-O4-C38
36	c	519	LMG	C32-C33-C34-C35
39	h	102	DGD	C7A-C8A-C9A-CAA
30	19	307	CLA	C13-C15-C16-C17
32	B	616	BCR	C16-C17-C18-C36
32	B	616	BCR	C20-C21-C22-C37
32	B	618	BCR	C16-C17-C18-C36
32	C	515	BCR	C20-C21-C22-C37
32	Y	101	BCR	C11-C10-C9-C34
32	Z	101	BCR	C11-C10-C9-C34
32	Z	101	BCR	C20-C21-C22-C37
32	b	617	BCR	C16-C17-C18-C36
32	c	515	BCR	C11-C10-C9-C34
32	c	515	BCR	C20-C21-C22-C37
32	c	516	BCR	C20-C21-C22-C37
32	c	520	BCR	C11-C10-C9-C34
32	m	103	BCR	C16-C17-C18-C36
32	m	103	BCR	C20-C21-C22-C37
30	18	309	CLA	C3-C5-C6-C7
33	A	406	SQD	C11-C12-C13-C14
33	a	405	SQD	C11-C12-C13-C14
35	B	622	LHG	C11-C10-C9-C8
35	a	407	LHG	C29-C30-C31-C32
35	b	621	LHG	C11-C10-C9-C8
36	B	619	LMG	C31-C32-C33-C34
36	Q	301	LMG	C32-C33-C34-C35
36	b	618	LMG	C31-C32-C33-C34
36	d	410	LMG	C35-C36-C37-C38
36	12	301	LMG	C12-C13-C14-C15
37	B	625	LMU	C5-C6-C7-C8
37	12	302	LMU	C5-C6-C7-C8
39	H	102	DGD	C7A-C8A-C9A-CAA
30	B	611	CLA	C16-C17-C18-C19
33	A	406	SQD	C10-C11-C12-C13
33	a	405	SQD	C10-C11-C12-C13
35	A	408	LHG	C29-C30-C31-C32
35	a	407	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	D	408	LMG	C35-C36-C37-C38
33	L	103	SQD	C46-C45-O47-C7
33	l	101	SQD	C46-C45-O47-C7
30	C	512	CLA	O1D-CGD-O2D-CED
39	h	102	DGD	C1B-C2B-C3B-C4B
30	20	203	CLA	CBD-CGD-O2D-CED
35	A	408	LHG	C15-C16-C17-C18
35	l	102	LHG	C16-C17-C18-C19
36	1	101	LMG	C12-C13-C14-C15
30	c	512	CLA	O1D-CGD-O2D-CED
30	18	310	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	C15-C16-C17-C18
33	l	101	SQD	C15-C16-C17-C18
35	L	102	LHG	C16-C17-C18-C19
36	W	101	LMG	C20-C21-C22-C23
30	20	207	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	C32-C33-C34-C35
33	l	101	SQD	C32-C33-C34-C35
36	M	102	LMG	C15-C16-C17-C18
36	M	102	LMG	C33-C34-C35-C36
36	m	102	LMG	C15-C16-C17-C18
36	m	102	LMG	C33-C34-C35-C36
36	w	101	LMG	C20-C21-C22-C23
35	L	102	LHG	C23-C24-C25-C26
35	l	102	LHG	C23-C24-C25-C26
36	B	620	LMG	C28-C29-C30-C31
36	b	619	LMG	C28-C29-C30-C31
32	A	405	BCR	C20-C21-C22-C23
32	B	624	BCR	C12-C13-C14-C15
32	B	624	BCR	C16-C17-C18-C19
32	F	101	BCR	C20-C21-C22-C23
32	Y	101	BCR	C12-C13-C14-C15
32	Y	101	BCR	C20-C21-C22-C23
32	Z	101	BCR	C12-C13-C14-C15
32	Z	101	BCR	C16-C17-C18-C19
32	a	404	BCR	C20-C21-C22-C23
32	b	623	BCR	C12-C13-C14-C15
32	b	623	BCR	C16-C17-C18-C19
32	c	515	BCR	C12-C13-C14-C15
32	c	515	BCR	C16-C17-C18-C19
32	c	520	BCR	C12-C13-C14-C15
32	c	520	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
32	f	101	BCR	C20-C21-C22-C23
39	C	517	DGD	C2E-C1E-O5D-C6D
39	J	101	DGD	C2E-C1E-O5D-C6D
39	c	518	DGD	C2E-C1E-O5D-C6D
39	j	101	DGD	C2E-C1E-O5D-C6D
30	B	612	CLA	CBA-CGA-O2A-C1
30	b	612	CLA	CBA-CGA-O2A-C1
39	C	517	DGD	C2A-C3A-C4A-C5A
39	c	518	DGD	C2A-C3A-C4A-C5A
30	A	404	CLA	C5-C6-C7-C8
30	a	403	CLA	C5-C6-C7-C8
30	B	607	CLA	O1A-CGA-O2A-C1
30	W	103	CLA	O1A-CGA-O2A-C1
30	b	607	CLA	O1A-CGA-O2A-C1
30	w	103	CLA	O1A-CGA-O2A-C1
36	M	102	LMG	O10-C28-O8-C9
36	m	102	LMG	O10-C28-O8-C9
30	B	605	CLA	C16-C17-C18-C20
30	b	605	CLA	C16-C17-C18-C20
30	15	305	CLA	O1D-CGD-O2D-CED
30	C	507	CLA	C4-C3-C5-C6
30	c	507	CLA	C4-C3-C5-C6
35	l	102	LHG	C32-C33-C34-C35
30	C	504	CLA	C6-C7-C8-C9
30	c	504	CLA	C6-C7-C8-C9
30	21	303	CLA	CBD-CGD-O2D-CED
35	A	408	LHG	C23-C24-C25-C26
35	a	407	LHG	C23-C24-C25-C26
33	L	103	SQD	C33-C34-C35-C36
33	l	101	SQD	C33-C34-C35-C36
35	L	102	LHG	C32-C33-C34-C35
35	a	407	LHG	C28-C29-C30-C31
36	D	408	LMG	C36-C37-C38-C39
36	d	410	LMG	C36-C37-C38-C39
30	D	406	CLA	O1A-CGA-O2A-C1
30	d	407	CLA	O1A-CGA-O2A-C1
42	17	315	A86	C7-C6-C8-C9
42	19	311	A86	C7-C6-C8-C9
42	20	212	A86	C-C1-C24-C25
42	20	213	A86	C-C1-C24-C25
42	21	314	A86	C-C1-C24-C25
35	A	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
35	L	101	LHG	C24-C25-C26-C27
35	d	409	LHG	C24-C25-C26-C27
36	D	408	LMG	C30-C31-C32-C33
36	W	101	LMG	C19-C20-C21-C22
32	B	616	BCR	C21-C22-C23-C24
32	B	624	BCR	C21-C22-C23-C24
32	Y	101	BCR	C11-C12-C13-C14
32	b	623	BCR	C21-C22-C23-C24
32	c	520	BCR	C11-C12-C13-C14
32	m	103	BCR	C21-C22-C23-C24
42	17	315	A86	C5-C6-C8-C9
42	19	311	A86	C5-C6-C8-C9
42	20	212	A86	C2-C1-C24-C25
30	16	304	CLA	C3-C5-C6-C7
35	L	101	LHG	C25-C26-C27-C28
35	d	409	LHG	C25-C26-C27-C28
36	M	102	LMG	C14-C15-C16-C17
36	W	101	LMG	C14-C15-C16-C17
36	d	410	LMG	C30-C31-C32-C33
36	m	102	LMG	C14-C15-C16-C17
36	m	102	LMG	C31-C32-C33-C34
36	w	101	LMG	C14-C15-C16-C17
36	w	101	LMG	C19-C20-C21-C22
42	20	211	A86	O5-C38-O4-C34
42	21	311	A86	O5-C38-O4-C34
35	A	408	LHG	C7-C8-C9-C10
35	B	622	LHG	C30-C31-C32-C33
35	L	102	LHG	C28-C29-C30-C31
35	b	621	LHG	C30-C31-C32-C33
35	l	102	LHG	C28-C29-C30-C31
36	M	102	LMG	C31-C32-C33-C34
30	B	623	CLA	C4B-C3B-CAB-CBB
30	C	505	CLA	C4B-C3B-CAB-CBB
30	C	513	CLA	C4B-C3B-CAB-CBB
30	D	406	CLA	C4B-C3B-CAB-CBB
30	W	103	CLA	C4B-C3B-CAB-CBB
30	b	622	CLA	C4B-C3B-CAB-CBB
30	c	505	CLA	C4B-C3B-CAB-CBB
30	c	513	CLA	C4B-C3B-CAB-CBB
30	d	407	CLA	C4B-C3B-CAB-CBB
30	w	103	CLA	C4B-C3B-CAB-CBB
30	11	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	12	313	CLA	C4B-C3B-CAB-CBB
30	13	309	CLA	C4B-C3B-CAB-CBB
30	14	310	CLA	C4B-C3B-CAB-CBB
30	15	301	CLA	C4B-C3B-CAB-CBB
30	15	308	CLA	C4B-C3B-CAB-CBB
30	18	303	CLA	C4B-C3B-CAB-CBB
30	18	307	CLA	C4B-C3B-CAB-CBB
30	19	301	CLA	C4B-C3B-CAB-CBB
30	19	303	CLA	C4B-C3B-CAB-CBB
30	19	305	CLA	C4B-C3B-CAB-CBB
30	19	306	CLA	C4B-C3B-CAB-CBB
30	19	307	CLA	C4B-C3B-CAB-CBB
30	19	309	CLA	C4B-C3B-CAB-CBB
30	20	204	CLA	C4B-C3B-CAB-CBB
30	21	301	CLA	C4B-C3B-CAB-CBB
30	21	308	CLA	C4B-C3B-CAB-CBB
30	21	309	CLA	C4B-C3B-CAB-CBB
30	C	520	CLA	C16-C17-C18-C19
30	15	303	CLA	C16-C17-C18-C19
30	19	307	CLA	C16-C17-C18-C19
30	19	307	CLA	C16-C17-C18-C20
39	C	516	DGD	O6D-C1D-O3G-C3G
39	J	101	DGD	O6E-C1E-O5D-C6D
39	c	517	DGD	O6D-C1D-O3G-C3G
39	j	101	DGD	O6E-C1E-O5D-C6D
30	C	508	CLA	C13-C15-C16-C17
30	c	508	CLA	C13-C15-C16-C17
39	C	516	DGD	C3A-C4A-C5A-C6A
39	c	517	DGD	C3A-C4A-C5A-C6A
30	b	622	CLA	O1D-CGD-O2D-CED
30	17	301	CLA	O1D-CGD-O2D-CED
39	C	516	DGD	CCA-CDA-CEA-CFA
39	c	517	DGD	CCA-CDA-CEA-CFA
39	j	101	DGD	C8A-C9A-CAA-CBA
35	a	407	LHG	C7-C8-C9-C10
33	A	406	SQD	C32-C33-C34-C35
33	a	405	SQD	C32-C33-C34-C35
36	Q	301	LMG	C18-C19-C20-C21
36	c	519	LMG	C18-C19-C20-C21
39	J	101	DGD	C8A-C9A-CAA-CBA
39	C	516	DGD	C7B-C8B-C9B-CAB
39	c	517	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
39	h	102	DGD	C3A-C4A-C5A-C6A
30	B	610	CLA	O1D-CGD-O2D-CED
30	b	610	CLA	O1D-CGD-O2D-CED
30	m	101	CLA	O1D-CGD-O2D-CED
30	16	307	CLA	O1D-CGD-O2D-CED
30	B	623	CLA	C3A-C2A-CAA-CBA
30	D	405	CLA	C3A-C2A-CAA-CBA
30	W	102	CLA	C3A-C2A-CAA-CBA
30	W	103	CLA	C3A-C2A-CAA-CBA
30	d	406	CLA	C3A-C2A-CAA-CBA
30	w	102	CLA	C3A-C2A-CAA-CBA
30	w	103	CLA	C3A-C2A-CAA-CBA
30	11	303	CLA	C3A-C2A-CAA-CBA
30	11	304	CLA	C3A-C2A-CAA-CBA
30	11	306	CLA	C3A-C2A-CAA-CBA
30	11	308	CLA	C3A-C2A-CAA-CBA
30	12	307	CLA	C3A-C2A-CAA-CBA
30	12	308	CLA	C3A-C2A-CAA-CBA
30	12	310	CLA	C3A-C2A-CAA-CBA
30	12	313	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C3A-C2A-CAA-CBA
30	13	305	CLA	C3A-C2A-CAA-CBA
30	13	307	CLA	C3A-C2A-CAA-CBA
30	13	309	CLA	C3A-C2A-CAA-CBA
30	14	305	CLA	C3A-C2A-CAA-CBA
30	14	306	CLA	C3A-C2A-CAA-CBA
30	14	308	CLA	C3A-C2A-CAA-CBA
30	14	310	CLA	C3A-C2A-CAA-CBA
30	15	302	CLA	C3A-C2A-CAA-CBA
30	15	304	CLA	C3A-C2A-CAA-CBA
30	15	306	CLA	C3A-C2A-CAA-CBA
30	15	308	CLA	C3A-C2A-CAA-CBA
30	16	303	CLA	C3A-C2A-CAA-CBA
30	16	304	CLA	C3A-C2A-CAA-CBA
30	16	305	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C3A-C2A-CAA-CBA
30	17	304	CLA	C3A-C2A-CAA-CBA
30	17	305	CLA	C3A-C2A-CAA-CBA
30	17	306	CLA	C3A-C2A-CAA-CBA
30	17	307	CLA	C3A-C2A-CAA-CBA
30	18	305	CLA	C3A-C2A-CAA-CBA
30	18	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	18	308	CLA	C3A-C2A-CAA-CBA
30	18	311	CLA	C3A-C2A-CAA-CBA
30	19	304	CLA	C3A-C2A-CAA-CBA
30	19	306	CLA	C3A-C2A-CAA-CBA
30	20	205	CLA	C3A-C2A-CAA-CBA
30	20	206	CLA	C3A-C2A-CAA-CBA
30	20	207	CLA	C3A-C2A-CAA-CBA
30	20	208	CLA	C3A-C2A-CAA-CBA
30	21	302	CLA	C3A-C2A-CAA-CBA
30	21	304	CLA	C3A-C2A-CAA-CBA
30	21	305	CLA	C3A-C2A-CAA-CBA
30	21	309	CLA	C3A-C2A-CAA-CBA
30	C	504	CLA	C8-C10-C11-C12
30	c	504	CLA	C8-C10-C11-C12
30	11	307	CLA	C5-C6-C7-C8
30	12	311	CLA	C5-C6-C7-C8
30	18	309	CLA	C15-C16-C17-C18
37	B	625	LMU	C2-C1-O1'-C1'
36	W	101	LMG	C12-C13-C14-C15
36	w	101	LMG	C12-C13-C14-C15
39	H	102	DGD	C3A-C4A-C5A-C6A
30	M	101	CLA	O1D-CGD-O2D-CED
30	B	605	CLA	C16-C17-C18-C19
30	b	605	CLA	C16-C17-C18-C19
30	C	503	CLA	O1D-CGD-O2D-CED
30	c	505	CLA	CBD-CGD-O2D-CED
30	B	623	CLA	O1D-CGD-O2D-CED
30	B	601	CLA	C3-C5-C6-C7
30	b	601	CLA	C3-C5-C6-C7
30	13	308	CLA	C5-C6-C7-C8
30	14	309	CLA	C5-C6-C7-C8
30	C	511	CLA	C4-C3-C5-C6
30	c	511	CLA	C4-C3-C5-C6
30	C	507	CLA	C2-C3-C5-C6
30	C	511	CLA	C2-C3-C5-C6
30	c	507	CLA	C2-C3-C5-C6
30	c	511	CLA	C2-C3-C5-C6
30	C	505	CLA	CBD-CGD-O2D-CED
35	B	622	LHG	C9-C10-C11-C12
35	b	621	LHG	C9-C10-C11-C12
36	W	101	LMG	C37-C38-C39-C40
36	w	101	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
42	21	313	A86	C35-C34-O4-C38
39	c	518	DGD	O6E-C5E-C6E-O5E
33	L	103	SQD	C14-C15-C16-C17
33	l	101	SQD	C14-C15-C16-C17
35	A	408	LHG	C14-C15-C16-C17
35	L	101	LHG	C31-C32-C33-C34
35	a	407	LHG	C14-C15-C16-C17
35	d	409	LHG	C31-C32-C33-C34
39	C	517	DGD	O6E-C5E-C6E-O5E
30	17	301	CLA	C16-C17-C18-C20
30	B	602	CLA	C2B-C3B-CAB-CBB
30	B	623	CLA	C2B-C3B-CAB-CBB
30	C	505	CLA	C2B-C3B-CAB-CBB
30	W	103	CLA	C2B-C3B-CAB-CBB
30	b	602	CLA	C2B-C3B-CAB-CBB
30	c	505	CLA	C2B-C3B-CAB-CBB
30	w	103	CLA	C2B-C3B-CAB-CBB
30	11	308	CLA	C2B-C3B-CAB-CBB
30	11	309	CLA	C2B-C3B-CAB-CBB
30	12	313	CLA	C2B-C3B-CAB-CBB
30	12	314	CLA	C2B-C3B-CAB-CBB
30	13	309	CLA	C2B-C3B-CAB-CBB
30	13	310	CLA	C2B-C3B-CAB-CBB
30	14	310	CLA	C2B-C3B-CAB-CBB
30	14	311	CLA	C2B-C3B-CAB-CBB
30	15	301	CLA	C2B-C3B-CAB-CBB
30	15	308	CLA	C2B-C3B-CAB-CBB
30	16	306	CLA	C2B-C3B-CAB-CBB
30	17	310	CLA	C2B-C3B-CAB-CBB
30	18	303	CLA	C2B-C3B-CAB-CBB
30	18	305	CLA	C2B-C3B-CAB-CBB
30	18	307	CLA	C2B-C3B-CAB-CBB
30	18	308	CLA	C2B-C3B-CAB-CBB
30	19	301	CLA	C2B-C3B-CAB-CBB
30	19	304	CLA	C2B-C3B-CAB-CBB
30	19	305	CLA	C2B-C3B-CAB-CBB
30	19	306	CLA	C2B-C3B-CAB-CBB
30	19	307	CLA	C2B-C3B-CAB-CBB
30	19	309	CLA	C2B-C3B-CAB-CBB
30	20	204	CLA	C2B-C3B-CAB-CBB
30	20	206	CLA	C2B-C3B-CAB-CBB
30	21	301	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	21	307	CLA	C2B-C3B-CAB-CBB
30	21	308	CLA	C2B-C3B-CAB-CBB
30	21	309	CLA	C2B-C3B-CAB-CBB
33	B	621	SQD	C11-C10-C9-C8
33	L	103	SQD	C31-C32-C33-C34
33	l	101	SQD	C31-C32-C33-C34
36	b	619	LMG	C18-C19-C20-C21
39	C	517	DGD	CAA-CBA-CCA-CDA
30	c	503	CLA	O1D-CGD-O2D-CED
33	b	620	SQD	C11-C10-C9-C8
35	L	101	LHG	C13-C14-C15-C16
35	L	101	LHG	C29-C30-C31-C32
35	d	409	LHG	C29-C30-C31-C32
36	B	620	LMG	C18-C19-C20-C21
37	12	302	LMU	C2-C3-C4-C5
39	c	518	DGD	CAA-CBA-CCA-CDA
42	12	304	A86	C33-C34-O4-C38
42	13	301	A86	C33-C34-O4-C38
42	18	302	A86	C33-C34-O4-C38
35	d	409	LHG	C13-C14-C15-C16
36	D	408	LMG	C17-C18-C19-C20
36	Q	301	LMG	C19-C20-C21-C22
36	c	519	LMG	C19-C20-C21-C22
36	d	410	LMG	C17-C18-C19-C20
35	L	101	LHG	O9-C7-O7-C5
35	d	409	LHG	O9-C7-O7-C5
30	B	612	CLA	C2-C1-O2A-CGA
30	b	612	CLA	C2-C1-O2A-CGA
33	A	406	SQD	C12-C13-C14-C15
33	a	405	SQD	C12-C13-C14-C15
30	C	512	CLA	C5-C6-C7-C8
30	c	512	CLA	C5-C6-C7-C8
30	20	202	CLA	C8-C10-C11-C12
30	B	612	CLA	O1A-CGA-O2A-C1
30	b	612	CLA	O1A-CGA-O2A-C1
36	Q	301	LMG	C4-C5-C6-O5
33	a	405	SQD	C17-C18-C19-C20
30	15	303	CLA	C16-C17-C18-C20
30	18	310	CLA	C16-C17-C18-C19
33	L	103	SQD	C7-C8-C9-C10
33	l	101	SQD	C7-C8-C9-C10
32	A	405	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	A	405	BCR	C5-C6-C7-C8
32	A	409	BCR	C1-C6-C7-C8
32	A	409	BCR	C5-C6-C7-C8
32	B	616	BCR	C1-C6-C7-C8
32	B	616	BCR	C5-C6-C7-C8
32	B	616	BCR	C23-C24-C25-C26
32	B	617	BCR	C5-C6-C7-C8
32	B	618	BCR	C5-C6-C7-C8
32	B	624	BCR	C1-C6-C7-C8
32	B	624	BCR	C5-C6-C7-C8
32	C	515	BCR	C5-C6-C7-C8
32	C	518	BCR	C5-C6-C7-C8
32	C	518	BCR	C23-C24-C25-C26
32	C	518	BCR	C23-C24-C25-C30
32	F	101	BCR	C1-C6-C7-C8
32	F	101	BCR	C5-C6-C7-C8
32	H	101	BCR	C5-C6-C7-C8
32	Y	101	BCR	C5-C6-C7-C8
32	Z	101	BCR	C1-C6-C7-C8
32	Z	101	BCR	C5-C6-C7-C8
32	Z	101	BCR	C23-C24-C25-C26
32	a	404	BCR	C1-C6-C7-C8
32	a	404	BCR	C5-C6-C7-C8
32	a	408	BCR	C1-C6-C7-C8
32	a	408	BCR	C5-C6-C7-C8
32	b	616	BCR	C5-C6-C7-C8
32	b	617	BCR	C5-C6-C7-C8
32	b	623	BCR	C1-C6-C7-C8
32	b	623	BCR	C5-C6-C7-C8
32	c	515	BCR	C1-C6-C7-C8
32	c	515	BCR	C5-C6-C7-C8
32	c	515	BCR	C23-C24-C25-C26
32	c	516	BCR	C5-C6-C7-C8
32	c	520	BCR	C5-C6-C7-C8
32	c	521	BCR	C5-C6-C7-C8
32	c	521	BCR	C23-C24-C25-C26
32	c	521	BCR	C23-C24-C25-C30
32	f	101	BCR	C1-C6-C7-C8
32	f	101	BCR	C5-C6-C7-C8
32	h	101	BCR	C5-C6-C7-C8
32	m	103	BCR	C1-C6-C7-C8
32	m	103	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	m	103	BCR	C23-C24-C25-C26
33	A	406	SQD	C17-C18-C19-C20
36	b	618	LMG	C29-C30-C31-C32
30	C	504	CLA	CBA-CGA-O2A-C1
30	M	101	CLA	CBA-CGA-O2A-C1
30	c	504	CLA	CBA-CGA-O2A-C1
30	m	101	CLA	CBA-CGA-O2A-C1
42	11	316	A86	C33-C34-O4-C38
42	13	315	A86	C33-C34-O4-C38
42	15	315	A86	C33-C34-O4-C38
42	15	316	A86	C33-C34-O4-C38
30	16	301	CLA	C5-C6-C7-C8
36	c	519	LMG	C4-C5-C6-O5
36	B	619	LMG	C29-C30-C31-C32
37	B	625	LMU	C2-C3-C4-C5
36	Q	301	LMG	C10-C11-C12-C13
36	c	519	LMG	C10-C11-C12-C13
30	19	306	CLA	O1D-CGD-O2D-CED
30	C	508	CLA	C11-C10-C8-C7
30	W	102	CLA	C12-C13-C15-C16
30	W	103	CLA	C6-C7-C8-C10
30	W	103	CLA	C11-C12-C13-C15
30	c	508	CLA	C11-C10-C8-C7
30	w	102	CLA	C12-C13-C15-C16
30	w	103	CLA	C6-C7-C8-C10
30	w	103	CLA	C11-C12-C13-C15
31	A	403	PHO	C2-C3-C5-C6
31	d	403	PHO	C2-C3-C5-C6
40	D	404	PL9	C28-C29-C31-C32
40	d	405	PL9	C28-C29-C31-C32
30	c	510	CLA	C3-C5-C6-C7
30	M	101	CLA	O1A-CGA-O2A-C1
30	m	101	CLA	O1A-CGA-O2A-C1
33	A	406	SQD	C14-C15-C16-C17
33	a	405	SQD	C14-C15-C16-C17
42	11	316	A86	C3-C4-C5-C6
42	12	304	A86	C3-C4-C5-C6
42	13	301	A86	C3-C4-C5-C6
42	13	315	A86	C3-C4-C5-C6
42	15	315	A86	C3-C4-C5-C6
42	15	316	A86	C3-C4-C5-C6
42	18	302	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
42	19	311	A86	C11-C10-C9-C8
42	19	312	A86	C1-C2-C3-C4
42	20	210	A86	C1-C2-C3-C4
30	20	202	CLA	CBD-CGD-O2D-CED
30	B	602	CLA	C16-C17-C18-C19
30	B	611	CLA	C16-C17-C18-C20
30	b	602	CLA	C16-C17-C18-C19
30	b	611	CLA	C16-C17-C18-C20
30	18	305	CLA	C16-C17-C18-C19
39	H	102	DGD	O6D-C5D-C6D-O5D
39	h	102	DGD	O6D-C5D-C6D-O5D
30	B	602	CLA	CBA-CGA-O2A-C1
30	Z	102	CLA	CBA-CGA-O2A-C1
30	b	602	CLA	CBA-CGA-O2A-C1
36	B	619	LMG	C29-C28-O8-C9
36	b	618	LMG	C29-C28-O8-C9
30	B	615	CLA	C2A-CAA-CBA-CGA
30	b	615	CLA	C2A-CAA-CBA-CGA
30	17	303	CLA	C2A-CAA-CBA-CGA
30	17	307	CLA	C2A-CAA-CBA-CGA
30	18	307	CLA	C2A-CAA-CBA-CGA
30	c	502	CLA	C10-C11-C12-C13
30	19	307	CLA	C8-C10-C11-C12
35	d	409	LHG	C33-C34-C35-C36
36	12	301	LMG	C32-C33-C34-C35
35	L	101	LHG	C33-C34-C35-C36
30	C	502	CLA	C10-C11-C12-C13
30	W	102	CLA	C5-C6-C7-C8
30	w	102	CLA	C5-C6-C7-C8
30	18	309	CLA	C10-C11-C12-C13
30	C	510	CLA	C3-C5-C6-C7
36	1	101	LMG	C32-C33-C34-C35
36	b	619	LMG	C11-C12-C13-C14
36	12	301	LMG	C14-C15-C16-C17
39	J	101	DGD	C6A-C7A-C8A-C9A
30	D	405	CLA	C5-C6-C7-C8
30	d	406	CLA	C5-C6-C7-C8
33	L	103	SQD	C17-C18-C19-C20
33	l	101	SQD	C17-C18-C19-C20
36	B	620	LMG	C11-C12-C13-C14
36	Q	301	LMG	C17-C18-C19-C20
36	c	519	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
39	j	101	DGD	C6A-C7A-C8A-C9A
33	A	406	SQD	C7-C8-C9-C10
33	a	405	SQD	C7-C8-C9-C10
36	B	620	LMG	C11-C10-O7-C8
36	b	619	LMG	C11-C10-O7-C8
33	L	103	SQD	C12-C13-C14-C15
33	l	101	SQD	C12-C13-C14-C15
39	C	516	DGD	C3B-C4B-C5B-C6B
30	M	101	CLA	C5-C6-C7-C8
30	b	614	CLA	C15-C16-C17-C18
30	c	507	CLA	C13-C15-C16-C17
30	21	305	CLA	CBD-CGD-O2D-CED
35	a	407	LHG	C13-C14-C15-C16
39	c	517	DGD	C3B-C4B-C5B-C6B
36	Q	301	LMG	O9-C10-O7-C8
36	W	101	LMG	O9-C10-O7-C8
36	w	101	LMG	O9-C10-O7-C8
35	A	408	LHG	C13-C14-C15-C16
37	12	302	LMU	C4-C5-C6-C7
30	B	614	CLA	C15-C16-C17-C18
30	C	507	CLA	C13-C15-C16-C17
30	c	514	CLA	C15-C16-C17-C18
30	m	101	CLA	C5-C6-C7-C8
33	B	621	SQD	O47-C45-C46-O48
33	b	620	SQD	O47-C45-C46-O48
30	14	305	CLA	CBA-CGA-O2A-C1
30	C	520	CLA	C16-C17-C18-C20
30	C	503	CLA	C13-C15-C16-C17
30	C	514	CLA	C15-C16-C17-C18
30	c	503	CLA	C13-C15-C16-C17
30	18	303	CLA	C8-C10-C11-C12
30	19	307	CLA	C10-C11-C12-C13
30	B	609	CLA	C2-C3-C5-C6
30	D	406	CLA	C2-C3-C5-C6
30	b	609	CLA	C2-C3-C5-C6
30	d	407	CLA	C2-C3-C5-C6
30	B	615	CLA	C6-C7-C8-C9
30	C	503	CLA	C11-C12-C13-C14
30	C	505	CLA	C6-C7-C8-C9
30	Z	102	CLA	C14-C13-C15-C16
30	W	102	CLA	C14-C13-C15-C16
30	W	103	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	b	615	CLA	C6-C7-C8-C9
30	c	503	CLA	C11-C12-C13-C14
30	c	505	CLA	C6-C7-C8-C9
30	w	102	CLA	C14-C13-C15-C16
30	w	103	CLA	C6-C7-C8-C9
30	11	307	CLA	C6-C7-C8-C9
30	12	311	CLA	C6-C7-C8-C9
30	13	308	CLA	C6-C7-C8-C9
30	14	309	CLA	C6-C7-C8-C9
30	19	303	CLA	C11-C12-C13-C14
30	20	209	CLA	C11-C10-C8-C9
30	21	307	CLA	C14-C13-C15-C16
30	C	507	CLA	C2A-CAA-CBA-CGA
30	M	101	CLA	C2A-CAA-CBA-CGA
30	c	507	CLA	C2A-CAA-CBA-CGA
30	m	101	CLA	C2A-CAA-CBA-CGA
30	15	302	CLA	C2A-CAA-CBA-CGA
35	L	101	LHG	C28-C29-C30-C31
35	d	409	LHG	C28-C29-C30-C31
36	W	101	LMG	C18-C19-C20-C21
36	w	101	LMG	C18-C19-C20-C21
42	19	310	A86	C-C1-C24-C25
42	19	310	A86	C2-C1-C24-C25
30	19	309	CLA	O1D-CGD-O2D-CED
30	A	404	CLA	C1A-C2A-CAA-CBA
30	B	604	CLA	C1A-C2A-CAA-CBA
30	B	606	CLA	C1A-C2A-CAA-CBA
30	B	607	CLA	C1A-C2A-CAA-CBA
30	B	611	CLA	C1A-C2A-CAA-CBA
30	B	623	CLA	C1A-C2A-CAA-CBA
30	C	504	CLA	C1A-C2A-CAA-CBA
30	C	512	CLA	C1A-C2A-CAA-CBA
30	C	513	CLA	C1A-C2A-CAA-CBA
30	D	401	CLA	C1A-C2A-CAA-CBA
30	D	402	CLA	C1A-C2A-CAA-CBA
30	M	101	CLA	C1A-C2A-CAA-CBA
30	W	103	CLA	C1A-C2A-CAA-CBA
30	a	403	CLA	C1A-C2A-CAA-CBA
30	b	604	CLA	C1A-C2A-CAA-CBA
30	b	606	CLA	C1A-C2A-CAA-CBA
30	b	607	CLA	C1A-C2A-CAA-CBA
30	b	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	b	622	CLA	C1A-C2A-CAA-CBA
30	c	504	CLA	C1A-C2A-CAA-CBA
30	c	512	CLA	C1A-C2A-CAA-CBA
30	d	401	CLA	C1A-C2A-CAA-CBA
30	d	402	CLA	C1A-C2A-CAA-CBA
30	m	101	CLA	C1A-C2A-CAA-CBA
30	w	103	CLA	C1A-C2A-CAA-CBA
30	11	301	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	C1A-C2A-CAA-CBA
30	11	306	CLA	C1A-C2A-CAA-CBA
30	12	305	CLA	C1A-C2A-CAA-CBA
30	12	308	CLA	C1A-C2A-CAA-CBA
30	12	310	CLA	C1A-C2A-CAA-CBA
30	13	302	CLA	C1A-C2A-CAA-CBA
30	13	305	CLA	C1A-C2A-CAA-CBA
30	13	307	CLA	C1A-C2A-CAA-CBA
30	14	303	CLA	C1A-C2A-CAA-CBA
30	14	306	CLA	C1A-C2A-CAA-CBA
30	14	308	CLA	C1A-C2A-CAA-CBA
30	15	304	CLA	C1A-C2A-CAA-CBA
30	15	306	CLA	C1A-C2A-CAA-CBA
30	15	308	CLA	C1A-C2A-CAA-CBA
30	16	305	CLA	C1A-C2A-CAA-CBA
30	16	306	CLA	C1A-C2A-CAA-CBA
30	17	306	CLA	C1A-C2A-CAA-CBA
30	17	307	CLA	C1A-C2A-CAA-CBA
30	18	306	CLA	C1A-C2A-CAA-CBA
30	18	308	CLA	C1A-C2A-CAA-CBA
30	18	309	CLA	C1A-C2A-CAA-CBA
30	18	311	CLA	C1A-C2A-CAA-CBA
30	19	304	CLA	C1A-C2A-CAA-CBA
30	19	306	CLA	C1A-C2A-CAA-CBA
30	20	205	CLA	C1A-C2A-CAA-CBA
30	20	206	CLA	C1A-C2A-CAA-CBA
30	21	304	CLA	C1A-C2A-CAA-CBA
30	21	305	CLA	C1A-C2A-CAA-CBA
30	21	309	CLA	C1A-C2A-CAA-CBA
30	B	602	CLA	C16-C17-C18-C20
30	B	610	CLA	C16-C17-C18-C20
30	b	602	CLA	C16-C17-C18-C20
30	b	610	CLA	C16-C17-C18-C20
30	17	301	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	18	305	CLA	C16-C17-C18-C20
36	c	519	LMG	O9-C10-O7-C8
36	1	101	LMG	C15-C16-C17-C18
32	B	624	BCR	C13-C14-C15-C16
32	b	623	BCR	C13-C14-C15-C16
42	20	212	A86	C3-C4-C5-C6
42	20	213	A86	C11-C10-C9-C8
42	21	314	A86	C11-C10-C9-C8
30	C	507	CLA	C8-C10-C11-C12
37	12	302	LMU	C1-C2-C3-C4
35	A	408	LHG	C3-O3-P-O6
35	B	622	LHG	C3-O3-P-O6
35	a	407	LHG	C3-O3-P-O6
35	b	621	LHG	C3-O3-P-O6
35	B	622	LHG	C33-C34-C35-C36
35	L	101	LHG	C32-C33-C34-C35
35	d	409	LHG	C32-C33-C34-C35
39	C	516	DGD	CBA-CCA-CDA-CEA
39	c	517	DGD	CBA-CCA-CDA-CEA
36	w	101	LMG	C17-C18-C19-C20
30	C	505	CLA	C10-C11-C12-C13
30	c	505	CLA	C10-C11-C12-C13
30	c	507	CLA	C8-C10-C11-C12
35	B	622	LHG	O6-C4-C5-C6
35	b	621	LHG	O6-C4-C5-C6
35	b	621	LHG	C33-C34-C35-C36
36	W	101	LMG	C17-C18-C19-C20
30	Z	102	CLA	O1A-CGA-O2A-C1
36	D	408	LMG	O6-C5-C6-O5
36	d	410	LMG	O6-C5-C6-O5
36	B	620	LMG	C31-C32-C33-C34
36	b	619	LMG	C31-C32-C33-C34
37	B	625	LMU	C4-C5-C6-C7
30	B	601	CLA	C10-C11-C12-C13
30	b	601	CLA	C10-C11-C12-C13
39	J	101	DGD	O1B-C1B-O2G-C2G
39	j	101	DGD	O1B-C1B-O2G-C2G
36	w	101	LMG	C30-C31-C32-C33
30	20	209	CLA	C15-C16-C17-C18
36	W	101	LMG	C30-C31-C32-C33
30	B	602	CLA	O1A-CGA-O2A-C1
30	C	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	b	602	CLA	O1A-CGA-O2A-C1
30	c	504	CLA	O1A-CGA-O2A-C1
30	14	305	CLA	O1A-CGA-O2A-C1
30	B	610	CLA	C16-C17-C18-C19
30	b	610	CLA	C16-C17-C18-C19
35	A	408	LHG	C4-C5-C6-O8
35	A	408	LHG	C30-C31-C32-C33
35	a	407	LHG	C4-C5-C6-O8
35	a	407	LHG	C30-C31-C32-C33
36	B	619	LMG	C30-C31-C32-C33
36	D	408	LMG	O1-C7-C8-C9
36	W	101	LMG	O1-C7-C8-C9
36	W	101	LMG	C7-C8-C9-O8
36	d	410	LMG	O1-C7-C8-C9
36	w	101	LMG	O1-C7-C8-C9
36	w	101	LMG	C7-C8-C9-O8
30	C	511	CLA	C5-C6-C7-C8
30	M	101	CLA	C10-C11-C12-C13
30	c	511	CLA	C5-C6-C7-C8
30	m	101	CLA	C10-C11-C12-C13
36	B	620	LMG	C34-C35-C36-C37
36	b	618	LMG	C30-C31-C32-C33
36	b	619	LMG	C34-C35-C36-C37
39	H	102	DGD	C1A-C2A-C3A-C4A
39	h	102	DGD	C1A-C2A-C3A-C4A
39	C	517	DGD	C5D-C6D-O5D-C1E
39	c	518	DGD	C5D-C6D-O5D-C1E
30	B	604	CLA	C13-C15-C16-C17
30	Z	102	CLA	C13-C15-C16-C17
30	b	604	CLA	C13-C15-C16-C17
36	B	620	LMG	C13-C14-C15-C16
36	Q	301	LMG	C37-C38-C39-C40
36	b	619	LMG	C13-C14-C15-C16
30	11	307	CLA	CAA-CBA-CGA-O2A
30	12	311	CLA	CAA-CBA-CGA-O2A
30	13	308	CLA	CAA-CBA-CGA-O2A
30	14	309	CLA	CAA-CBA-CGA-O2A
36	c	519	LMG	C37-C38-C39-C40
35	l	102	LHG	C13-C14-C15-C16
39	H	102	DGD	CBA-CCA-CDA-CEA
35	L	101	LHG	O1-C1-C2-O2
35	d	409	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
42	20	211	A86	C24-C25-C26-C27
42	21	311	A86	C24-C25-C26-C27
35	L	102	LHG	C13-C14-C15-C16
39	h	102	DGD	CBA-CCA-CDA-CEA
37	B	625	LMU	C1-C2-C3-C4
35	B	622	LHG	C27-C28-C29-C30
35	b	621	LHG	C27-C28-C29-C30
39	H	102	DGD	CBB-CCB-CDB-CEB
39	h	102	DGD	CBB-CCB-CDB-CEB
30	C	509	CLA	C5-C6-C7-C8
39	C	516	DGD	O6E-C5E-C6E-O5E
39	c	517	DGD	O6E-C5E-C6E-O5E
30	B	609	CLA	C4-C3-C5-C6
30	b	609	CLA	C4-C3-C5-C6
31	A	403	PHO	C4-C3-C5-C6
31	d	403	PHO	C4-C3-C5-C6
30	C	502	CLA	CBA-CGA-O2A-C1
30	c	502	CLA	CBA-CGA-O2A-C1
30	c	509	CLA	C5-C6-C7-C8
30	11	307	CLA	C15-C16-C17-C18
30	12	311	CLA	C15-C16-C17-C18
30	13	308	CLA	C15-C16-C17-C18
30	14	309	CLA	C15-C16-C17-C18
31	A	403	PHO	C8-C10-C11-C12
31	d	403	PHO	C8-C10-C11-C12
30	18	303	CLA	C5-C6-C7-C8
31	D	403	PHO	C5-C6-C7-C8
31	d	404	PHO	C5-C6-C7-C8
30	11	306	CLA	O1D-CGD-O2D-CED
30	12	310	CLA	O1D-CGD-O2D-CED
30	13	307	CLA	O1D-CGD-O2D-CED
30	14	308	CLA	O1D-CGD-O2D-CED
36	W	101	LMG	C15-C16-C17-C18
36	w	101	LMG	C15-C16-C17-C18
39	J	101	DGD	CDA-CEA-CFA-CGA
39	j	101	DGD	CDA-CEA-CFA-CGA
33	L	103	SQD	C24-C23-O48-C46
33	l	101	SQD	C24-C23-O48-C46
35	l	102	LHG	O10-C23-O8-C6
30	C	519	CLA	C16-C17-C18-C19
30	B	611	CLA	C15-C16-C17-C18
30	b	611	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	C	513	CLA	O1D-CGD-O2D-CED
30	c	513	CLA	O1D-CGD-O2D-CED
35	L	102	LHG	O10-C23-O8-C6
30	B	605	CLA	C5-C6-C7-C8
30	W	102	CLA	C15-C16-C17-C18
30	b	605	CLA	C5-C6-C7-C8
30	w	102	CLA	C15-C16-C17-C18
30	18	305	CLA	C10-C11-C12-C13
36	12	301	LMG	O1-C7-C8-O7
39	C	516	DGD	O2G-C2G-C3G-O3G
39	c	517	DGD	O2G-C2G-C3G-O3G
42	21	313	A86	C33-C34-O4-C38
35	L	101	LHG	C27-C28-C29-C30
30	z	101	CLA	C16-C17-C18-C19
35	d	409	LHG	C27-C28-C29-C30
30	C	506	CLA	C4-C3-C5-C6
30	c	506	CLA	C4-C3-C5-C6
30	B	601	CLA	C11-C10-C8-C7
30	B	610	CLA	C12-C13-C15-C16
30	B	612	CLA	C6-C7-C8-C10
30	B	623	CLA	C11-C10-C8-C7
30	C	503	CLA	C11-C12-C13-C15
30	C	505	CLA	C11-C12-C13-C15
30	C	506	CLA	C2-C3-C5-C6
30	C	513	CLA	C11-C10-C8-C7
30	C	519	CLA	C11-C12-C13-C15
30	D	402	CLA	C12-C13-C15-C16
30	M	101	CLA	C6-C7-C8-C10
30	b	601	CLA	C11-C10-C8-C7
30	b	610	CLA	C12-C13-C15-C16
30	b	612	CLA	C6-C7-C8-C10
30	b	622	CLA	C11-C10-C8-C7
30	c	503	CLA	C11-C12-C13-C15
30	c	505	CLA	C11-C12-C13-C15
30	c	506	CLA	C2-C3-C5-C6
30	c	513	CLA	C11-C10-C8-C7
30	d	402	CLA	C12-C13-C15-C16
30	m	101	CLA	C6-C7-C8-C10
30	z	101	CLA	C11-C12-C13-C15
30	11	301	CLA	C11-C10-C8-C7
30	12	305	CLA	C11-C10-C8-C7
30	13	302	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	14	303	CLA	C11-C10-C8-C7
30	16	302	CLA	C11-C10-C8-C7
30	17	308	CLA	C6-C7-C8-C10
30	18	301	CLA	C12-C13-C15-C16
30	18	303	CLA	C12-C13-C15-C16
30	18	305	CLA	C6-C7-C8-C10
30	19	303	CLA	C11-C12-C13-C15
30	19	307	CLA	C11-C10-C8-C7
30	20	204	CLA	C12-C13-C15-C16
30	20	209	CLA	C11-C10-C8-C7
30	21	303	CLA	C11-C10-C8-C7
30	21	303	CLA	C11-C12-C13-C15
30	21	307	CLA	C12-C13-C15-C16
30	16	301	CLA	C3-C5-C6-C7
36	B	620	LMG	C21-C22-C23-C24
36	b	619	LMG	C21-C22-C23-C24
30	B	605	CLA	C11-C12-C13-C14
30	B	606	CLA	C11-C10-C8-C9
30	B	607	CLA	C14-C13-C15-C16
30	B	610	CLA	C14-C13-C15-C16
30	B	623	CLA	C6-C7-C8-C9
30	B	623	CLA	C11-C10-C8-C9
30	C	505	CLA	C11-C12-C13-C14
30	C	506	CLA	C14-C13-C15-C16
30	C	507	CLA	C11-C12-C13-C14
30	C	508	CLA	C11-C10-C8-C9
30	C	513	CLA	C11-C10-C8-C9
30	C	519	CLA	C6-C7-C8-C9
30	Z	102	CLA	C6-C7-C8-C9
30	Z	102	CLA	C11-C12-C13-C14
30	W	103	CLA	C11-C12-C13-C14
30	W	103	CLA	C14-C13-C15-C16
30	b	605	CLA	C11-C12-C13-C14
30	b	606	CLA	C11-C10-C8-C9
30	b	607	CLA	C14-C13-C15-C16
30	b	610	CLA	C14-C13-C15-C16
30	b	622	CLA	C6-C7-C8-C9
30	b	622	CLA	C11-C10-C8-C9
30	c	505	CLA	C11-C12-C13-C14
30	c	506	CLA	C14-C13-C15-C16
30	c	507	CLA	C11-C12-C13-C14
30	c	508	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	513	CLA	C11-C10-C8-C9
30	z	101	CLA	C6-C7-C8-C9
30	w	103	CLA	C11-C12-C13-C14
30	w	103	CLA	C14-C13-C15-C16
30	11	301	CLA	C11-C10-C8-C9
30	12	305	CLA	C11-C10-C8-C9
30	13	302	CLA	C11-C10-C8-C9
30	14	303	CLA	C11-C10-C8-C9
30	16	304	CLA	C6-C7-C8-C9
30	17	301	CLA	C14-C13-C15-C16
30	17	308	CLA	C6-C7-C8-C9
30	18	301	CLA	C14-C13-C15-C16
30	18	303	CLA	C14-C13-C15-C16
30	18	305	CLA	C6-C7-C8-C9
30	18	310	CLA	C14-C13-C15-C16
30	19	301	CLA	C11-C10-C8-C9
30	19	303	CLA	C14-C13-C15-C16
30	20	204	CLA	C14-C13-C15-C16
30	21	303	CLA	C11-C10-C8-C9
30	11	303	CLA	CBA-CGA-O2A-C1
30	11	315	CLA	CBA-CGA-O2A-C1
30	12	303	CLA	CBA-CGA-O2A-C1
30	12	307	CLA	CBA-CGA-O2A-C1
30	12	312	CLA	CBA-CGA-O2A-C1
30	13	304	CLA	CBA-CGA-O2A-C1
30	14	302	CLA	CBA-CGA-O2A-C1
39	h	102	DGD	C5A-C6A-C7A-C8A
32	B	618	BCR	C7-C8-C9-C34
32	b	617	BCR	C7-C8-C9-C34
42	11	316	A86	C7-C6-C8-C9
42	12	304	A86	C7-C6-C8-C9
42	13	301	A86	C7-C6-C8-C9
42	13	315	A86	C7-C6-C8-C9
42	15	315	A86	C7-C6-C8-C9
42	15	316	A86	C7-C6-C8-C9
42	18	302	A86	C7-C6-C8-C9
42	20	201	A86	C-C1-C24-C25
42	20	212	A86	C7-C6-C8-C9
42	21	310	A86	C-C1-C24-C25
30	B	608	CLA	C13-C15-C16-C17
35	A	408	LHG	C32-C33-C34-C35
35	a	407	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	M	102	LMG	C16-C17-C18-C19
36	m	102	LMG	C16-C17-C18-C19
39	H	102	DGD	C5A-C6A-C7A-C8A
32	A	405	BCR	C11-C12-C13-C14
32	H	101	BCR	C21-C22-C23-C24
32	a	404	BCR	C11-C12-C13-C14
32	h	101	BCR	C21-C22-C23-C24
42	11	314	A86	C2-C1-C24-C25
42	12	319	A86	C2-C1-C24-C25
42	14	301	A86	C2-C1-C24-C25
42	14	316	A86	C2-C1-C24-C25
42	15	314	A86	C2-C1-C24-C25
42	16	313	A86	C2-C1-C24-C25
42	17	316	A86	C2-C1-C24-C25
42	20	212	A86	C5-C6-C8-C9
42	21	310	A86	C2-C1-C24-C25
39	C	517	DGD	C5A-C6A-C7A-C8A
30	b	608	CLA	C13-C15-C16-C17
39	H	102	DGD	CCB-CDB-CEB-CFB
39	c	518	DGD	C5A-C6A-C7A-C8A
30	17	301	CLA	CBA-CGA-O2A-C1
36	M	102	LMG	C29-C28-O8-C9
36	m	102	LMG	C29-C28-O8-C9
39	h	102	DGD	CCB-CDB-CEB-CFB
30	B	602	CLA	C4B-C3B-CAB-CBB
30	B	609	CLA	C4B-C3B-CAB-CBB
30	B	610	CLA	C4B-C3B-CAB-CBB
30	B	611	CLA	C4B-C3B-CAB-CBB
30	C	506	CLA	C4B-C3B-CAB-CBB
30	C	512	CLA	C4B-C3B-CAB-CBB
30	b	602	CLA	C4B-C3B-CAB-CBB
30	b	609	CLA	C4B-C3B-CAB-CBB
30	b	610	CLA	C4B-C3B-CAB-CBB
30	b	611	CLA	C4B-C3B-CAB-CBB
30	c	506	CLA	C4B-C3B-CAB-CBB
30	c	512	CLA	C4B-C3B-CAB-CBB
30	11	301	CLA	C4B-C3B-CAB-CBB
30	11	306	CLA	C4B-C3B-CAB-CBB
30	12	305	CLA	C4B-C3B-CAB-CBB
30	12	310	CLA	C4B-C3B-CAB-CBB
30	13	302	CLA	C4B-C3B-CAB-CBB
30	13	307	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	14	303	CLA	C4B-C3B-CAB-CBB
30	14	308	CLA	C4B-C3B-CAB-CBB
30	15	303	CLA	C4B-C3B-CAB-CBB
30	15	305	CLA	C4B-C3B-CAB-CBB
30	16	304	CLA	C4B-C3B-CAB-CBB
30	17	301	CLA	C4B-C3B-CAB-CBB
30	17	305	CLA	C4B-C3B-CAB-CBB
30	20	207	CLA	C4B-C3B-CAB-CBB
30	21	302	CLA	C4B-C3B-CAB-CBB
30	21	305	CLA	C4B-C3B-CAB-CBB
30	C	519	CLA	C16-C17-C18-C20
30	z	101	CLA	C16-C17-C18-C20
30	c	513	CLA	C13-C15-C16-C17
35	L	101	LHG	O6-C4-C5-C6
35	d	409	LHG	O6-C4-C5-C6
35	B	622	LHG	C32-C33-C34-C35
35	L	102	LHG	C30-C31-C32-C33
35	b	621	LHG	C32-C33-C34-C35
35	l	102	LHG	C30-C31-C32-C33
36	d	410	LMG	C20-C21-C22-C23
39	C	516	DGD	C5A-C6A-C7A-C8A
39	c	517	DGD	C5A-C6A-C7A-C8A
39	c	518	DGD	C4A-C5A-C6A-C7A
36	B	619	LMG	C13-C14-C15-C16
36	D	408	LMG	C20-C21-C22-C23
36	b	618	LMG	C13-C14-C15-C16
39	C	517	DGD	C4A-C5A-C6A-C7A
30	B	606	CLA	C13-C15-C16-C17
30	C	513	CLA	C13-C15-C16-C17
30	b	606	CLA	C13-C15-C16-C17
30	20	203	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	C36-C37-C38-C39
36	Q	301	LMG	C29-C30-C31-C32
36	b	618	LMG	C36-C37-C38-C39
30	b	611	CLA	CBA-CGA-O2A-C1
30	B	601	CLA	C3A-C2A-CAA-CBA
30	C	513	CLA	C3A-C2A-CAA-CBA
30	b	601	CLA	C3A-C2A-CAA-CBA
30	b	622	CLA	C3A-C2A-CAA-CBA
30	c	513	CLA	C3A-C2A-CAA-CBA
30	15	305	CLA	C3A-C2A-CAA-CBA
30	21	301	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	c	519	LMG	C29-C30-C31-C32
42	11	310	A86	O-C13-C14-C15
42	11	312	A86	O-C13-C14-C15
42	12	315	A86	O-C13-C14-C15
42	12	317	A86	O-C13-C14-C15
42	13	311	A86	O-C13-C14-C15
42	13	313	A86	O-C13-C14-C15
42	14	312	A86	O-C13-C14-C15
42	14	314	A86	O-C13-C14-C15
42	15	310	A86	O-C13-C14-C15
42	15	312	A86	O-C13-C14-C15
42	16	312	A86	O-C13-C14-C15
42	17	302	A86	O-C13-C14-C15
42	17	313	A86	O-C13-C14-C15
42	18	313	A86	O-C13-C14-C15
42	19	310	A86	O-C13-C14-C15
42	20	213	A86	O-C13-C14-C15
42	21	310	A86	O-C13-C14-C15
42	21	314	A86	O-C13-C14-C15
35	A	408	LHG	C12-C13-C14-C15
35	a	407	LHG	C12-C13-C14-C15
30	18	301	CLA	O1D-CGD-O2D-CED
30	17	305	CLA	C10-C11-C12-C13
30	B	611	CLA	CBA-CGA-O2A-C1
30	17	308	CLA	C13-C15-C16-C17
33	B	621	SQD	C44-C45-C46-O48
33	L	103	SQD	C44-C45-C46-O48
33	b	620	SQD	C44-C45-C46-O48
33	l	101	SQD	C44-C45-C46-O48
36	Q	301	LMG	O1-C7-C8-C9
36	c	519	LMG	O1-C7-C8-C9
39	C	516	DGD	C1G-C2G-C3G-O3G
39	c	517	DGD	C1G-C2G-C3G-O3G
33	L	103	SQD	C25-C26-C27-C28
33	a	405	SQD	C28-C29-C30-C31
33	l	101	SQD	C25-C26-C27-C28
35	l	102	LHG	C9-C10-C11-C12
36	d	410	LMG	C34-C35-C36-C37
36	w	101	LMG	C32-C33-C34-C35
40	D	407	PL9	C32-C33-C34-C36
40	d	408	PL9	C32-C33-C34-C36
33	A	406	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
35	L	102	LHG	C9-C10-C11-C12
36	D	408	LMG	C34-C35-C36-C37
36	W	101	LMG	C32-C33-C34-C35
30	B	609	CLA	C5-C6-C7-C8
30	c	505	CLA	O1D-CGD-O2D-CED
30	18	307	CLA	CBD-CGD-O2D-CED
30	b	609	CLA	C5-C6-C7-C8
36	Q	301	LMG	C28-C29-C30-C31
36	c	519	LMG	C28-C29-C30-C31
30	C	502	CLA	O1A-CGA-O2A-C1
30	11	303	CLA	O1A-CGA-O2A-C1
30	12	307	CLA	O1A-CGA-O2A-C1
30	13	304	CLA	O1A-CGA-O2A-C1
30	C	505	CLA	O1D-CGD-O2D-CED
30	W	102	CLA	O1D-CGD-O2D-CED
30	w	102	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	O6-C4-C5-O7
35	L	101	LHG	O6-C4-C5-O7
35	b	621	LHG	O6-C4-C5-O7
35	d	409	LHG	O6-C4-C5-O7
35	l	102	LHG	C29-C30-C31-C32
39	H	102	DGD	C6A-C7A-C8A-C9A
39	h	102	DGD	C6A-C7A-C8A-C9A
30	c	502	CLA	O1A-CGA-O2A-C1
36	B	620	LMG	C19-C20-C21-C22
30	B	609	CLA	C2B-C3B-CAB-CBB
30	B	611	CLA	C2B-C3B-CAB-CBB
30	C	512	CLA	C2B-C3B-CAB-CBB
30	D	406	CLA	C2B-C3B-CAB-CBB
30	b	609	CLA	C2B-C3B-CAB-CBB
30	b	611	CLA	C2B-C3B-CAB-CBB
30	b	622	CLA	C2B-C3B-CAB-CBB
30	c	512	CLA	C2B-C3B-CAB-CBB
30	d	407	CLA	C2B-C3B-CAB-CBB
30	11	306	CLA	C2B-C3B-CAB-CBB
30	16	304	CLA	C2B-C3B-CAB-CBB
30	17	301	CLA	C2B-C3B-CAB-CBB
30	17	305	CLA	C2B-C3B-CAB-CBB
30	19	303	CLA	C2B-C3B-CAB-CBB
30	20	207	CLA	C2B-C3B-CAB-CBB
30	21	302	CLA	C2B-C3B-CAB-CBB
30	21	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	W	101	LMG	C22-C23-C24-C25
36	w	101	LMG	C22-C23-C24-C25
30	11	315	CLA	O1A-CGA-O2A-C1
30	12	303	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	O1A-CGA-O2A-C1
30	14	302	CLA	O1A-CGA-O2A-C1
36	b	619	LMG	C19-C20-C21-C22
35	L	102	LHG	C29-C30-C31-C32
33	L	103	SQD	O47-C45-C46-O48
33	l	101	SQD	O47-C45-C46-O48
35	A	408	LHG	O7-C5-C6-O8
35	a	407	LHG	O7-C5-C6-O8
36	D	408	LMG	O1-C7-C8-O7
36	d	410	LMG	O1-C7-C8-O7
30	B	605	CLA	CBD-CGD-O2D-CED
30	C	514	CLA	CBA-CGA-O2A-C1
30	c	514	CLA	CBA-CGA-O2A-C1
42	17	302	A86	C11-C10-C9-C8
42	17	315	A86	C11-C10-C9-C8
42	17	315	A86	C24-C25-C26-C27
42	19	311	A86	C3-C4-C5-C6
35	A	408	LHG	C8-C7-O7-C5
36	Q	301	LMG	C11-C10-O7-C8
42	11	313	A86	C10-C11-C13-C14
42	12	318	A86	C10-C11-C13-C14
42	13	314	A86	C10-C11-C13-C14
42	14	315	A86	C10-C11-C13-C14
42	15	313	A86	C10-C11-C13-C14
42	17	302	A86	C10-C11-C13-C14
42	17	314	A86	C10-C11-C13-C14
42	18	315	A86	C10-C11-C13-C14
30	A	402	CLA	C2-C1-O2A-CGA
30	B	615	CLA	C2-C1-O2A-CGA
30	a	402	CLA	C2-C1-O2A-CGA
30	b	615	CLA	C2-C1-O2A-CGA
30	18	303	CLA	C2-C1-O2A-CGA
30	21	301	CLA	C2-C1-O2A-CGA
30	21	305	CLA	O1D-CGD-O2D-CED
30	B	613	CLA	C8-C10-C11-C12
30	b	613	CLA	C8-C10-C11-C12
30	A	404	CLA	C11-C10-C8-C9
30	B	605	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	C	514	CLA	C14-C13-C15-C16
30	C	520	CLA	C11-C10-C8-C9
30	D	402	CLA	C11-C10-C8-C9
30	D	402	CLA	C14-C13-C15-C16
30	a	403	CLA	C11-C10-C8-C9
30	b	605	CLA	C6-C7-C8-C9
30	c	514	CLA	C14-C13-C15-C16
30	d	402	CLA	C11-C10-C8-C9
30	d	402	CLA	C14-C13-C15-C16
30	11	303	CLA	C11-C12-C13-C14
30	11	315	CLA	C14-C13-C15-C16
30	12	303	CLA	C14-C13-C15-C16
30	12	307	CLA	C11-C12-C13-C14
30	12	312	CLA	C14-C13-C15-C16
30	13	304	CLA	C11-C12-C13-C14
30	14	302	CLA	C14-C13-C15-C16
30	14	305	CLA	C11-C12-C13-C14
30	18	303	CLA	C11-C10-C8-C9
30	18	309	CLA	C11-C10-C8-C9
30	20	202	CLA	C11-C10-C8-C9
30	21	303	CLA	C11-C12-C13-C14
35	L	102	LHG	C10-C11-C12-C13
30	b	605	CLA	CBD-CGD-O2D-CED
30	17	301	CLA	O1A-CGA-O2A-C1
35	l	102	LHG	C10-C11-C12-C13
36	B	619	LMG	C38-C39-C40-C41
36	b	618	LMG	C38-C39-C40-C41
30	11	302	CLA	C2A-CAA-CBA-CGA
30	12	306	CLA	C2A-CAA-CBA-CGA
30	13	303	CLA	C2A-CAA-CBA-CGA
30	14	304	CLA	C2A-CAA-CBA-CGA
30	D	402	CLA	C16-C17-C18-C19
30	d	402	CLA	C16-C17-C18-C19
30	21	306	CLA	C16-C17-C18-C19
32	A	405	BCR	C23-C24-C25-C26
32	A	405	BCR	C23-C24-C25-C30
32	A	409	BCR	C23-C24-C25-C26
32	A	409	BCR	C23-C24-C25-C30
32	B	617	BCR	C23-C24-C25-C26
32	B	618	BCR	C23-C24-C25-C26
32	F	101	BCR	C23-C24-C25-C26
32	F	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
32	H	101	BCR	C23-C24-C25-C26
32	Y	101	BCR	C1-C6-C7-C8
32	Y	101	BCR	C23-C24-C25-C26
32	Y	101	BCR	C23-C24-C25-C30
32	a	404	BCR	C23-C24-C25-C26
32	a	404	BCR	C23-C24-C25-C30
32	a	408	BCR	C23-C24-C25-C26
32	a	408	BCR	C23-C24-C25-C30
32	b	616	BCR	C23-C24-C25-C26
32	b	617	BCR	C23-C24-C25-C26
32	c	520	BCR	C1-C6-C7-C8
32	c	520	BCR	C23-C24-C25-C26
32	c	520	BCR	C23-C24-C25-C30
32	f	101	BCR	C23-C24-C25-C26
32	f	101	BCR	C23-C24-C25-C30
32	h	101	BCR	C23-C24-C25-C26
35	L	101	LHG	C17-C18-C19-C20
35	d	409	LHG	C17-C18-C19-C20
36	D	408	LMG	C39-C40-C41-C42
36	Q	301	LMG	C30-C31-C32-C33
36	c	519	LMG	C30-C31-C32-C33
36	d	410	LMG	C39-C40-C41-C42
30	21	303	CLA	O1D-CGD-O2D-CED
39	C	517	DGD	C4E-C5E-C6E-O5E
39	c	518	DGD	C4E-C5E-C6E-O5E
36	B	620	LMG	C17-C18-C19-C20
39	H	102	DGD	C3B-C4B-C5B-C6B
42	20	201	A86	C2-C1-C24-C25
36	b	619	LMG	C17-C18-C19-C20
39	c	517	DGD	C6B-C7B-C8B-C9B
39	h	102	DGD	C3B-C4B-C5B-C6B
35	a	407	LHG	C8-C7-O7-C5
36	c	519	LMG	C11-C10-O7-C8
39	C	516	DGD	C6B-C7B-C8B-C9B
39	C	516	DGD	C9A-CAA-CBA-CCA
30	B	613	CLA	CBD-CGD-O2D-CED
30	17	303	CLA	C8-C10-C11-C12
42	20	201	A86	C33-C34-O4-C38
36	12	301	LMG	C13-C14-C15-C16
39	c	517	DGD	C9A-CAA-CBA-CCA
35	L	102	LHG	O6-C4-C5-C6
35	l	102	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
36	Q	301	LMG	C33-C34-C35-C36
36	1	101	LMG	C11-C12-C13-C14
36	c	519	LMG	C33-C34-C35-C36
30	B	605	CLA	C11-C12-C13-C15
30	B	606	CLA	C11-C10-C8-C7
30	B	607	CLA	C12-C13-C15-C16
30	B	612	CLA	C11-C10-C8-C7
30	B	614	CLA	C11-C10-C8-C7
30	B	623	CLA	C6-C7-C8-C10
30	C	506	CLA	C12-C13-C15-C16
30	C	507	CLA	C11-C12-C13-C15
30	C	508	CLA	C12-C13-C15-C16
30	C	510	CLA	C12-C13-C15-C16
30	C	514	CLA	C12-C13-C15-C16
30	C	519	CLA	C6-C7-C8-C10
30	C	520	CLA	C11-C10-C8-C7
30	D	402	CLA	C11-C10-C8-C7
30	D	405	CLA	C11-C12-C13-C15
30	Z	102	CLA	C6-C7-C8-C10
30	b	605	CLA	C11-C12-C13-C15
30	b	606	CLA	C11-C10-C8-C7
30	b	607	CLA	C12-C13-C15-C16
30	b	612	CLA	C11-C10-C8-C7
30	b	614	CLA	C11-C10-C8-C7
30	b	622	CLA	C6-C7-C8-C10
30	c	506	CLA	C12-C13-C15-C16
30	c	507	CLA	C11-C12-C13-C15
30	c	508	CLA	C12-C13-C15-C16
30	c	510	CLA	C12-C13-C15-C16
30	c	514	CLA	C12-C13-C15-C16
30	d	402	CLA	C11-C10-C8-C7
30	d	406	CLA	C11-C12-C13-C15
30	z	101	CLA	C6-C7-C8-C10
30	11	303	CLA	C11-C12-C13-C15
30	11	307	CLA	C12-C13-C15-C16
30	11	315	CLA	C12-C13-C15-C16
30	12	303	CLA	C12-C13-C15-C16
30	12	307	CLA	C11-C12-C13-C15
30	12	311	CLA	C12-C13-C15-C16
30	12	312	CLA	C12-C13-C15-C16
30	13	304	CLA	C11-C12-C13-C15
30	13	308	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	14	302	CLA	C12-C13-C15-C16
30	14	305	CLA	C11-C12-C13-C15
30	14	309	CLA	C12-C13-C15-C16
30	15	301	CLA	C11-C10-C8-C7
30	16	301	CLA	C12-C13-C15-C16
30	16	304	CLA	C6-C7-C8-C10
30	17	301	CLA	C12-C13-C15-C16
30	18	303	CLA	C11-C10-C8-C7
30	18	309	CLA	C11-C10-C8-C7
30	18	310	CLA	C12-C13-C15-C16
30	19	301	CLA	C11-C10-C8-C7
30	19	303	CLA	C12-C13-C15-C16
30	20	202	CLA	C11-C10-C8-C7
30	20	202	CLA	C12-C13-C15-C16
30	21	301	CLA	C11-C10-C8-C7
36	12	301	LMG	C11-C12-C13-C14
42	11	312	A86	C3-C4-C5-C6
42	11	314	A86	C1-C2-C3-C4
42	12	317	A86	C3-C4-C5-C6
42	12	319	A86	C1-C2-C3-C4
42	13	313	A86	C3-C4-C5-C6
42	14	301	A86	C1-C2-C3-C4
42	14	314	A86	C3-C4-C5-C6
42	14	316	A86	C1-C2-C3-C4
42	15	312	A86	C3-C4-C5-C6
42	15	314	A86	C1-C2-C3-C4
42	16	312	A86	C3-C4-C5-C6
42	16	313	A86	C1-C2-C3-C4
42	17	313	A86	C3-C4-C5-C6
42	17	316	A86	C1-C2-C3-C4
42	20	212	A86	C11-C10-C9-C8
42	20	213	A86	C3-C4-C5-C6
42	21	314	A86	C3-C4-C5-C6
30	17	308	CLA	C16-C17-C18-C20
39	C	517	DGD	C1B-C2B-C3B-C4B
30	18	301	CLA	C5-C6-C7-C8
30	D	405	CLA	C2A-CAA-CBA-CGA
30	d	406	CLA	C2A-CAA-CBA-CGA
30	b	613	CLA	CBD-CGD-O2D-CED
32	C	515	BCR	C35-C13-C14-C15
32	c	516	BCR	C35-C13-C14-C15
39	J	101	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
39	c	518	DGD	C1B-C2B-C3B-C4B
35	B	622	LHG	C34-C35-C36-C37
35	b	621	LHG	C34-C35-C36-C37
39	j	101	DGD	C4A-C5A-C6A-C7A
30	A	402	CLA	C13-C15-C16-C17
30	B	604	CLA	CBA-CGA-O2A-C1
30	C	503	CLA	CBA-CGA-O2A-C1
30	b	604	CLA	CBA-CGA-O2A-C1
30	c	503	CLA	CBA-CGA-O2A-C1
30	D	401	CLA	C10-C11-C12-C13
30	a	402	CLA	C13-C15-C16-C17
30	B	601	CLA	CAD-CBD-CGD-O2D
30	B	613	CLA	CAD-CBD-CGD-O2D
30	C	513	CLA	CAD-CBD-CGD-O2D
30	C	514	CLA	CAD-CBD-CGD-O2D
30	W	102	CLA	CAD-CBD-CGD-O2D
30	W	103	CLA	CAD-CBD-CGD-O2D
30	b	601	CLA	CAD-CBD-CGD-O2D
30	b	613	CLA	CAD-CBD-CGD-O2D
30	c	513	CLA	CAD-CBD-CGD-O2D
30	c	514	CLA	CAD-CBD-CGD-O2D
30	w	102	CLA	CAD-CBD-CGD-O2D
30	w	103	CLA	CAD-CBD-CGD-O2D
30	11	306	CLA	CAD-CBD-CGD-O2D
30	12	310	CLA	CAD-CBD-CGD-O2D
30	13	307	CLA	CAD-CBD-CGD-O2D
30	14	308	CLA	CAD-CBD-CGD-O2D
30	17	307	CLA	CAD-CBD-CGD-O2D
30	18	304	CLA	CAD-CBD-CGD-O2D
30	18	308	CLA	CAD-CBD-CGD-O2D
30	19	305	CLA	CAD-CBD-CGD-O2D
30	21	306	CLA	CAD-CBD-CGD-O2D
31	A	403	PHO	CAD-CBD-CGD-O2D
31	d	403	PHO	CAD-CBD-CGD-O2D
42	21	312	A86	C28-C27-C29-C30
30	C	509	CLA	C13-C15-C16-C17
30	D	402	CLA	C13-C15-C16-C17
30	d	401	CLA	C10-C11-C12-C13
30	d	402	CLA	C13-C15-C16-C17
32	B	617	BCR	C6-C7-C8-C9
32	B	618	BCR	C22-C23-C24-C25
32	b	616	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	b	617	BCR	C22-C23-C24-C25
30	C	504	CLA	C4-C3-C5-C6
30	c	504	CLA	C4-C3-C5-C6
39	J	101	DGD	O6D-C1D-O3G-C3G
39	j	101	DGD	O6D-C1D-O3G-C3G
30	c	509	CLA	C13-C15-C16-C17
36	B	620	LMG	O1-C7-C8-C9
36	1	101	LMG	O1-C7-C8-C9
36	b	619	LMG	O1-C7-C8-C9
42	11	316	A86	C12-C11-C13-O
42	12	304	A86	C12-C11-C13-O
42	13	301	A86	C12-C11-C13-O
42	13	315	A86	C12-C11-C13-O
42	15	315	A86	C12-C11-C13-O
42	15	316	A86	C12-C11-C13-O
42	16	310	A86	C12-C11-C13-O
42	17	311	A86	C12-C11-C13-O
42	18	302	A86	C12-C11-C13-O
42	19	311	A86	C12-C11-C13-O
41	V	201	HEM	C4C-C3C-CAC-CBC
41	v	201	HEM	C4C-C3C-CAC-CBC
30	18	303	CLA	C2A-CAA-CBA-CGA
30	c	514	CLA	O1A-CGA-O2A-C1
30	C	507	CLA	C16-C17-C18-C19
30	D	402	CLA	C16-C17-C18-C20
30	c	507	CLA	C16-C17-C18-C19
30	d	402	CLA	C16-C17-C18-C20
35	L	102	LHG	C33-C34-C35-C36
35	l	102	LHG	C33-C34-C35-C36
30	B	609	CLA	CHA-CBD-CGD-O1D
30	B	609	CLA	CHA-CBD-CGD-O2D
30	B	610	CLA	CHA-CBD-CGD-O1D
30	B	612	CLA	CHA-CBD-CGD-O1D
30	B	612	CLA	CHA-CBD-CGD-O2D
30	B	615	CLA	CHA-CBD-CGD-O1D
30	C	503	CLA	CHA-CBD-CGD-O1D
30	C	503	CLA	CHA-CBD-CGD-O2D
30	C	507	CLA	CHA-CBD-CGD-O1D
30	C	508	CLA	CHA-CBD-CGD-O1D
30	C	509	CLA	CHA-CBD-CGD-O1D
30	C	509	CLA	CHA-CBD-CGD-O2D
30	C	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	C	510	CLA	CHA-CBD-CGD-O2D
30	C	512	CLA	CHA-CBD-CGD-O2D
30	b	609	CLA	CHA-CBD-CGD-O1D
30	b	609	CLA	CHA-CBD-CGD-O2D
30	b	610	CLA	CHA-CBD-CGD-O1D
30	b	612	CLA	CHA-CBD-CGD-O1D
30	b	612	CLA	CHA-CBD-CGD-O2D
30	b	615	CLA	CHA-CBD-CGD-O1D
30	c	503	CLA	CHA-CBD-CGD-O1D
30	c	503	CLA	CHA-CBD-CGD-O2D
30	c	507	CLA	CHA-CBD-CGD-O1D
30	c	508	CLA	CHA-CBD-CGD-O1D
30	c	509	CLA	CHA-CBD-CGD-O1D
30	c	509	CLA	CHA-CBD-CGD-O2D
30	c	510	CLA	CHA-CBD-CGD-O1D
30	c	510	CLA	CHA-CBD-CGD-O2D
30	c	512	CLA	CHA-CBD-CGD-O2D
30	11	303	CLA	CHA-CBD-CGD-O1D
30	11	303	CLA	CHA-CBD-CGD-O2D
30	11	305	CLA	CHA-CBD-CGD-O2D
30	11	308	CLA	CHA-CBD-CGD-O1D
30	11	308	CLA	CHA-CBD-CGD-O2D
30	12	307	CLA	CHA-CBD-CGD-O1D
30	12	307	CLA	CHA-CBD-CGD-O2D
30	12	309	CLA	CHA-CBD-CGD-O2D
30	12	313	CLA	CHA-CBD-CGD-O1D
30	12	313	CLA	CHA-CBD-CGD-O2D
30	13	304	CLA	CHA-CBD-CGD-O1D
30	13	304	CLA	CHA-CBD-CGD-O2D
30	13	306	CLA	CHA-CBD-CGD-O2D
30	13	309	CLA	CHA-CBD-CGD-O1D
30	13	309	CLA	CHA-CBD-CGD-O2D
30	14	305	CLA	CHA-CBD-CGD-O1D
30	14	305	CLA	CHA-CBD-CGD-O2D
30	14	307	CLA	CHA-CBD-CGD-O2D
30	14	310	CLA	CHA-CBD-CGD-O1D
30	14	310	CLA	CHA-CBD-CGD-O2D
30	15	305	CLA	CHA-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O2D
30	16	308	CLA	CHA-CBD-CGD-O1D
30	16	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	17	309	CLA	CHA-CBD-CGD-O1D
30	17	310	CLA	CHA-CBD-CGD-O1D
30	18	309	CLA	CHA-CBD-CGD-O1D
30	19	303	CLA	CHA-CBD-CGD-O1D
30	19	303	CLA	CHA-CBD-CGD-O2D
30	21	303	CLA	CHA-CBD-CGD-O1D
30	c	510	CLA	C5-C6-C7-C8
30	14	303	CLA	C5-C6-C7-C8
30	B	611	CLA	O1A-CGA-O2A-C1
30	C	514	CLA	O1A-CGA-O2A-C1
30	b	611	CLA	O1A-CGA-O2A-C1
39	C	517	DGD	O1A-C1A-O1G-C1G
39	c	518	DGD	O1A-C1A-O1G-C1G
32	A	409	BCR	C11-C10-C9-C8
32	a	408	BCR	C11-C10-C9-C8
33	A	406	SQD	O6-C44-C45-O47
33	a	405	SQD	O6-C44-C45-O47
36	B	620	LMG	O1-C7-C8-O7
36	Q	301	LMG	O1-C7-C8-O7
36	W	101	LMG	O7-C8-C9-O8
36	1	101	LMG	O1-C7-C8-O7
36	b	619	LMG	O1-C7-C8-O7
36	c	519	LMG	O1-C7-C8-O7
36	w	101	LMG	O7-C8-C9-O8
30	18	301	CLA	CBA-CGA-O2A-C1
35	L	102	LHG	C27-C28-C29-C30
35	l	102	LHG	C27-C28-C29-C30
36	B	619	LMG	C12-C13-C14-C15
30	C	510	CLA	C5-C6-C7-C8
30	11	301	CLA	C5-C6-C7-C8
36	b	618	LMG	C12-C13-C14-C15
31	D	403	PHO	C16-C17-C18-C20
42	11	313	A86	C10-C11-C13-O
42	11	316	A86	C10-C11-C13-O
42	11	316	A86	C13-C14-C15-O1
42	12	304	A86	C10-C11-C13-O
42	12	304	A86	C13-C14-C15-O1
42	12	318	A86	C10-C11-C13-O
42	13	301	A86	C10-C11-C13-O
42	13	301	A86	C13-C14-C15-O1
42	13	314	A86	C10-C11-C13-O
42	13	315	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
42	13	315	A86	C13-C14-C15-O1
42	14	315	A86	C10-C11-C13-O
42	15	313	A86	C10-C11-C13-O
42	15	315	A86	C10-C11-C13-O
42	15	315	A86	C13-C14-C15-O1
42	15	316	A86	C10-C11-C13-O
42	15	316	A86	C13-C14-C15-O1
42	16	310	A86	C10-C11-C13-O
42	17	302	A86	C13-C14-C15-O1
42	17	314	A86	C10-C11-C13-O
42	17	315	A86	C13-C14-C15-O1
42	18	302	A86	C10-C11-C13-O
42	18	302	A86	C13-C14-C15-O1
42	18	315	A86	C10-C11-C13-O
42	19	311	A86	C13-C14-C15-O1
42	19	312	A86	C13-C14-C15-O1
42	20	201	A86	C13-C14-C15-O1
30	20	202	CLA	O1D-CGD-O2D-CED
36	W	101	LMG	C16-C17-C18-C19
30	D	401	CLA	C4-C3-C5-C6
30	d	401	CLA	C4-C3-C5-C6
36	w	101	LMG	C16-C17-C18-C19
30	13	302	CLA	C5-C6-C7-C8
30	B	614	CLA	C11-C10-C8-C9
30	C	504	CLA	C11-C12-C13-C14
30	C	510	CLA	C14-C13-C15-C16
30	b	614	CLA	C11-C10-C8-C9
30	c	504	CLA	C11-C12-C13-C14
30	c	510	CLA	C14-C13-C15-C16
30	15	301	CLA	C11-C10-C8-C9
30	20	202	CLA	C14-C13-C15-C16
30	21	301	CLA	C11-C12-C13-C14
30	21	303	CLA	C6-C7-C8-C9
30	12	305	CLA	C5-C6-C7-C8
30	B	613	CLA	O1D-CGD-O2D-CED
30	C	503	CLA	O1A-CGA-O2A-C1
30	c	503	CLA	O1A-CGA-O2A-C1
32	B	617	BCR	C11-C12-C13-C35
32	b	616	BCR	C11-C12-C13-C35
42	11	314	A86	C-C1-C24-C25
42	12	319	A86	C-C1-C24-C25
42	14	301	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
42	14	316	A86	C-C1-C24-C25
42	15	314	A86	C-C1-C24-C25
42	16	313	A86	C-C1-C24-C25
42	17	315	A86	C-C1-C24-C25
42	17	316	A86	C-C1-C24-C25
42	20	201	A86	C35-C34-O4-C38
42	11	316	A86	C5-C6-C8-C9
42	12	304	A86	C5-C6-C8-C9
42	13	301	A86	C5-C6-C8-C9
42	13	315	A86	C5-C6-C8-C9
42	15	315	A86	C5-C6-C8-C9
42	15	316	A86	C5-C6-C8-C9
42	17	315	A86	C2-C1-C24-C25
42	18	302	A86	C5-C6-C8-C9
30	C	509	CLA	C1A-C2A-CAA-CBA
30	c	509	CLA	C1A-C2A-CAA-CBA
30	C	507	CLA	C16-C17-C18-C20
30	c	507	CLA	C16-C17-C18-C20
30	21	306	CLA	C16-C17-C18-C20
31	d	404	PHO	C16-C17-C18-C20
30	12	307	CLA	C10-C11-C12-C13
30	D	401	CLA	C2-C1-O2A-CGA
30	W	103	CLA	C2-C1-O2A-CGA
30	d	401	CLA	C2-C1-O2A-CGA
30	w	103	CLA	C2-C1-O2A-CGA
30	z	101	CLA	CBD-CGD-O2D-CED
35	b	621	LHG	C28-C29-C30-C31
36	B	619	LMG	C19-C20-C21-C22
39	c	518	DGD	C6B-C7B-C8B-C9B
39	c	518	DGD	CBB-CCB-CDB-CEB
42	21	313	A86	C1-C2-C3-C4
30	b	613	CLA	O1D-CGD-O2D-CED
30	11	303	CLA	C10-C11-C12-C13
30	13	304	CLA	C10-C11-C12-C13
30	14	305	CLA	C10-C11-C12-C13
36	b	618	LMG	C19-C20-C21-C22
39	C	517	DGD	C6B-C7B-C8B-C9B
39	C	517	DGD	CBB-CCB-CDB-CEB
35	B	622	LHG	C28-C29-C30-C31
30	B	608	CLA	C4B-C3B-CAB-CBB
30	W	102	CLA	C4B-C3B-CAB-CBB
30	b	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	w	102	CLA	C4B-C3B-CAB-CBB
30	11	315	CLA	C4B-C3B-CAB-CBB
30	12	303	CLA	C4B-C3B-CAB-CBB
30	12	312	CLA	C4B-C3B-CAB-CBB
30	14	302	CLA	C4B-C3B-CAB-CBB
35	A	408	LHG	C3-O3-P-O4
35	A	408	LHG	C4-O6-P-O4
35	B	622	LHG	C3-O3-P-O5
35	L	101	LHG	C4-O6-P-O5
35	L	102	LHG	C3-O3-P-O5
35	a	407	LHG	C3-O3-P-O4
35	a	407	LHG	C4-O6-P-O4
35	b	621	LHG	C3-O3-P-O5
35	d	409	LHG	C4-O6-P-O5
35	l	102	LHG	C3-O3-P-O5
30	C	519	CLA	CBD-CGD-O2D-CED
36	B	619	LMG	C18-C19-C20-C21
36	b	618	LMG	C18-C19-C20-C21
30	b	604	CLA	O1A-CGA-O2A-C1
30	D	405	CLA	C13-C15-C16-C17
30	d	406	CLA	C13-C15-C16-C17
36	12	301	LMG	C30-C31-C32-C33
41	f	102	HEM	C2A-CAA-CBA-CGA
30	B	604	CLA	O1A-CGA-O2A-C1
30	18	301	CLA	O1A-CGA-O2A-C1
30	D	401	CLA	C16-C17-C18-C19
30	d	401	CLA	C16-C17-C18-C19
30	21	301	CLA	C16-C17-C18-C19
30	19	309	CLA	C4C-C3C-CAC-CBC
30	B	604	CLA	CAD-CBD-CGD-O1D
30	B	609	CLA	CAD-CBD-CGD-O1D
30	B	612	CLA	CAD-CBD-CGD-O1D
30	C	503	CLA	CAD-CBD-CGD-O1D
30	C	505	CLA	CAD-CBD-CGD-O1D
30	C	506	CLA	CAD-CBD-CGD-O1D
30	C	507	CLA	CAD-CBD-CGD-O1D
30	C	508	CLA	CAD-CBD-CGD-O1D
30	C	520	CLA	CAD-CBD-CGD-O1D
30	b	604	CLA	CAD-CBD-CGD-O1D
30	b	609	CLA	CAD-CBD-CGD-O1D
30	b	612	CLA	CAD-CBD-CGD-O1D
30	c	503	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	c	505	CLA	CAD-CBD-CGD-O1D
30	c	506	CLA	CAD-CBD-CGD-O1D
30	c	507	CLA	CAD-CBD-CGD-O1D
30	c	508	CLA	CAD-CBD-CGD-O1D
30	11	303	CLA	CAD-CBD-CGD-O1D
30	11	305	CLA	CAD-CBD-CGD-O1D
30	12	307	CLA	CAD-CBD-CGD-O1D
30	12	309	CLA	CAD-CBD-CGD-O1D
30	13	304	CLA	CAD-CBD-CGD-O1D
30	13	306	CLA	CAD-CBD-CGD-O1D
30	14	305	CLA	CAD-CBD-CGD-O1D
30	14	307	CLA	CAD-CBD-CGD-O1D
30	15	302	CLA	CAD-CBD-CGD-O1D
30	15	303	CLA	CAD-CBD-CGD-O1D
30	16	307	CLA	CAD-CBD-CGD-O1D
30	17	304	CLA	CAD-CBD-CGD-O1D
30	17	305	CLA	CAD-CBD-CGD-O1D
30	18	305	CLA	CAD-CBD-CGD-O1D
30	19	303	CLA	CAD-CBD-CGD-O1D
30	21	303	CLA	CAD-CBD-CGD-O1D
42	17	311	A86	C26-C27-C29-C30
30	C	508	CLA	C5-C6-C7-C8
30	c	508	CLA	C5-C6-C7-C8
30	21	303	CLA	C10-C11-C12-C13
39	H	102	DGD	CCA-CDA-CEA-CFA
39	h	102	DGD	CCA-CDA-CEA-CFA
36	b	619	LMG	C22-C23-C24-C25
39	C	516	DGD	C4D-C5D-C6D-O5D
39	c	517	DGD	C4D-C5D-C6D-O5D
30	B	601	CLA	C12-C13-C15-C16
30	C	504	CLA	C11-C12-C13-C15
30	C	506	CLA	C11-C12-C13-C15
30	C	509	CLA	C6-C7-C8-C10
30	C	519	CLA	C12-C13-C15-C16
30	b	601	CLA	C12-C13-C15-C16
30	c	504	CLA	C11-C12-C13-C15
30	c	506	CLA	C11-C12-C13-C15
30	c	509	CLA	C6-C7-C8-C10
30	z	101	CLA	C12-C13-C15-C16
30	11	309	CLA	C3A-C2A-CAA-CBA
30	12	314	CLA	C3A-C2A-CAA-CBA
30	13	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	14	311	CLA	C3A-C2A-CAA-CBA
30	15	303	CLA	C11-C12-C13-C15
30	16	302	CLA	C6-C7-C8-C10
30	18	305	CLA	C11-C12-C13-C15
30	19	307	CLA	C12-C13-C15-C16
30	21	301	CLA	C11-C12-C13-C15
30	21	303	CLA	C6-C7-C8-C10
31	A	403	PHO	C11-C10-C8-C7
31	d	403	PHO	C11-C10-C8-C7
35	L	101	LHG	C23-C24-C25-C26
35	L	102	LHG	O6-C4-C5-O7
35	d	409	LHG	C23-C24-C25-C26
35	l	102	LHG	O6-C4-C5-O7
36	B	620	LMG	C22-C23-C24-C25
36	1	101	LMG	C16-C17-C18-C19
32	C	518	BCR	C19-C20-C21-C22
32	c	521	BCR	C19-C20-C21-C22
42	11	316	A86	C24-C25-C26-C27
42	12	304	A86	C24-C25-C26-C27
42	13	301	A86	C24-C25-C26-C27
42	13	315	A86	C24-C25-C26-C27
42	15	315	A86	C24-C25-C26-C27
42	15	316	A86	C24-C25-C26-C27
42	18	302	A86	C24-C25-C26-C27
39	C	516	DGD	O6D-C5D-C6D-O5D
39	c	517	DGD	O6D-C5D-C6D-O5D
35	l	102	LHG	C35-C36-C37-C38
30	15	307	CLA	C13-C15-C16-C17
35	L	102	LHG	C35-C36-C37-C38
39	C	517	DGD	C7B-C8B-C9B-CAB
39	c	518	DGD	C7B-C8B-C9B-CAB
30	21	307	CLA	C15-C16-C17-C18
30	C	514	CLA	C16-C17-C18-C19
39	C	517	DGD	C1A-C2A-C3A-C4A
39	c	518	DGD	C1A-C2A-C3A-C4A
39	C	516	DGD	C2D-C1D-O3G-C3G
39	c	517	DGD	C2D-C1D-O3G-C3G
36	B	619	LMG	C16-C17-C18-C19
36	b	618	LMG	C16-C17-C18-C19
36	w	101	LMG	C38-C39-C40-C41
36	W	101	LMG	C38-C39-C40-C41
39	h	102	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
30	c	514	CLA	C16-C17-C18-C19
30	17	308	CLA	C16-C17-C18-C19
30	18	303	CLA	C10-C11-C12-C13
30	19	301	CLA	C13-C15-C16-C17
30	21	306	CLA	C5-C6-C7-C8
31	A	403	PHO	C5-C6-C7-C8
30	16	301	CLA	O1A-CGA-O2A-C1
31	d	403	PHO	C5-C6-C7-C8
40	D	404	PL9	C30-C29-C31-C32
40	d	405	PL9	C30-C29-C31-C32
30	16	301	CLA	CBA-CGA-O2A-C1
39	H	102	DGD	C5B-C6B-C7B-C8B
30	B	612	CLA	C11-C10-C8-C9
30	B	623	CLA	C11-C12-C13-C14
30	C	502	CLA	C14-C13-C15-C16
30	C	508	CLA	C14-C13-C15-C16
30	C	519	CLA	C14-C13-C15-C16
30	D	405	CLA	C11-C12-C13-C14
30	b	612	CLA	C11-C10-C8-C9
30	b	622	CLA	C11-C12-C13-C14
30	c	502	CLA	C14-C13-C15-C16
30	c	508	CLA	C14-C13-C15-C16
30	d	406	CLA	C11-C12-C13-C14
30	z	101	CLA	C14-C13-C15-C16
30	11	307	CLA	C14-C13-C15-C16
30	12	311	CLA	C14-C13-C15-C16
30	13	308	CLA	C14-C13-C15-C16
30	14	309	CLA	C14-C13-C15-C16
30	16	301	CLA	C14-C13-C15-C16
30	21	301	CLA	C11-C10-C8-C9
30	11	315	CLA	O1D-CGD-O2D-CED
35	L	102	LHG	C12-C13-C14-C15
41	F	102	HEM	C2A-CAA-CBA-CGA
30	11	304	CLA	C2A-CAA-CBA-CGA
30	12	308	CLA	C2A-CAA-CBA-CGA
30	13	305	CLA	C2A-CAA-CBA-CGA
30	14	306	CLA	C2A-CAA-CBA-CGA
36	w	101	LMG	C36-C37-C38-C39
39	J	101	DGD	CDB-CEB-CFB-CGB
39	j	101	DGD	CDB-CEB-CFB-CGB
35	l	102	LHG	C12-C13-C14-C15
42	19	311	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
30	21	303	CLA	C3-C5-C6-C7
36	W	101	LMG	C36-C37-C38-C39
36	w	101	LMG	C21-C22-C23-C24
30	19	309	CLA	C2C-C3C-CAC-CBC
36	W	101	LMG	C21-C22-C23-C24
30	B	610	CLA	C2B-C3B-CAB-CBB
30	C	506	CLA	C2B-C3B-CAB-CBB
30	C	507	CLA	C2B-C3B-CAB-CBB
30	C	513	CLA	C2B-C3B-CAB-CBB
30	C	520	CLA	C2B-C3B-CAB-CBB
30	M	101	CLA	C2B-C3B-CAB-CBB
30	b	610	CLA	C2B-C3B-CAB-CBB
30	c	506	CLA	C2B-C3B-CAB-CBB
30	c	507	CLA	C2B-C3B-CAB-CBB
30	c	513	CLA	C2B-C3B-CAB-CBB
30	m	101	CLA	C2B-C3B-CAB-CBB
30	11	301	CLA	C2B-C3B-CAB-CBB
30	11	303	CLA	C2B-C3B-CAB-CBB
30	11	305	CLA	C2B-C3B-CAB-CBB
30	11	307	CLA	C2B-C3B-CAB-CBB
30	12	305	CLA	C2B-C3B-CAB-CBB
30	12	307	CLA	C2B-C3B-CAB-CBB
30	12	309	CLA	C2B-C3B-CAB-CBB
30	12	310	CLA	C2B-C3B-CAB-CBB
30	12	311	CLA	C2B-C3B-CAB-CBB
30	13	302	CLA	C2B-C3B-CAB-CBB
30	13	304	CLA	C2B-C3B-CAB-CBB
30	13	306	CLA	C2B-C3B-CAB-CBB
30	13	307	CLA	C2B-C3B-CAB-CBB
30	13	308	CLA	C2B-C3B-CAB-CBB
30	14	303	CLA	C2B-C3B-CAB-CBB
30	14	305	CLA	C2B-C3B-CAB-CBB
30	14	307	CLA	C2B-C3B-CAB-CBB
30	14	308	CLA	C2B-C3B-CAB-CBB
30	14	309	CLA	C2B-C3B-CAB-CBB
30	15	302	CLA	C2B-C3B-CAB-CBB
30	15	303	CLA	C2B-C3B-CAB-CBB
30	15	305	CLA	C2B-C3B-CAB-CBB
30	15	307	CLA	C2B-C3B-CAB-CBB
30	20	205	CLA	C2B-C3B-CAB-CBB
30	12	312	CLA	O1D-CGD-O2D-CED
30	C	513	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	c	513	CLA	C10-C11-C12-C13
30	19	307	CLA	O1A-CGA-O2A-C1
30	D	401	CLA	C2-C3-C5-C6
30	d	401	CLA	C2-C3-C5-C6
30	B	615	CLA	C5-C6-C7-C8
30	b	615	CLA	C5-C6-C7-C8
35	b	621	LHG	C29-C30-C31-C32
41	F	102	HEM	C3A-C2A-CAA-CBA
30	b	608	CLA	CBD-CGD-O2D-CED
30	21	307	CLA	C13-C15-C16-C17
30	14	302	CLA	O1D-CGD-O2D-CED
33	l	101	SQD	C24-C25-C26-C27
39	h	102	DGD	O2G-C1B-C2B-C3B
35	B	622	LHG	C29-C30-C31-C32
39	H	102	DGD	C4A-C5A-C6A-C7A
30	17	301	CLA	C8-C10-C11-C12
30	B	608	CLA	CBD-CGD-O2D-CED
30	12	303	CLA	O1D-CGD-O2D-CED
30	B	603	CLA	C2A-CAA-CBA-CGA
30	C	506	CLA	C2A-CAA-CBA-CGA
30	b	603	CLA	C2A-CAA-CBA-CGA
30	c	506	CLA	C2A-CAA-CBA-CGA
33	L	103	SQD	C24-C25-C26-C27
36	b	619	LMG	O10-C28-O8-C9
39	h	102	DGD	C4A-C5A-C6A-C7A
39	H	102	DGD	O2G-C1B-C2B-C3B
36	B	620	LMG	O10-C28-O8-C9
39	C	516	DGD	C8A-C9A-CAA-CBA
36	1	101	LMG	C13-C14-C15-C16
42	11	313	A86	C12-C11-C13-C14
42	12	318	A86	C12-C11-C13-C14
42	13	314	A86	C12-C11-C13-C14
42	14	315	A86	C12-C11-C13-C14
42	15	313	A86	C12-C11-C13-C14
42	17	302	A86	C12-C11-C13-C14
42	17	314	A86	C12-C11-C13-C14
42	18	315	A86	C12-C11-C13-C14
42	21	313	A86	C12-C11-C13-C14
39	c	517	DGD	C8A-C9A-CAA-CBA
30	19	307	CLA	CBA-CGA-O2A-C1
30	b	605	CLA	O1D-CGD-O2D-CED
30	C	519	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	11	315	CLA	C13-C15-C16-C17
30	12	303	CLA	C13-C15-C16-C17
30	14	302	CLA	C13-C15-C16-C17
30	B	605	CLA	O1D-CGD-O2D-CED
30	C	519	CLA	O1D-CGD-O2D-CED
32	H	101	BCR	C23-C24-C25-C30
32	h	101	BCR	C23-C24-C25-C30
30	z	101	CLA	O1D-CGD-O2D-CED
30	z	101	CLA	C5-C6-C7-C8
30	12	312	CLA	C13-C15-C16-C17
41	f	102	HEM	C3A-C2A-CAA-CBA
30	16	303	CLA	C2A-CAA-CBA-CGA
36	b	619	LMG	C32-C33-C34-C35
36	B	620	LMG	C32-C33-C34-C35
35	L	102	LHG	C4-O6-P-O3
35	l	102	LHG	C4-O6-P-O3
36	12	301	LMG	C7-C8-C9-O8
30	C	511	CLA	C11-C12-C13-C15
30	c	511	CLA	C11-C12-C13-C15
30	17	305	CLA	C11-C10-C8-C7
30	17	305	CLA	C11-C12-C13-C15
30	20	209	CLA	CAA-CBA-CGA-O2A
30	19	303	CLA	C3-C5-C6-C7
36	B	619	LMG	C20-C21-C22-C23
30	C	509	CLA	C6-C7-C8-C9
30	c	509	CLA	C6-C7-C8-C9
30	15	303	CLA	C11-C12-C13-C14
30	16	302	CLA	C11-C10-C8-C9
30	18	305	CLA	C11-C12-C13-C14
30	B	606	CLA	C8-C10-C11-C12
30	18	301	CLA	C13-C15-C16-C17
32	C	518	BCR	C9-C10-C11-C12
32	c	521	BCR	C9-C10-C11-C12
30	B	603	CLA	C16-C17-C18-C20
30	b	603	CLA	C16-C17-C18-C20
30	21	301	CLA	C16-C17-C18-C20
35	L	101	LHG	C10-C11-C12-C13
35	d	409	LHG	C10-C11-C12-C13
36	b	618	LMG	C20-C21-C22-C23
39	C	517	DGD	C5B-C6B-C7B-C8B
39	c	518	DGD	C5B-C6B-C7B-C8B
30	b	606	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	19	303	CLA	CBD-CGD-O2D-CED
30	B	614	CLA	C13-C15-C16-C17
35	L	101	LHG	C30-C31-C32-C33
30	18	307	CLA	O1D-CGD-O2D-CED
35	d	409	LHG	C30-C31-C32-C33
30	b	614	CLA	C13-C15-C16-C17
30	C	509	CLA	CBA-CGA-O2A-C1
33	L	103	SQD	C11-C12-C13-C14
30	11	315	CLA	C3-C5-C6-C7
30	12	303	CLA	C3-C5-C6-C7
36	12	301	LMG	C15-C16-C17-C18
30	b	605	CLA	C8-C10-C11-C12
30	20	209	CLA	C8-C10-C11-C12
33	l	101	SQD	C11-C12-C13-C14
30	D	401	CLA	C16-C17-C18-C20
30	d	401	CLA	C16-C17-C18-C20
30	c	509	CLA	CBA-CGA-O2A-C1
30	19	303	CLA	CBA-CGA-O2A-C1
35	A	408	LHG	C24-C23-O8-C6
35	a	407	LHG	C24-C23-O8-C6
36	Q	301	LMG	C29-C28-O8-C9
36	c	519	LMG	C29-C28-O8-C9
33	B	621	SQD	O10-C23-O48-C46
30	15	306	CLA	CAA-CBA-CGA-O2A
39	H	102	DGD	C2B-C3B-C4B-C5B
39	c	517	DGD	C8B-C9B-CAB-CBB
30	B	601	CLA	CAA-CBA-CGA-O2A
30	b	601	CLA	CAA-CBA-CGA-O2A
39	C	516	DGD	C8B-C9B-CAB-CBB
39	h	102	DGD	C2B-C3B-C4B-C5B
33	b	620	SQD	O10-C23-O48-C46
35	a	407	LHG	C31-C32-C33-C34
30	B	603	CLA	C4B-C3B-CAB-CBB
30	b	603	CLA	C4B-C3B-CAB-CBB
30	11	303	CLA	C4B-C3B-CAB-CBB
30	12	307	CLA	C4B-C3B-CAB-CBB
30	13	304	CLA	C4B-C3B-CAB-CBB
30	14	305	CLA	C4B-C3B-CAB-CBB
30	15	302	CLA	C4B-C3B-CAB-CBB
30	20	205	CLA	C4B-C3B-CAB-CBB
30	13	308	CLA	CAA-CBA-CGA-O1A
30	B	605	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
42	21	312	A86	C11-C10-C9-C8
30	12	312	CLA	C3-C5-C6-C7
30	14	302	CLA	C3-C5-C6-C7
35	A	408	LHG	C31-C32-C33-C34
39	j	101	DGD	C3A-C4A-C5A-C6A
30	C	509	CLA	C10-C11-C12-C13
30	c	509	CLA	C10-C11-C12-C13
39	J	101	DGD	C3A-C4A-C5A-C6A
33	b	620	SQD	C12-C13-C14-C15
30	B	623	CLA	O1A-CGA-O2A-C1
30	19	303	CLA	O1A-CGA-O2A-C1
30	Z	102	CLA	C3-C5-C6-C7
30	12	311	CLA	CAA-CBA-CGA-O1A
30	14	309	CLA	CAA-CBA-CGA-O1A
30	17	303	CLA	C4-C3-C5-C6
30	11	304	CLA	CAA-CBA-CGA-O2A
30	12	308	CLA	CAA-CBA-CGA-O2A
30	13	305	CLA	CAA-CBA-CGA-O2A
30	14	306	CLA	CAA-CBA-CGA-O2A
30	17	306	CLA	CAA-CBA-CGA-O1A
30	b	612	CLA	C5-C6-C7-C8
33	B	621	SQD	C12-C13-C14-C15
30	b	622	CLA	O1A-CGA-O2A-C1
30	B	612	CLA	C5-C6-C7-C8
30	C	514	CLA	C10-C11-C12-C13
30	c	514	CLA	C10-C11-C12-C13
30	12	312	CLA	C8-C10-C11-C12
30	11	307	CLA	CAA-CBA-CGA-O1A
30	11	304	CLA	CAA-CBA-CGA-O1A
30	13	305	CLA	CAA-CBA-CGA-O1A
30	14	306	CLA	CAA-CBA-CGA-O1A
41	F	102	HEM	CAD-CBD-CGD-O1D
41	f	102	HEM	CAD-CBD-CGD-O1D
30	A	404	CLA	C2-C1-O2A-CGA
30	B	610	CLA	C2-C1-O2A-CGA
30	C	506	CLA	C2-C1-O2A-CGA
30	C	511	CLA	C2-C1-O2A-CGA
30	a	403	CLA	C2-C1-O2A-CGA
30	b	610	CLA	C2-C1-O2A-CGA
30	c	506	CLA	C2-C1-O2A-CGA
30	c	511	CLA	C2-C1-O2A-CGA
31	d	403	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	11	315	CLA	C8-C10-C11-C12
30	14	302	CLA	C8-C10-C11-C12
31	A	403	PHO	C13-C15-C16-C17
30	12	308	CLA	CAA-CBA-CGA-O1A
30	16	305	CLA	CAA-CBA-CGA-O2A
30	21	304	CLA	CAA-CBA-CGA-O2A
30	C	511	CLA	C2A-CAA-CBA-CGA
30	c	511	CLA	C2A-CAA-CBA-CGA
36	12	301	LMG	O7-C8-C9-O8
36	W	101	LMG	C34-C35-C36-C37
39	c	518	DGD	C8B-C9B-CAB-CBB
39	C	517	DGD	C8B-C9B-CAB-CBB
30	C	507	CLA	C3A-C2A-CAA-CBA
30	c	507	CLA	C3A-C2A-CAA-CBA
30	16	309	CLA	C3A-C2A-CAA-CBA
30	20	204	CLA	C3A-C2A-CAA-CBA
30	21	303	CLA	C3A-C2A-CAA-CBA
30	12	303	CLA	C8-C10-C11-C12
36	w	101	LMG	C34-C35-C36-C37
42	16	310	A86	O-C13-C14-C15
42	17	311	A86	O-C13-C14-C15
42	20	210	A86	O-C13-C14-C15
42	20	212	A86	O-C13-C14-C15
39	C	516	DGD	C2A-C3A-C4A-C5A
39	c	517	DGD	C2A-C3A-C4A-C5A
30	C	520	CLA	C4-C3-C5-C6
40	D	404	PL9	C4-C3-C7-C8
40	d	405	PL9	C4-C3-C7-C8
30	B	605	CLA	C11-C10-C8-C9
30	b	605	CLA	C11-C10-C8-C9
30	15	307	CLA	C14-C13-C15-C16
30	17	308	CLA	C11-C10-C8-C9
30	18	303	CLA	C11-C12-C13-C14
30	21	302	CLA	CAA-CBA-CGA-O1A
36	12	301	LMG	O1-C7-C8-C9
42	19	311	A86	C25-C26-C27-C28
35	L	101	LHG	C35-C36-C37-C38
30	11	308	CLA	CAA-CBA-CGA-O1A
30	12	313	CLA	CAA-CBA-CGA-O1A
30	14	310	CLA	CAA-CBA-CGA-O1A
30	19	304	CLA	CAA-CBA-CGA-O1A
30	21	304	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	19	303	CLA	O1D-CGD-O2D-CED
35	d	409	LHG	C35-C36-C37-C38
39	J	101	DGD	O1A-C1A-O1G-C1G
30	B	603	CLA	C16-C17-C18-C19
30	b	603	CLA	C16-C17-C18-C19
36	B	620	LMG	O6-C1-O1-C7
36	Q	301	LMG	O6-C1-O1-C7
36	b	619	LMG	O6-C1-O1-C7
36	c	519	LMG	O6-C1-O1-C7
30	17	306	CLA	CAA-CBA-CGA-O2A
30	18	306	CLA	CAA-CBA-CGA-O1A
30	18	311	CLA	CAA-CBA-CGA-O1A
30	12	303	CLA	CBD-CGD-O2D-CED
39	j	101	DGD	C3B-C4B-C5B-C6B
30	13	309	CLA	CAA-CBA-CGA-O1A
30	16	306	CLA	CAA-CBA-CGA-O2A
30	20	208	CLA	CAA-CBA-CGA-O1A
30	B	603	CLA	C1A-C2A-CAA-CBA
30	C	519	CLA	C1A-C2A-CAA-CBA
30	b	603	CLA	C1A-C2A-CAA-CBA
30	z	101	CLA	C1A-C2A-CAA-CBA
30	11	302	CLA	C1A-C2A-CAA-CBA
30	12	306	CLA	C1A-C2A-CAA-CBA
30	13	303	CLA	C1A-C2A-CAA-CBA
30	14	304	CLA	C1A-C2A-CAA-CBA
30	15	305	CLA	C1A-C2A-CAA-CBA
30	21	307	CLA	C1A-C2A-CAA-CBA
30	C	510	CLA	C6-C7-C8-C10
30	W	102	CLA	C11-C12-C13-C15
30	c	510	CLA	C6-C7-C8-C10
30	w	102	CLA	C11-C12-C13-C15
30	C	509	CLA	O1A-CGA-O2A-C1
30	c	509	CLA	O1A-CGA-O2A-C1
39	j	101	DGD	O1A-C1A-O1G-C1G
30	15	304	CLA	CAA-CBA-CGA-O2A
30	18	311	CLA	CAA-CBA-CGA-O2A
30	19	304	CLA	CAA-CBA-CGA-O2A
30	20	208	CLA	CAA-CBA-CGA-O2A
32	Z	101	BCR	C19-C20-C21-C22
32	c	515	BCR	C19-C20-C21-C22
39	J	101	DGD	C3B-C4B-C5B-C6B
30	18	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	20	205	CLA	CAA-CBA-CGA-O1A
30	20	205	CLA	CAA-CBA-CGA-O2A
36	D	408	LMG	C15-C16-C17-C18
36	d	410	LMG	C15-C16-C17-C18
30	C	519	CLA	C2A-CAA-CBA-CGA
30	z	101	CLA	C2A-CAA-CBA-CGA
30	20	202	CLA	C10-C11-C12-C13
36	B	619	LMG	C11-C12-C13-C14
30	16	306	CLA	CAA-CBA-CGA-O1A
30	19	302	CLA	CAA-CBA-CGA-O2A
35	L	101	LHG	C9-C10-C11-C12
35	d	409	LHG	C9-C10-C11-C12
30	21	306	CLA	C10-C11-C12-C13
30	21	307	CLA	CBA-CGA-O2A-C1
36	b	618	LMG	C11-C12-C13-C14
30	16	302	CLA	C15-C16-C17-C18
30	16	305	CLA	CAA-CBA-CGA-O1A
41	F	102	HEM	CAD-CBD-CGD-O2D
41	f	102	HEM	CAD-CBD-CGD-O2D
35	b	621	LHG	C14-C15-C16-C17
30	w	102	CLA	C4-C3-C5-C6
35	B	622	LHG	C14-C15-C16-C17
36	D	408	LMG	C28-C29-C30-C31
36	d	410	LMG	C28-C29-C30-C31
30	C	520	CLA	C2-C3-C5-C6
40	D	404	PL9	C12-C11-C9-C8
40	d	405	PL9	C12-C11-C9-C8
30	B	603	CLA	C2B-C3B-CAB-CBB
30	W	102	CLA	C2B-C3B-CAB-CBB
30	b	603	CLA	C2B-C3B-CAB-CBB
30	w	102	CLA	C2B-C3B-CAB-CBB
30	11	315	CLA	C2B-C3B-CAB-CBB
30	12	303	CLA	C2B-C3B-CAB-CBB
30	12	312	CLA	C2B-C3B-CAB-CBB
30	14	302	CLA	C2B-C3B-CAB-CBB
30	18	309	CLA	C2B-C3B-CAB-CBB
30	15	304	CLA	CAA-CBA-CGA-O1A
30	18	304	CLA	CAA-CBA-CGA-O2A
30	19	308	CLA	CAA-CBA-CGA-O2A
41	F	102	HEM	CAA-CBA-CGA-O1A
41	f	102	HEM	CAA-CBA-CGA-O1A
30	11	315	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	12	312	CLA	CBD-CGD-O2D-CED
42	11	310	A86	C13-C14-C15-C16
42	11	313	A86	C13-C14-C15-C16
42	12	315	A86	C13-C14-C15-C16
42	12	318	A86	C13-C14-C15-C16
42	13	311	A86	C13-C14-C15-C16
42	13	314	A86	C13-C14-C15-C16
42	14	312	A86	C13-C14-C15-C16
42	14	315	A86	C13-C14-C15-C16
42	15	310	A86	C13-C14-C15-C16
42	15	313	A86	C13-C14-C15-C16
42	17	314	A86	C13-C14-C15-C16
42	18	313	A86	C13-C14-C15-C16
42	18	315	A86	C13-C14-C15-C16
42	19	311	A86	C25-C26-C27-C29
42	21	310	A86	C13-C14-C15-C16
30	15	306	CLA	CAA-CBA-CGA-O1A
30	16	309	CLA	CAA-CBA-CGA-O2A
30	21	302	CLA	CAA-CBA-CGA-O2A
33	L	103	SQD	C9-C10-C11-C12
33	l	101	SQD	C9-C10-C11-C12
36	Q	301	LMG	C35-C36-C37-C38
30	16	302	CLA	C8-C10-C11-C12
30	15	305	CLA	CAA-CBA-CGA-O2A
30	19	308	CLA	CAA-CBA-CGA-O1A
36	12	301	LMG	C31-C32-C33-C34
30	C	514	CLA	C16-C17-C18-C20
30	c	514	CLA	C16-C17-C18-C20
36	c	519	LMG	C35-C36-C37-C38
39	H	102	DGD	C9B-CAB-CBB-CCB
36	B	620	LMG	C36-C37-C38-C39
30	b	601	CLA	CBA-CGA-O2A-C1
30	14	302	CLA	CBD-CGD-O2D-CED
40	D	407	PL9	C39-C41-C42-C43
40	d	408	PL9	C39-C41-C42-C43
42	11	316	A86	C10-C11-C13-C14
42	12	304	A86	C10-C11-C13-C14
42	13	315	A86	C10-C11-C13-C14
42	15	316	A86	C10-C11-C13-C14
42	16	310	A86	C10-C11-C13-C14
30	17	307	CLA	CAA-CBA-CGA-O2A
30	20	207	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	b	619	LMG	C36-C37-C38-C39
30	W	102	CLA	C4-C3-C5-C6
30	21	306	CLA	C2-C1-O2A-CGA
39	h	102	DGD	C9B-CAB-CBB-CCB
30	B	601	CLA	O1A-CGA-O2A-C1
30	b	601	CLA	O1A-CGA-O2A-C1
30	21	307	CLA	O1A-CGA-O2A-C1
30	18	304	CLA	CAA-CBA-CGA-O1A
30	20	206	CLA	CAA-CBA-CGA-O2A
30	20	204	CLA	C16-C17-C18-C19
30	18	309	CLA	C14-C13-C15-C16
30	B	601	CLA	CBA-CGA-O2A-C1
33	L	103	SQD	C19-C20-C21-C22
30	19	302	CLA	CAA-CBA-CGA-O1A
30	20	206	CLA	CAA-CBA-CGA-O1A
30	20	207	CLA	CAA-CBA-CGA-O1A
33	l	101	SQD	C19-C20-C21-C22
30	18	301	CLA	C8-C10-C11-C12
31	D	403	PHO	O1D-CGD-O2D-CED
41	F	102	HEM	CAA-CBA-CGA-O2A
41	f	102	HEM	CAA-CBA-CGA-O2A
36	B	619	LMG	C34-C35-C36-C37
30	A	404	CLA	O1A-CGA-O2A-C1
30	a	403	CLA	O1A-CGA-O2A-C1
32	B	617	BCR	C23-C24-C25-C30
32	B	618	BCR	C23-C24-C25-C30
32	B	624	BCR	C23-C24-C25-C26
32	B	624	BCR	C23-C24-C25-C30
32	C	515	BCR	C23-C24-C25-C26
32	C	515	BCR	C23-C24-C25-C30
32	b	616	BCR	C23-C24-C25-C30
32	b	617	BCR	C23-C24-C25-C30
32	b	623	BCR	C23-C24-C25-C26
32	b	623	BCR	C23-C24-C25-C30
32	c	516	BCR	C23-C24-C25-C26
32	c	516	BCR	C23-C24-C25-C30
36	b	618	LMG	C34-C35-C36-C37
39	c	518	DGD	CCB-CDB-CEB-CFB
30	b	608	CLA	O1D-CGD-O2D-CED
31	D	403	PHO	CAA-CBA-CGA-O2A
31	d	404	PHO	CAA-CBA-CGA-O2A
39	H	102	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
39	h	102	DGD	C1G-C2G-C3G-O3G
39	C	517	DGD	CCB-CDB-CEB-CFB
40	D	407	PL9	C15-C14-C16-C17
40	d	408	PL9	C15-C14-C16-C17
32	A	409	BCR	C17-C18-C19-C20
32	a	408	BCR	C17-C18-C19-C20
30	16	309	CLA	CAA-CBA-CGA-O1A
30	20	203	CLA	CAA-CBA-CGA-O2A
36	Q	301	LMG	C16-C17-C18-C19
36	c	519	LMG	C16-C17-C18-C19
30	a	403	CLA	CBA-CGA-O2A-C1
30	11	308	CLA	CAA-CBA-CGA-O2A
30	17	307	CLA	C4C-C3C-CAC-CBC
30	B	608	CLA	O1D-CGD-O2D-CED
31	d	404	PHO	O1D-CGD-O2D-CED
30	12	313	CLA	CAA-CBA-CGA-O2A
30	13	309	CLA	CAA-CBA-CGA-O2A
30	14	310	CLA	CAA-CBA-CGA-O2A
30	B	605	CLA	C2A-CAA-CBA-CGA
30	b	605	CLA	C2A-CAA-CBA-CGA
30	11	305	CLA	C2A-CAA-CBA-CGA
30	12	309	CLA	C2A-CAA-CBA-CGA
30	13	306	CLA	C2A-CAA-CBA-CGA
30	14	307	CLA	C2A-CAA-CBA-CGA
30	21	306	CLA	C2A-CAA-CBA-CGA
30	21	307	CLA	C2A-CAA-CBA-CGA
30	15	305	CLA	CAA-CBA-CGA-O1A
30	C	507	CLA	C4B-C3B-CAB-CBB
30	C	520	CLA	C4B-C3B-CAB-CBB
30	M	101	CLA	C4B-C3B-CAB-CBB
30	c	507	CLA	C4B-C3B-CAB-CBB
30	m	101	CLA	C4B-C3B-CAB-CBB
30	11	305	CLA	C4B-C3B-CAB-CBB
30	11	307	CLA	C4B-C3B-CAB-CBB
30	12	309	CLA	C4B-C3B-CAB-CBB
30	12	311	CLA	C4B-C3B-CAB-CBB
30	13	306	CLA	C4B-C3B-CAB-CBB
30	13	308	CLA	C4B-C3B-CAB-CBB
30	14	307	CLA	C4B-C3B-CAB-CBB
30	14	309	CLA	C4B-C3B-CAB-CBB
30	15	307	CLA	C4B-C3B-CAB-CBB
30	A	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	B	623	CLA	CBA-CGA-O2A-C1
36	1	101	LMG	C2-C1-O1-C7
30	19	306	CLA	CAA-CBA-CGA-O2A
30	21	305	CLA	CAA-CBA-CGA-O1A
39	H	102	DGD	C4B-C5B-C6B-C7B
30	19	305	CLA	CAA-CBA-CGA-O1A
30	20	203	CLA	CAA-CBA-CGA-O1A
30	21	305	CLA	CAA-CBA-CGA-O2A
30	B	611	CLA	C2A-CAA-CBA-CGA
30	b	611	CLA	C2A-CAA-CBA-CGA
30	17	307	CLA	CAA-CBA-CGA-O1A
32	Y	101	BCR	C16-C17-C18-C36
32	c	520	BCR	C16-C17-C18-C36
39	h	102	DGD	C4B-C5B-C6B-C7B
30	C	520	CLA	CAA-CBA-CGA-O2A
30	20	202	CLA	CAA-CBA-CGA-O2A
30	B	604	CLA	C4-C3-C5-C6
30	Z	102	CLA	C4-C3-C5-C6
30	b	604	CLA	C4-C3-C5-C6
30	C	505	CLA	C5-C6-C7-C8
30	c	505	CLA	C5-C6-C7-C8
30	11	306	CLA	CAA-CBA-CGA-O2A
30	12	310	CLA	CAA-CBA-CGA-O2A
30	13	307	CLA	CAA-CBA-CGA-O2A
30	C	504	CLA	C2-C3-C5-C6
30	W	102	CLA	C2-C3-C5-C6
30	c	504	CLA	C2-C3-C5-C6
30	w	102	CLA	C2-C3-C5-C6
30	17	305	CLA	C16-C17-C18-C19
30	15	307	CLA	CAA-CBA-CGA-O2A
39	J	101	DGD	O1G-C1A-C2A-C3A
39	j	101	DGD	O1G-C1A-C2A-C3A
30	B	601	CLA	C14-C13-C15-C16
30	B	602	CLA	C6-C7-C8-C9
30	B	615	CLA	C14-C13-C15-C16
30	C	519	CLA	C11-C10-C8-C9
30	b	601	CLA	C14-C13-C15-C16
30	b	602	CLA	C6-C7-C8-C9
30	b	615	CLA	C14-C13-C15-C16
30	z	101	CLA	C11-C10-C8-C9
30	17	305	CLA	C11-C12-C13-C14
30	19	307	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	14	308	CLA	CAA-CBA-CGA-O2A
30	15	303	CLA	C3A-C2A-CAA-CBA
30	19	303	CLA	C3A-C2A-CAA-CBA
36	w	101	LMG	O10-C28-O8-C9
30	C	502	CLA	CAA-CBA-CGA-O2A
35	A	408	LHG	C16-C17-C18-C19
35	B	622	LHG	C10-C11-C12-C13
35	a	407	LHG	C16-C17-C18-C19
36	w	101	LMG	C39-C40-C41-C42
30	18	308	CLA	CAA-CBA-CGA-O1A
30	18	308	CLA	CAA-CBA-CGA-O2A
30	C	502	CLA	CAD-CBD-CGD-O2D
30	C	504	CLA	CAD-CBD-CGD-O2D
30	C	519	CLA	CAD-CBD-CGD-O2D
30	c	502	CLA	CAD-CBD-CGD-O2D
30	c	504	CLA	CAD-CBD-CGD-O2D
30	z	101	CLA	CAD-CBD-CGD-O2D
30	11	302	CLA	CAD-CBD-CGD-O2D
30	11	307	CLA	CAD-CBD-CGD-O2D
30	12	306	CLA	CAD-CBD-CGD-O2D
30	12	311	CLA	CAD-CBD-CGD-O2D
30	13	303	CLA	CAD-CBD-CGD-O2D
30	13	308	CLA	CAD-CBD-CGD-O2D
30	14	304	CLA	CAD-CBD-CGD-O2D
30	14	309	CLA	CAD-CBD-CGD-O2D
30	15	305	CLA	CAD-CBD-CGD-O2D
30	15	306	CLA	CAD-CBD-CGD-O2D
30	16	303	CLA	CAD-CBD-CGD-O2D
30	16	309	CLA	CAD-CBD-CGD-O2D
30	17	306	CLA	CAD-CBD-CGD-O2D
30	17	308	CLA	CAD-CBD-CGD-O2D
30	19	308	CLA	CAD-CBD-CGD-O2D
30	20	209	CLA	CAD-CBD-CGD-O2D
30	21	304	CLA	CAD-CBD-CGD-O2D
30	21	305	CLA	CAD-CBD-CGD-O2D
42	20	211	A86	C28-C27-C29-C30
42	21	311	A86	C28-C27-C29-C30
30	b	622	CLA	CBA-CGA-O2A-C1
30	17	305	CLA	C16-C17-C18-C20
39	C	517	DGD	O1B-C1B-O2G-C2G
39	c	518	DGD	O1B-C1B-O2G-C2G
35	b	621	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	W	101	LMG	C39-C40-C41-C42
30	B	605	CLA	C13-C15-C16-C17
30	b	605	CLA	C13-C15-C16-C17
33	b	620	SQD	C24-C25-C26-C27
30	A	404	CLA	CAA-CBA-CGA-O2A
30	W	103	CLA	CAA-CBA-CGA-O2A
30	a	403	CLA	CAA-CBA-CGA-O2A
30	c	502	CLA	CAA-CBA-CGA-O2A
30	c	513	CLA	C15-C16-C17-C18
33	B	621	SQD	C24-C25-C26-C27
30	Z	102	CLA	C2-C3-C5-C6
40	D	407	PL9	C28-C29-C31-C32
40	d	408	PL9	C28-C29-C31-C32
30	w	103	CLA	CAA-CBA-CGA-O2A
42	11	314	A86	C5-C6-C8-C9
42	12	319	A86	C5-C6-C8-C9
42	14	301	A86	C5-C6-C8-C9
42	14	316	A86	C5-C6-C8-C9
42	15	314	A86	C5-C6-C8-C9
42	16	313	A86	C5-C6-C8-C9
42	17	316	A86	C5-C6-C8-C9
40	D	407	PL9	C29-C31-C32-C33
40	d	408	PL9	C29-C31-C32-C33
42	21	313	A86	C12-C11-C13-O
30	12	310	CLA	CAA-CBA-CGA-O1A
30	14	308	CLA	CAA-CBA-CGA-O1A
30	15	302	CLA	CAA-CBA-CGA-O1A
30	17	310	CLA	CAA-CBA-CGA-O1A
30	17	310	CLA	CAA-CBA-CGA-O2A
30	21	309	CLA	CAA-CBA-CGA-O1A
31	D	403	PHO	CBD-CGD-O2D-CED
31	d	404	PHO	CBD-CGD-O2D-CED
36	W	101	LMG	O10-C28-O8-C9
30	C	513	CLA	C15-C16-C17-C18
30	C	509	CLA	C3-C5-C6-C7
30	11	306	CLA	CAA-CBA-CGA-O1A
30	13	307	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	CAA-CBA-CGA-O2A
30	18	310	CLA	C13-C15-C16-C17
30	C	504	CLA	O2A-C1-C2-C3
30	C	510	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	c	504	CLA	O2A-C1-C2-C3
30	c	510	CLA	O2A-C1-C2-C3
31	A	403	PHO	O2A-C1-C2-C3
31	d	403	PHO	O2A-C1-C2-C3
30	16	307	CLA	C2A-CAA-CBA-CGA
30	17	301	CLA	C13-C15-C16-C17
30	16	302	CLA	CAA-CBA-CGA-O2A
30	c	509	CLA	C3-C5-C6-C7
30	16	307	CLA	CAA-CBA-CGA-O1A
30	16	307	CLA	CAA-CBA-CGA-O2A
30	18	307	CLA	CAA-CBA-CGA-O1A
30	18	307	CLA	CAA-CBA-CGA-O2A
30	19	306	CLA	CAA-CBA-CGA-O1A
30	B	607	CLA	CHA-CBD-CGD-O1D
30	C	507	CLA	CHA-CBD-CGD-O2D
30	C	508	CLA	CHA-CBD-CGD-O2D
30	C	513	CLA	CHA-CBD-CGD-O2D
30	b	607	CLA	CHA-CBD-CGD-O1D
30	c	507	CLA	CHA-CBD-CGD-O2D
30	c	508	CLA	CHA-CBD-CGD-O2D
30	c	513	CLA	CHA-CBD-CGD-O2D
30	16	302	CLA	CHA-CBD-CGD-O1D
30	16	302	CLA	CHA-CBD-CGD-O2D
30	16	305	CLA	CHA-CBD-CGD-O2D
30	16	307	CLA	CHA-CBD-CGD-O1D
30	17	310	CLA	CHA-CBD-CGD-O2D
30	18	306	CLA	CHA-CBD-CGD-O1D
30	18	306	CLA	CHA-CBD-CGD-O2D
30	18	309	CLA	CHA-CBD-CGD-O2D
30	18	310	CLA	CHA-CBD-CGD-O1D
30	18	310	CLA	CHA-CBD-CGD-O2D
30	19	304	CLA	CHA-CBD-CGD-O1D
30	19	304	CLA	CHA-CBD-CGD-O2D
30	19	306	CLA	CHA-CBD-CGD-O1D
30	19	306	CLA	CHA-CBD-CGD-O2D
30	20	205	CLA	CHA-CBD-CGD-O1D
30	20	205	CLA	CHA-CBD-CGD-O2D
30	20	206	CLA	CHA-CBD-CGD-O1D
30	20	206	CLA	CHA-CBD-CGD-O2D
30	20	207	CLA	CHA-CBD-CGD-O1D
30	20	208	CLA	CHA-CBD-CGD-O1D
30	20	208	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	21	303	CLA	CHA-CBD-CGD-O2D
30	21	308	CLA	CHA-CBD-CGD-O1D
30	21	308	CLA	CHA-CBD-CGD-O2D
30	21	309	CLA	CHA-CBD-CGD-O1D
30	21	309	CLA	CHA-CBD-CGD-O2D
32	B	616	BCR	C19-C20-C21-C22
32	m	103	BCR	C19-C20-C21-C22
30	d	402	CLA	C4C-C3C-CAC-CBC
40	d	405	PL9	C32-C33-C34-C36
30	D	402	CLA	C4C-C3C-CAC-CBC
32	F	101	BCR	C11-C10-C9-C8
32	f	101	BCR	C11-C10-C9-C8
30	21	307	CLA	C16-C17-C18-C20
30	14	303	CLA	C8-C10-C11-C12
30	16	304	CLA	CAA-CBA-CGA-O2A
30	17	301	CLA	CAA-CBA-CGA-O2A
36	D	408	LMG	C16-C17-C18-C19
39	C	517	DGD	O1G-C1G-C2G-O2G
39	c	518	DGD	O1G-C1G-C2G-O2G
36	d	410	LMG	C16-C17-C18-C19
30	21	305	CLA	C4C-C3C-CAC-CBC
30	d	401	CLA	CBD-CGD-O2D-CED
31	D	403	PHO	CHA-CBD-CGD-O1D
31	d	404	PHO	CHA-CBD-CGD-O1D
42	17	311	A86	C10-C11-C13-O
42	21	313	A86	C10-C11-C13-O
30	B	605	CLA	CBA-CGA-O2A-C1
30	b	605	CLA	CBA-CGA-O2A-C1
30	20	206	CLA	C4C-C3C-CAC-CBC
35	L	101	LHG	C11-C12-C13-C14
35	d	409	LHG	C11-C12-C13-C14
30	D	401	CLA	CBD-CGD-O2D-CED
30	15	302	CLA	CAA-CBA-CGA-O2A
30	21	309	CLA	CAA-CBA-CGA-O2A
30	11	301	CLA	C8-C10-C11-C12
30	A	404	CLA	C11-C10-C8-C7
30	B	604	CLA	C11-C10-C8-C7
30	B	623	CLA	C11-C12-C13-C15
30	a	403	CLA	C11-C10-C8-C7
30	b	604	CLA	C11-C10-C8-C7
30	b	622	CLA	C11-C12-C13-C15
30	19	307	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	20	202	CLA	C16-C17-C18-C19
39	h	102	DGD	CDB-CEB-CFB-CGB
30	13	302	CLA	C8-C10-C11-C12
30	19	305	CLA	CAA-CBA-CGA-O2A
30	21	305	CLA	C2C-C3C-CAC-CBC
30	17	305	CLA	C11-C10-C8-C9
35	l	102	LHG	C11-C10-C9-C8
30	12	305	CLA	C8-C10-C11-C12
39	H	102	DGD	CDB-CEB-CFB-CGB
30	12	314	CLA	CAA-CBA-CGA-O1A
33	A	406	SQD	C5-C6-S-O8
33	a	405	SQD	C5-C6-S-O8
30	11	309	CLA	CAA-CBA-CGA-O1A
30	W	103	CLA	CAA-CBA-CGA-O1A
30	w	103	CLA	CAA-CBA-CGA-O1A
35	L	102	LHG	C11-C10-C9-C8
30	13	310	CLA	CAA-CBA-CGA-O1A
30	14	311	CLA	CAA-CBA-CGA-O1A
42	12	317	A86	C-C1-C24-C25
42	13	313	A86	C-C1-C24-C25
30	C	506	CLA	C10-C11-C12-C13
30	B	608	CLA	C4-C3-C5-C6
30	b	608	CLA	C4-C3-C5-C6
33	A	406	SQD	C30-C31-C32-C33
30	C	520	CLA	CAA-CBA-CGA-O1A
33	A	406	SQD	C35-C36-C37-C38
33	a	405	SQD	C30-C31-C32-C33
30	c	506	CLA	C10-C11-C12-C13
30	21	303	CLA	C15-C16-C17-C18
35	B	622	LHG	C11-C12-C13-C14
35	b	621	LHG	C11-C12-C13-C14
30	19	303	CLA	C1A-C2A-CAA-CBA
30	20	203	CLA	C1A-C2A-CAA-CBA
30	21	308	CLA	C1A-C2A-CAA-CBA
33	a	405	SQD	C35-C36-C37-C38
36	B	619	LMG	C37-C38-C39-C40
36	b	618	LMG	C37-C38-C39-C40
30	20	202	CLA	CAA-CBA-CGA-O1A
30	19	307	CLA	C15-C16-C17-C18
36	Q	301	LMG	C39-C40-C41-C42
36	c	519	LMG	C39-C40-C41-C42
30	15	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	20	204	CLA	CAA-CBA-CGA-O2A
31	D	403	PHO	C8-C10-C11-C12
31	d	404	PHO	C8-C10-C11-C12
35	a	407	LHG	C18-C19-C20-C21
35	A	408	LHG	C18-C19-C20-C21
30	C	502	CLA	CAA-CBA-CGA-O1A
30	16	302	CLA	CAA-CBA-CGA-O1A
36	1	101	LMG	C31-C32-C33-C34
35	L	102	LHG	C17-C18-C19-C20
30	a	403	CLA	CAA-CBA-CGA-O1A
30	c	502	CLA	CAA-CBA-CGA-O1A
30	B	605	CLA	C10-C11-C12-C13
30	b	605	CLA	C10-C11-C12-C13
35	d	409	LHG	C34-C35-C36-C37
35	l	102	LHG	C17-C18-C19-C20
39	C	517	DGD	CCA-CDA-CEA-CFA
30	19	309	CLA	CAA-CBA-CGA-O2A
30	21	308	CLA	CAA-CBA-CGA-O2A
35	L	101	LHG	C16-C17-C18-C19
35	d	409	LHG	C16-C17-C18-C19
39	c	518	DGD	CCA-CDA-CEA-CFA
30	A	404	CLA	CAA-CBA-CGA-O1A
40	D	404	PL9	C32-C33-C34-C36
30	b	607	CLA	C8-C10-C11-C12
39	j	101	DGD	CCA-CDA-CEA-CFA
35	L	101	LHG	C34-C35-C36-C37
40	d	408	PL9	C12-C11-C9-C10
36	Q	301	LMG	C34-C35-C36-C37
36	12	301	LMG	C16-C17-C18-C19
30	16	304	CLA	C16-C17-C18-C19
30	B	607	CLA	CAD-CBD-CGD-O1D
30	b	607	CLA	CAD-CBD-CGD-O1D
30	11	307	CLA	CAD-CBD-CGD-O1D
30	12	311	CLA	CAD-CBD-CGD-O1D
30	13	308	CLA	CAD-CBD-CGD-O1D
30	14	309	CLA	CAD-CBD-CGD-O1D
30	18	307	CLA	CAD-CBD-CGD-O1D
30	18	309	CLA	CAD-CBD-CGD-O1D
30	19	301	CLA	CAD-CBD-CGD-O1D
30	21	302	CLA	CAD-CBD-CGD-O1D
42	20	211	A86	C26-C27-C29-C30
42	21	311	A86	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
30	c	508	CLA	CAA-CBA-CGA-O2A
30	B	607	CLA	C8-C10-C11-C12
30	B	607	CLA	C10-C11-C12-C13
30	b	607	CLA	C10-C11-C12-C13
30	17	305	CLA	C5-C6-C7-C8
36	c	519	LMG	C34-C35-C36-C37
30	B	605	CLA	O1A-CGA-O2A-C1
30	b	605	CLA	O1A-CGA-O2A-C1
39	J	101	DGD	CCA-CDA-CEA-CFA
30	C	504	CLA	C3-C5-C6-C7
30	C	506	CLA	CAA-CBA-CGA-O2A
30	C	508	CLA	CAA-CBA-CGA-O2A
30	c	506	CLA	CAA-CBA-CGA-O2A
30	17	301	CLA	CAA-CBA-CGA-O1A
36	M	102	LMG	C8-C9-O8-C28
36	m	102	LMG	C8-C9-O8-C28
30	C	511	CLA	CAA-CBA-CGA-O2A
30	C	514	CLA	CAA-CBA-CGA-O2A
30	C	519	CLA	CAA-CBA-CGA-O2A
30	Z	102	CLA	CAA-CBA-CGA-O2A
30	c	514	CLA	CAA-CBA-CGA-O2A
30	z	101	CLA	CAA-CBA-CGA-O2A
30	15	303	CLA	CAA-CBA-CGA-O2A
30	17	305	CLA	CAA-CBA-CGA-O2A
30	18	309	CLA	CAA-CBA-CGA-O2A
30	21	306	CLA	C13-C15-C16-C17
30	c	504	CLA	C3-C5-C6-C7
30	16	304	CLA	CAA-CBA-CGA-O1A
30	13	303	CLA	O1D-CGD-O2D-CED
40	D	407	PL9	C12-C11-C9-C10
42	17	313	A86	C-C1-C24-C25
30	B	604	CLA	C11-C12-C13-C15
30	B	610	CLA	C11-C10-C8-C7
30	B	610	CLA	C11-C12-C13-C15
30	C	502	CLA	C12-C13-C15-C16
30	b	604	CLA	C11-C12-C13-C15
30	b	610	CLA	C11-C10-C8-C7
30	b	610	CLA	C11-C12-C13-C15
30	c	502	CLA	C12-C13-C15-C16
30	11	302	CLA	C3A-C2A-CAA-CBA
30	12	306	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	14	304	CLA	C3A-C2A-CAA-CBA
30	15	301	CLA	C12-C13-C15-C16
30	17	303	CLA	C2-C3-C5-C6
30	18	305	CLA	C11-C10-C8-C7
30	18	305	CLA	CAA-CBA-CGA-O1A
36	D	408	LMG	O9-C10-C11-C12
36	d	410	LMG	O9-C10-C11-C12
30	11	309	CLA	CAA-CBA-CGA-O2A
30	12	314	CLA	CAA-CBA-CGA-O2A
30	13	310	CLA	CAA-CBA-CGA-O2A
30	14	311	CLA	CAA-CBA-CGA-O2A
30	15	309	CLA	CAA-CBA-CGA-O2A
30	18	312	CLA	CAA-CBA-CGA-O2A
30	19	309	CLA	CAA-CBA-CGA-O1A
30	c	511	CLA	CAA-CBA-CGA-O2A
30	11	303	CLA	CAA-CBA-CGA-O2A
30	12	307	CLA	CAA-CBA-CGA-O2A
30	13	304	CLA	CAA-CBA-CGA-O2A
30	14	305	CLA	CAA-CBA-CGA-O2A
30	18	305	CLA	CAA-CBA-CGA-O2A
30	21	303	CLA	CAA-CBA-CGA-O2A
30	21	306	CLA	CAA-CBA-CGA-O2A
30	20	204	CLA	C8-C10-C11-C12
30	17	303	CLA	C4C-C3C-CAC-CBC
32	B	618	BCR	C17-C18-C19-C20
32	C	515	BCR	C17-C18-C19-C20
32	b	617	BCR	C17-C18-C19-C20
32	c	516	BCR	C17-C18-C19-C20
42	11	310	A86	C2-C1-C24-C25
42	12	315	A86	C2-C1-C24-C25
42	13	311	A86	C2-C1-C24-C25
42	14	312	A86	C2-C1-C24-C25
42	15	310	A86	C2-C1-C24-C25
42	18	313	A86	C2-C1-C24-C25
42	19	311	A86	C2-C1-C24-C25
30	C	506	CLA	CAA-CBA-CGA-O1A
30	c	506	CLA	CAA-CBA-CGA-O1A
39	C	516	DGD	O1B-C1B-C2B-C3B
39	c	517	DGD	O1B-C1B-C2B-C3B
30	21	308	CLA	CAA-CBA-CGA-O1A
32	Y	101	BCR	C19-C20-C21-C22
32	c	520	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	b	619	LMG	C20-C21-C22-C23
30	20	202	CLA	C16-C17-C18-C20
42	11	316	A86	O-C13-C14-C15
42	12	304	A86	O-C13-C14-C15
42	13	301	A86	O-C13-C14-C15
42	13	315	A86	O-C13-C14-C15
42	15	315	A86	O-C13-C14-C15
42	15	316	A86	O-C13-C14-C15
42	17	315	A86	O-C13-C14-C15
42	18	302	A86	O-C13-C14-C15
30	19	303	CLA	CAA-CBA-CGA-O2A
39	C	517	DGD	O6D-C1D-O3G-C3G
39	c	518	DGD	O6D-C1D-O3G-C3G
30	11	302	CLA	O1D-CGD-O2D-CED
30	18	309	CLA	C13-C15-C16-C17
30	C	508	CLA	CAA-CBA-CGA-O1A
30	C	511	CLA	CAA-CBA-CGA-O1A
30	c	511	CLA	CAA-CBA-CGA-O1A
30	20	204	CLA	CAA-CBA-CGA-O1A
33	A	406	SQD	O49-C7-C8-C9
40	D	407	PL9	C44-C46-C47-C48
40	d	408	PL9	C44-C46-C47-C48
39	H	102	DGD	C8A-C9A-CAA-CBA
30	B	602	CLA	C13-C15-C16-C17
30	b	602	CLA	C13-C15-C16-C17
40	D	407	PL9	C31-C32-C33-C34
40	d	408	PL9	C31-C32-C33-C34
36	B	620	LMG	C20-C21-C22-C23
30	13	302	CLA	CAA-CBA-CGA-O2A
30	14	303	CLA	CAA-CBA-CGA-O2A
39	h	102	DGD	C8A-C9A-CAA-CBA
30	C	519	CLA	CAA-CBA-CGA-O1A
30	c	508	CLA	CAA-CBA-CGA-O1A
30	z	101	CLA	CAA-CBA-CGA-O1A
33	a	405	SQD	O49-C7-C8-C9
30	21	301	CLA	C2A-CAA-CBA-CGA
30	15	309	CLA	CAA-CBA-CGA-O1A
30	21	306	CLA	CAA-CBA-CGA-O1A
30	18	312	CLA	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	17	302	A86	C31-C32-C33-C34-C35-C36

284 monomers are involved in 862 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	619	LMG	3	0
32	h	101	BCR	3	0
42	17	315	A86	19	0
30	D	405	CLA	6	0
42	21	312	A86	4	0
30	15	305	CLA	1	0
30	14	310	CLA	3	0
30	c	507	CLA	5	0
32	A	409	BCR	2	0
30	14	302	CLA	2	0
35	d	409	LHG	3	0
30	d	407	CLA	1	0
40	D	404	PL9	3	0
42	21	313	A86	2	0
30	b	614	CLA	5	0
30	b	601	CLA	4	0
42	12	318	A86	4	0
30	c	511	CLA	5	0
30	B	605	CLA	2	0
42	15	311	A86	10	0
31	d	404	PHO	2	0
30	11	304	CLA	2	0
36	M	102	LMG	5	0
42	14	313	A86	10	0
36	Q	301	LMG	2	0
30	b	613	CLA	3	0
42	19	310	A86	6	0
42	13	315	A86	8	0
30	C	510	CLA	2	0
35	L	101	LHG	5	0
42	11	313	A86	6	0
32	a	408	BCR	1	0
30	18	310	CLA	2	0
30	20	209	CLA	2	0
30	17	303	CLA	11	0
30	12	306	CLA	2	0
30	17	308	CLA	5	0
32	Y	101	BCR	4	0
30	12	307	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	21	301	CLA	3	0
30	b	610	CLA	2	0
30	13	309	CLA	1	0
30	18	312	CLA	19	0
30	15	309	CLA	1	0
30	18	303	CLA	14	0
30	b	615	CLA	3	0
42	13	301	A86	9	0
30	14	304	CLA	3	0
42	13	312	A86	11	0
30	17	309	CLA	1	0
30	17	301	CLA	3	0
30	13	304	CLA	4	0
30	16	301	CLA	3	0
40	D	407	PL9	4	0
35	b	621	LHG	2	0
30	13	303	CLA	2	0
30	19	301	CLA	3	0
30	15	303	CLA	1	0
42	20	213	A86	1	0
42	13	313	A86	3	0
42	17	312	A86	12	0
41	F	102	HEM	3	0
42	15	313	A86	6	0
30	b	604	CLA	6	0
30	c	509	CLA	6	0
41	V	201	HEM	2	0
30	19	303	CLA	5	0
42	16	310	A86	7	0
42	19	312	A86	3	0
36	w	101	LMG	6	0
30	B	613	CLA	4	0
30	17	305	CLA	12	0
30	b	611	CLA	3	0
30	b	603	CLA	1	0
30	11	308	CLA	1	0
30	19	309	CLA	1	0
42	15	310	A86	2	0
42	12	316	A86	9	0
30	B	608	CLA	2	0
32	B	618	BCR	2	0
30	B	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	16	304	CLA	1	0
39	h	102	DGD	3	0
30	b	608	CLA	3	0
42	11	312	A86	3	0
30	14	308	CLA	1	0
30	15	301	CLA	8	0
30	c	502	CLA	4	0
35	B	622	LHG	1	0
30	C	506	CLA	4	0
30	C	511	CLA	4	0
30	W	103	CLA	4	0
32	b	617	BCR	2	0
30	C	504	CLA	4	0
30	12	310	CLA	3	0
32	m	103	BCR	3	0
32	Z	101	BCR	1	0
30	12	312	CLA	3	0
42	11	316	A86	10	0
30	B	604	CLA	6	0
38	c	501	OEX	1	0
40	d	405	PL9	3	0
30	17	306	CLA	4	0
30	21	302	CLA	4	0
32	b	616	BCR	1	0
30	11	306	CLA	1	0
30	C	503	CLA	3	0
30	B	610	CLA	2	0
33	L	103	SQD	3	0
42	20	201	A86	11	0
30	21	303	CLA	11	0
42	12	317	A86	4	0
30	21	308	CLA	1	0
42	21	310	A86	10	0
36	B	620	LMG	2	0
30	c	513	CLA	4	0
30	16	306	CLA	1	0
30	m	101	CLA	2	0
30	B	614	CLA	3	0
30	16	307	CLA	7	0
32	a	404	BCR	1	0
30	15	307	CLA	3	0
30	B	612	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	W	101	LMG	8	0
30	c	505	CLA	1	0
30	16	308	CLA	10	0
30	17	304	CLA	2	0
30	21	309	CLA	3	0
30	C	509	CLA	6	0
35	a	407	LHG	6	0
42	12	319	A86	2	0
30	d	401	CLA	3	0
32	c	520	BCR	2	0
30	z	101	CLA	4	0
42	14	316	A86	2	0
30	c	512	CLA	2	0
30	21	307	CLA	1	0
30	12	308	CLA	7	0
30	A	404	CLA	11	0
30	16	309	CLA	5	0
30	w	103	CLA	2	0
30	B	611	CLA	3	0
42	17	302	A86	18	0
30	13	302	CLA	9	0
32	b	623	BCR	4	0
42	18	314	A86	15	0
30	15	302	CLA	3	0
30	b	607	CLA	2	0
30	18	304	CLA	3	0
30	17	307	CLA	1	0
30	D	401	CLA	4	0
30	16	303	CLA	1	0
32	C	515	BCR	2	0
30	13	308	CLA	2	0
30	18	311	CLA	5	0
30	C	508	CLA	1	0
35	A	408	LHG	4	0
42	15	315	A86	7	0
32	B	617	BCR	1	0
31	A	403	PHO	1	0
39	J	101	DGD	1	0
30	b	605	CLA	1	0
30	B	602	CLA	6	0
34	a	406	BCT	2	0
30	20	203	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	601	CLA	4	0
32	B	616	BCR	2	0
30	14	305	CLA	4	0
30	C	514	CLA	10	0
42	20	211	A86	7	0
30	12	305	CLA	9	0
30	12	313	CLA	1	0
30	B	606	CLA	3	0
42	11	314	A86	3	0
36	c	519	LMG	1	0
30	13	307	CLA	2	0
30	C	512	CLA	3	0
30	C	507	CLA	11	0
32	H	101	BCR	5	0
39	H	102	DGD	5	0
30	21	304	CLA	5	0
30	13	306	CLA	2	0
32	c	521	BCR	2	0
30	15	308	CLA	6	0
30	C	502	CLA	3	0
32	A	405	BCR	1	0
30	B	623	CLA	3	0
30	18	308	CLA	1	0
42	14	314	A86	1	0
42	21	311	A86	9	0
42	17	313	A86	1	0
30	c	506	CLA	1	0
30	11	315	CLA	7	0
30	11	305	CLA	2	0
30	14	307	CLA	2	0
33	b	620	SQD	2	0
30	c	510	CLA	2	0
30	A	402	CLA	2	0
42	21	314	A86	19	0
30	12	311	CLA	2	0
42	18	302	A86	10	0
30	15	306	CLA	3	0
32	c	516	BCR	1	0
42	14	315	A86	3	0
30	b	622	CLA	3	0
30	16	302	CLA	7	0
30	C	505	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	519	CLA	1	0
36	m	102	LMG	2	0
42	18	315	A86	7	0
35	L	102	LHG	1	0
30	w	102	CLA	3	0
30	11	307	CLA	2	0
30	18	301	CLA	2	0
36	b	619	LMG	1	0
42	12	304	A86	7	0
42	20	212	A86	13	0
30	18	305	CLA	2	0
42	17	311	A86	6	0
30	C	513	CLA	2	0
30	b	612	CLA	4	0
30	21	306	CLA	3	0
30	B	609	CLA	1	0
32	F	101	BCR	2	0
30	Z	102	CLA	9	0
30	21	305	CLA	1	0
36	D	408	LMG	2	0
30	b	606	CLA	4	0
30	D	402	CLA	1	0
31	D	403	PHO	2	0
35	l	102	LHG	3	0
30	b	602	CLA	6	0
30	M	101	CLA	1	0
42	18	313	A86	1	0
33	l	101	SQD	3	0
30	18	309	CLA	4	0
30	a	403	CLA	6	0
30	b	609	CLA	2	0
30	d	406	CLA	5	0
30	11	301	CLA	8	0
30	11	302	CLA	1	0
42	15	316	A86	14	0
42	11	311	A86	9	0
30	W	102	CLA	5	0
42	13	314	A86	3	0
42	16	312	A86	5	0
32	f	101	BCR	1	0
42	20	210	A86	10	0
42	16	313	A86	2	0

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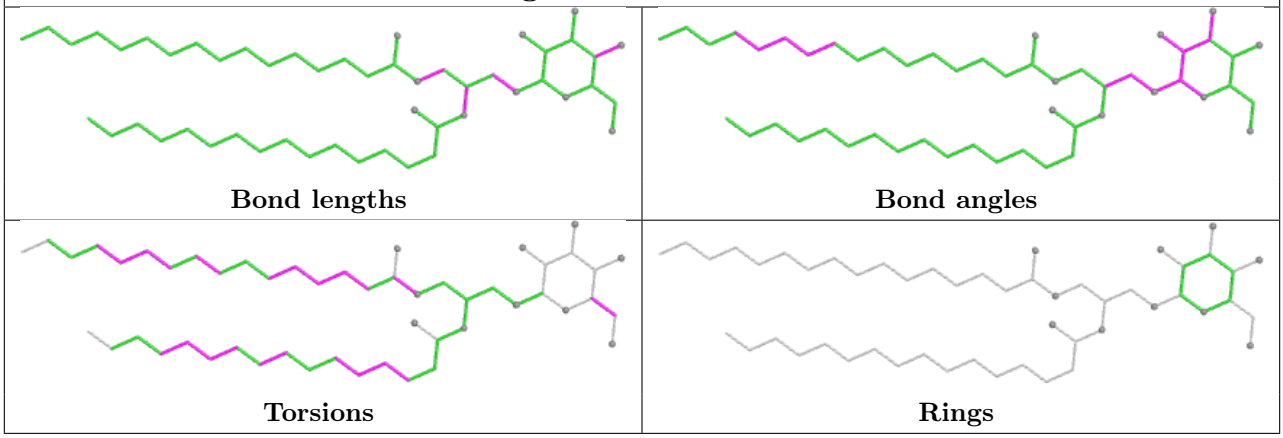
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	406	CLA	1	0
30	d	402	CLA	1	0
30	11	303	CLA	3	0
36	b	618	LMG	4	0
42	14	301	A86	2	0
41	f	102	HEM	4	0
34	A	407	BCT	1	0
32	c	515	BCR	3	0
36	d	410	LMG	1	0
30	14	309	CLA	2	0
30	C	520	CLA	3	0
42	17	316	A86	5	0
30	B	615	CLA	2	0
30	c	504	CLA	4	0
41	v	201	HEM	2	0
30	c	508	CLA	3	0
42	13	311	A86	2	0
30	14	303	CLA	9	0
42	15	314	A86	1	0
30	12	309	CLA	4	0
42	17	314	A86	2	0
30	20	207	CLA	2	0
40	d	408	PL9	5	0
30	20	202	CLA	5	0
42	16	311	A86	7	0
39	j	101	DGD	1	0
30	c	503	CLA	3	0
30	12	303	CLA	6	0
30	17	310	CLA	1	0
32	B	624	BCR	5	0
30	c	514	CLA	2	0
30	a	402	CLA	1	0
42	19	311	A86	13	0
36	12	301	LMG	8	0
32	C	518	BCR	3	0

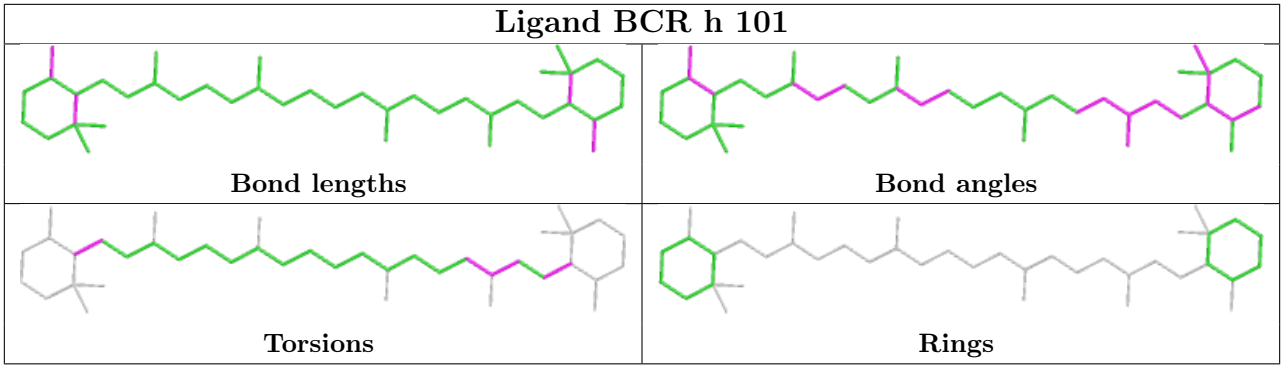
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

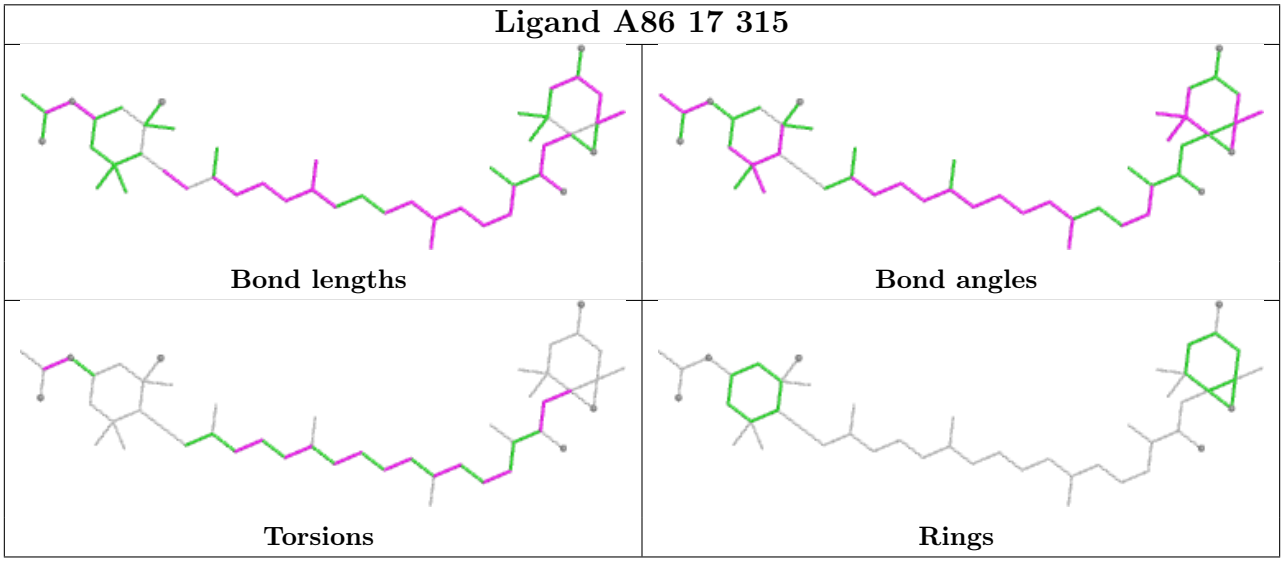
Ligand LMG B 619



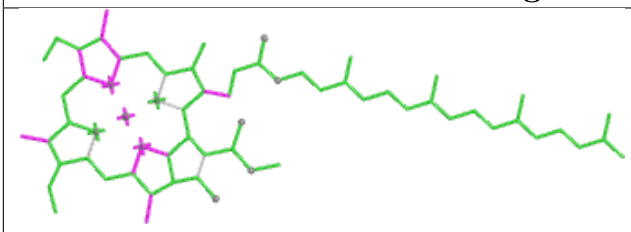
Ligand BCR h 101



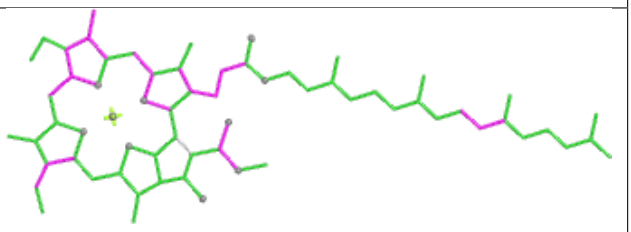
Ligand A86 17 315



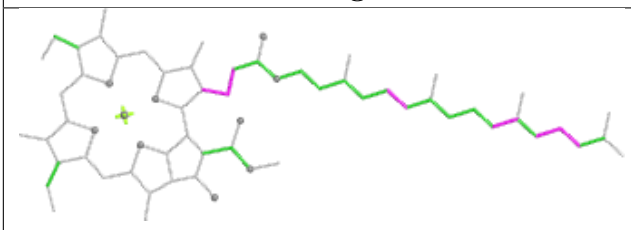
Ligand CLA D 405



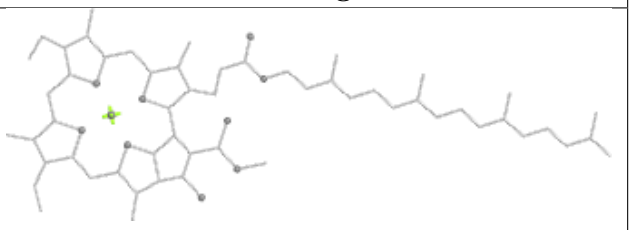
Bond lengths



Bond angles

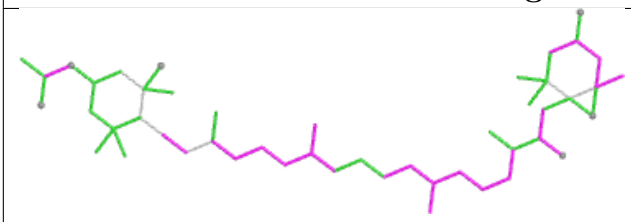


Torsions

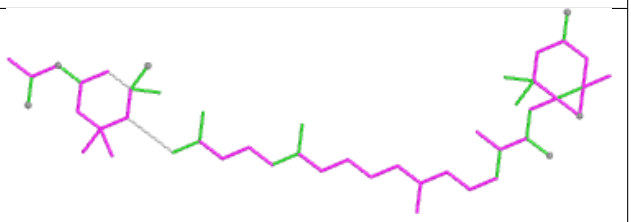


Rings

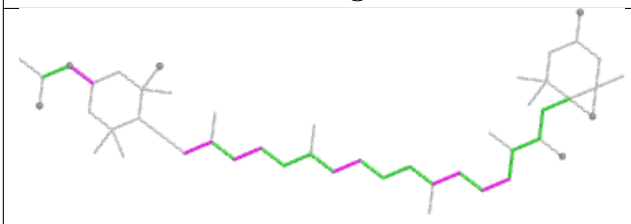
Ligand A86 21 312



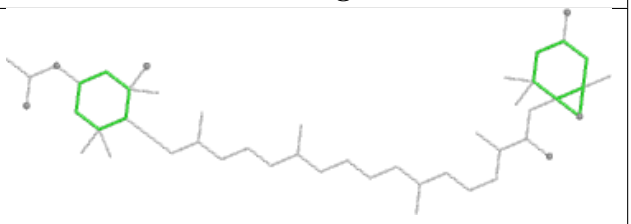
Bond lengths



Bond angles

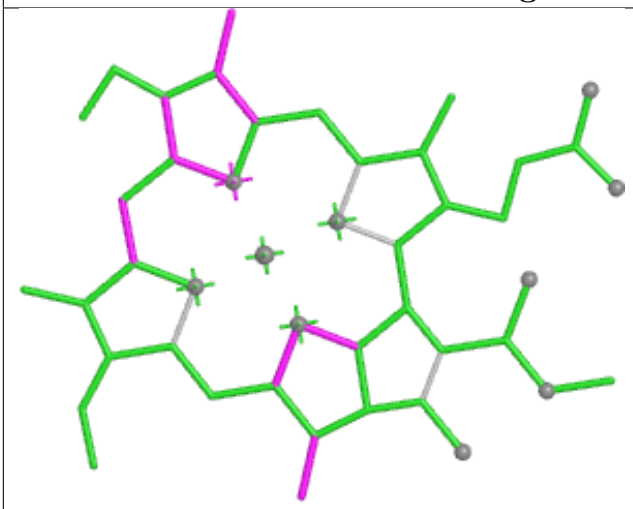


Torsions



Rings

Ligand CLA 15 305



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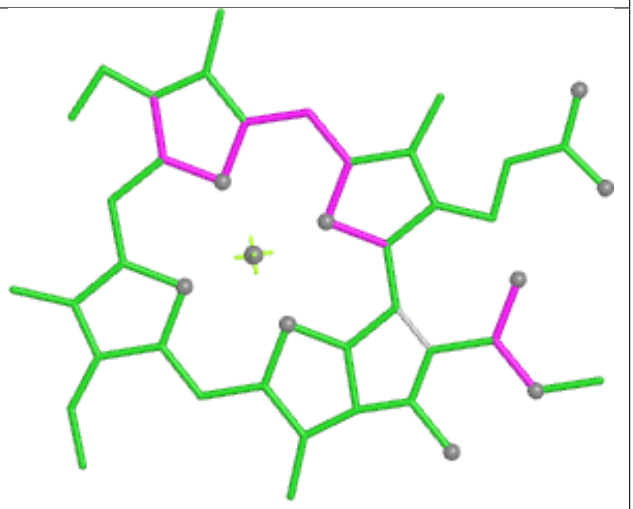

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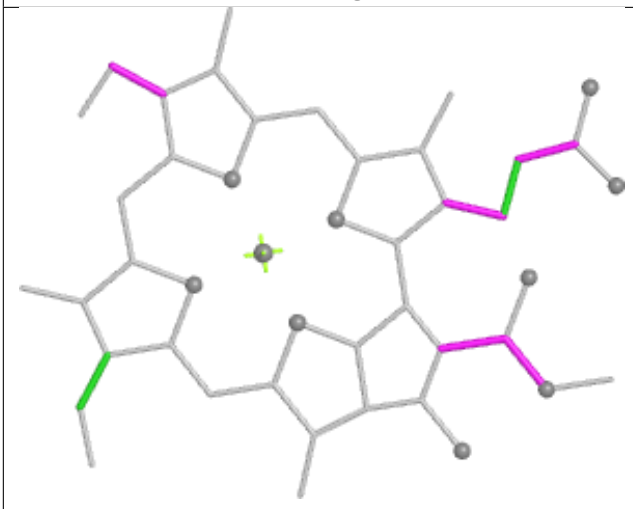
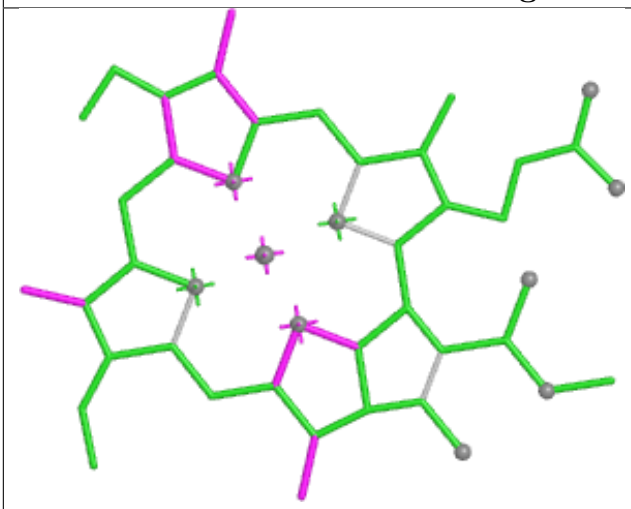


Torsions

Rings

Ligand CLA 14 310



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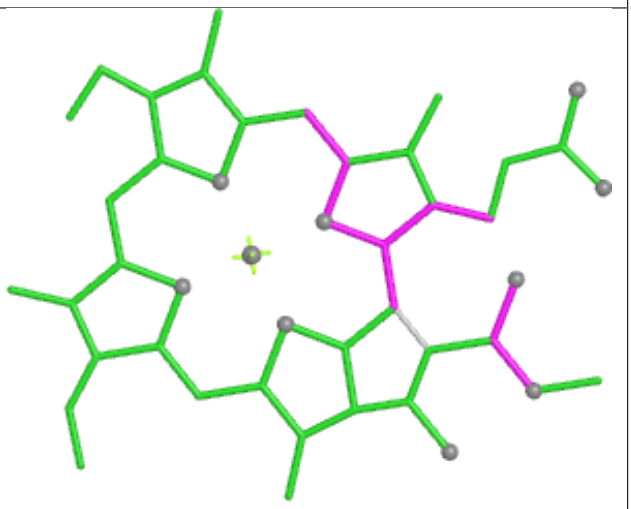

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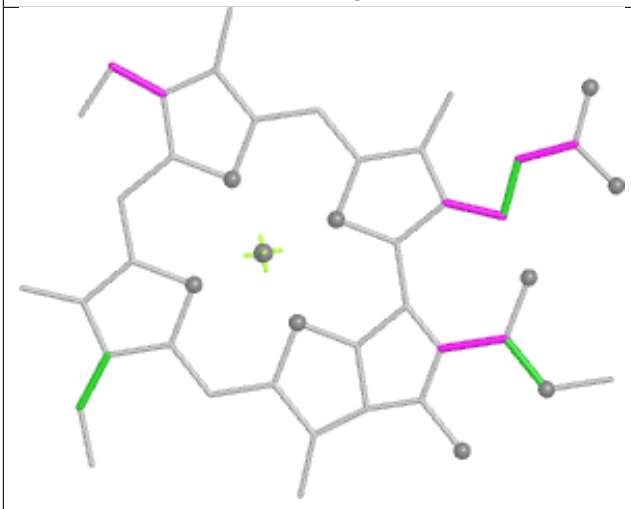
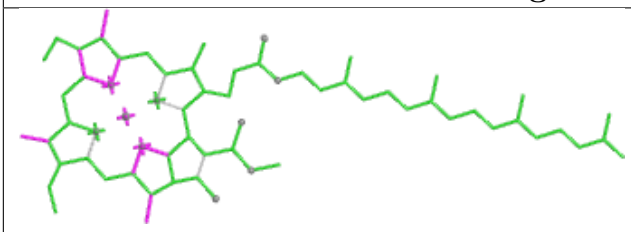


Torsions

Rings

Ligand CLA c 507



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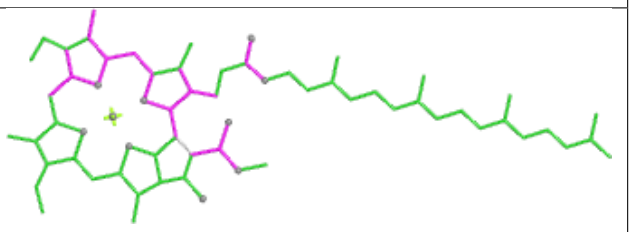

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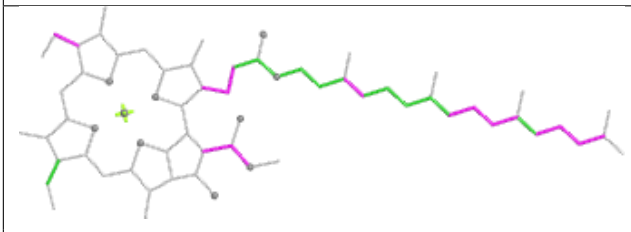

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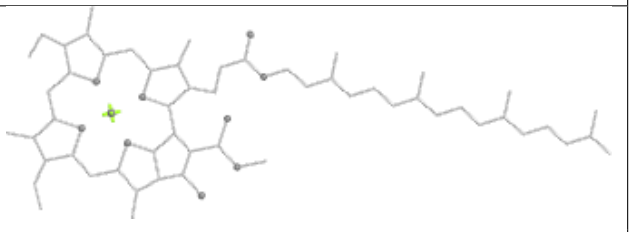
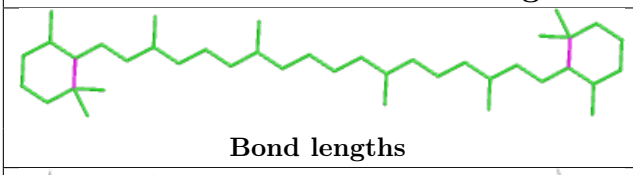


Rings

Ligand BCR A 409



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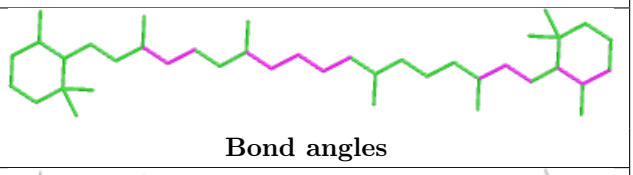
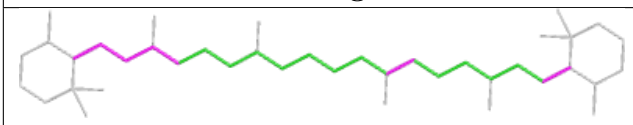


Bond angles



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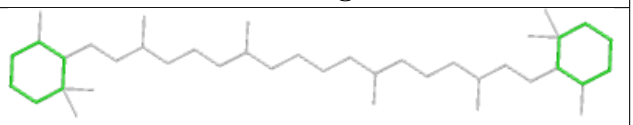
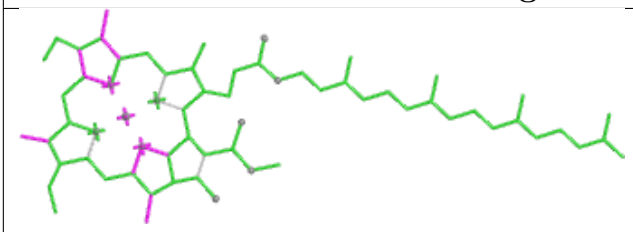


Rings

Ligand CLA 14 302



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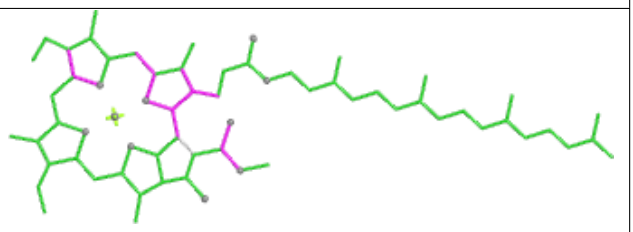

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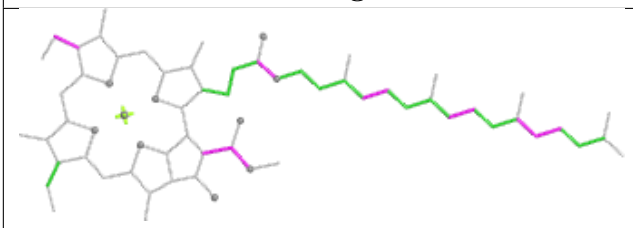

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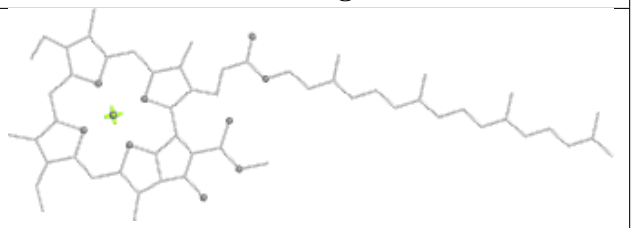
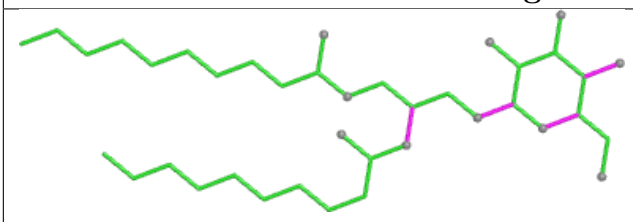


Rings

Ligand LMG 1 101



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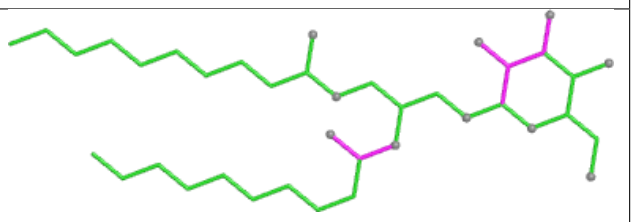

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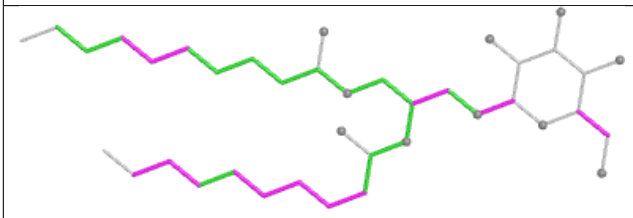

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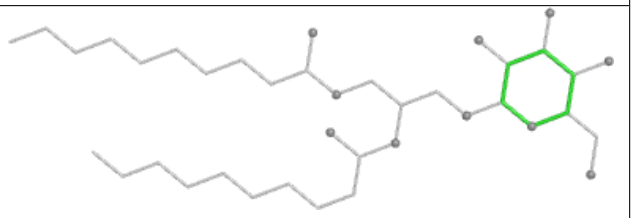
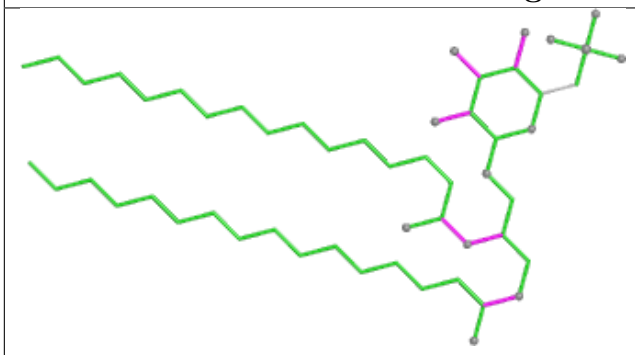


Rings

Ligand SQD A 406



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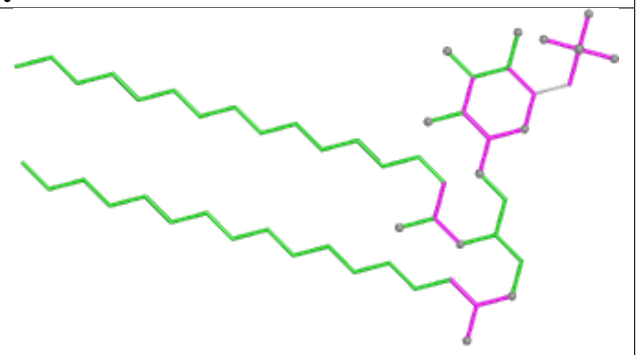

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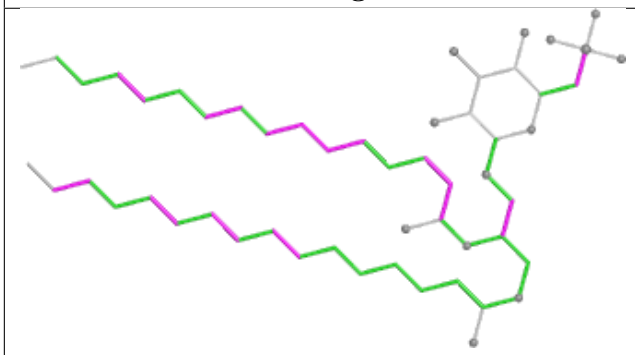

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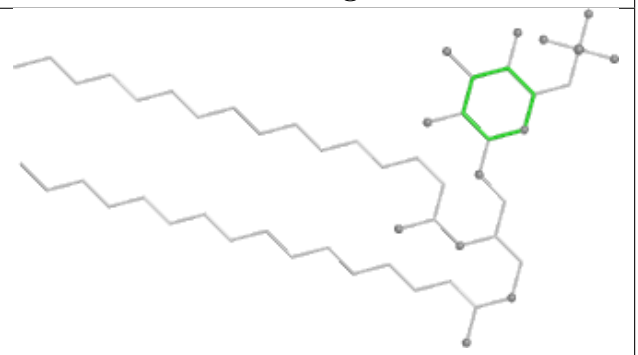
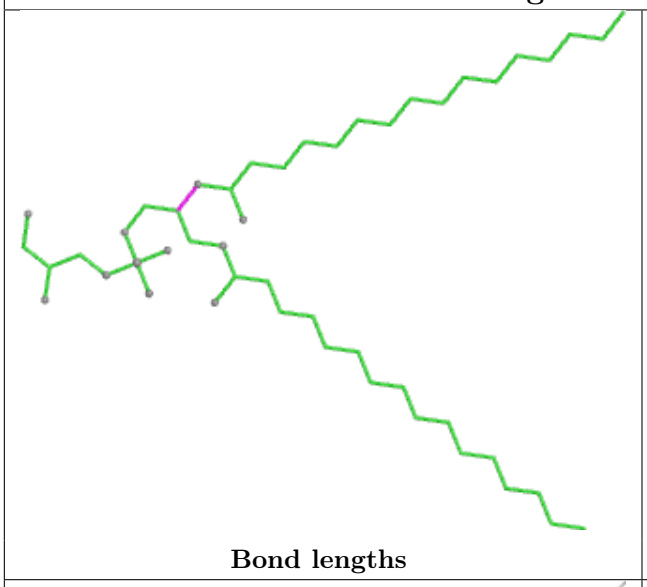


Rings

Ligand LHG d 409



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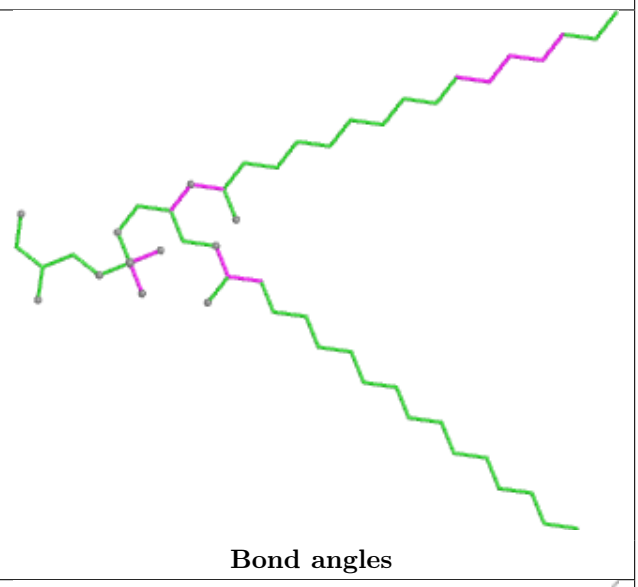

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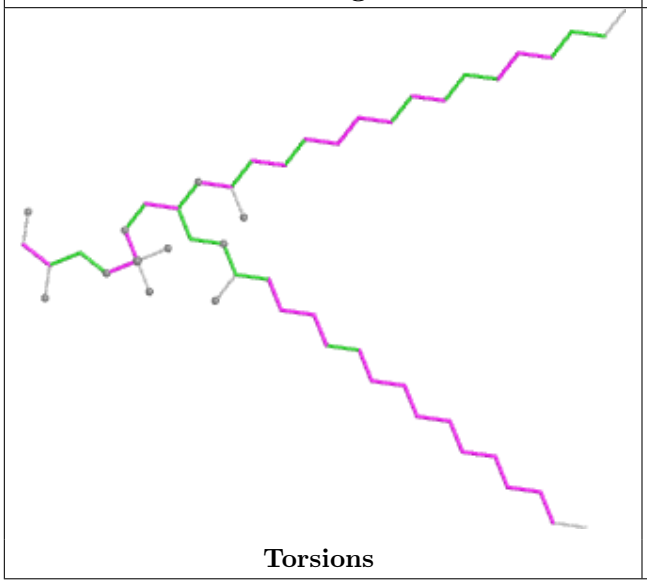

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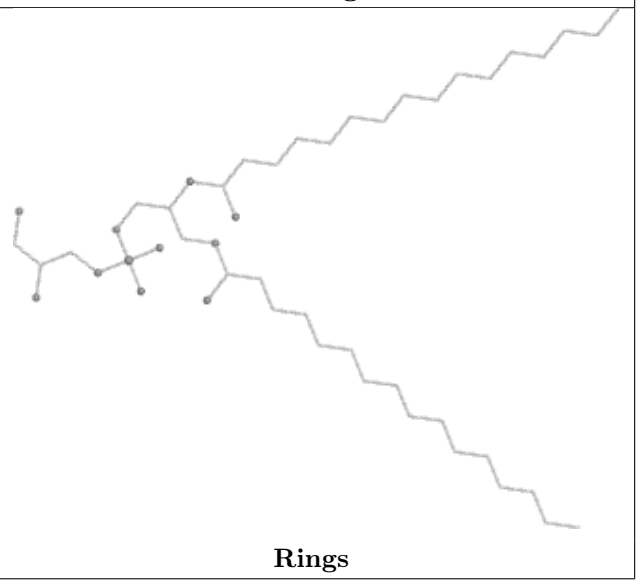
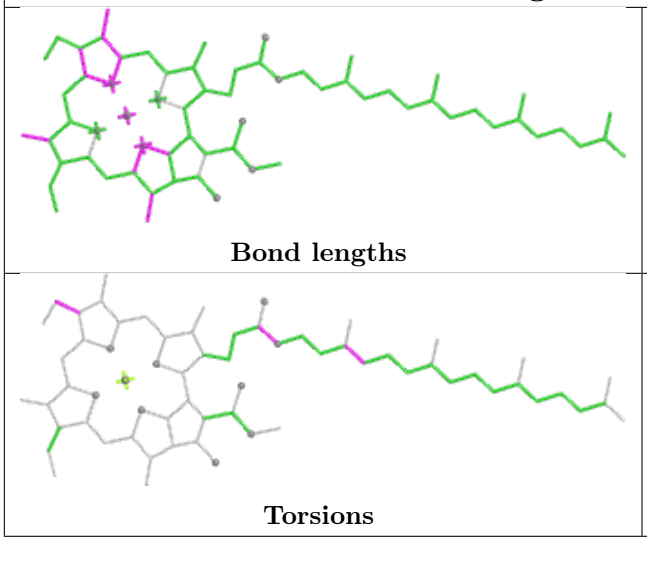


Rings

Ligand CLA d 407



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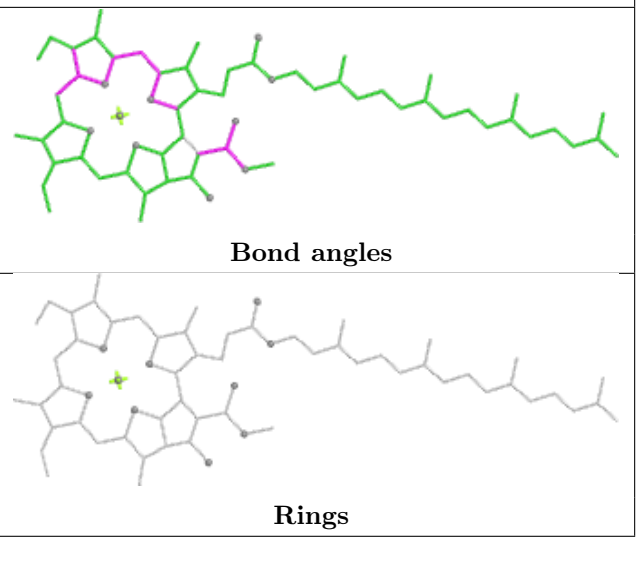
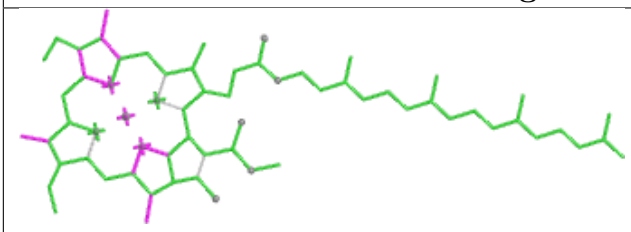


Bond angles

Torsions

Rings

Ligand CLA 20 204



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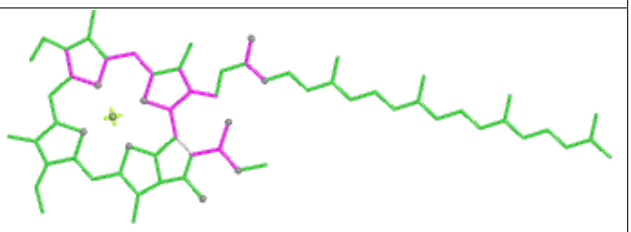
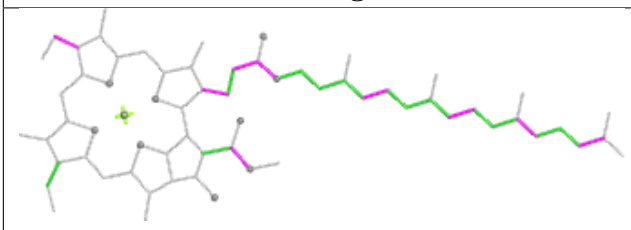


Bond angles



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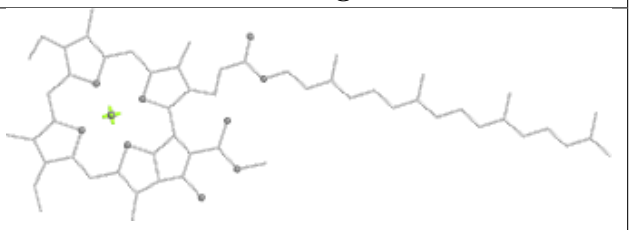
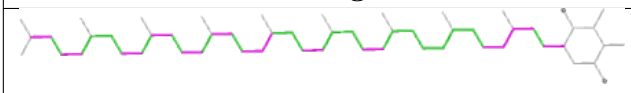


Rings

Ligand PL9 D 404

Bond lengths

Bond angles



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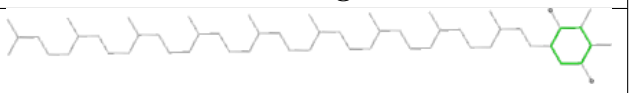
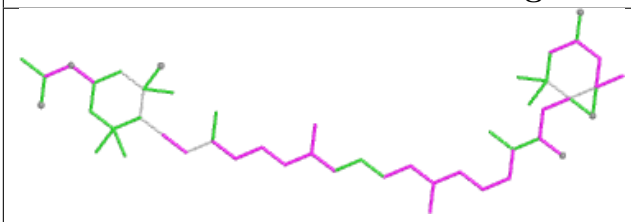


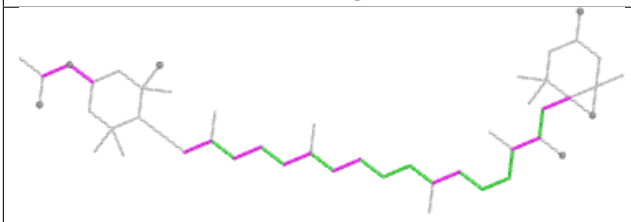
Rings

Ligand A86 21 313



Bond lengths

Bond angles



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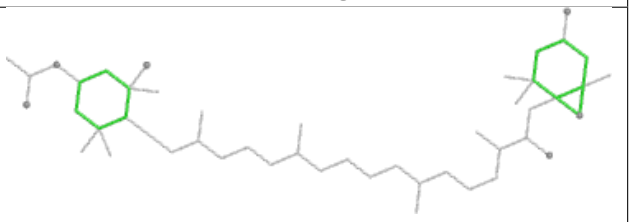
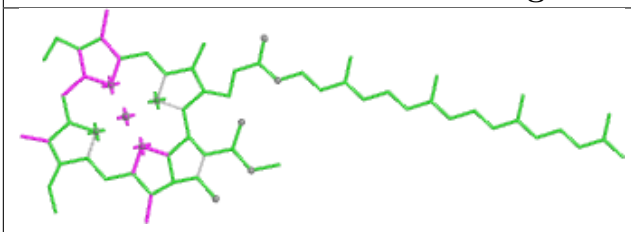


Rings

Ligand CLA b 614



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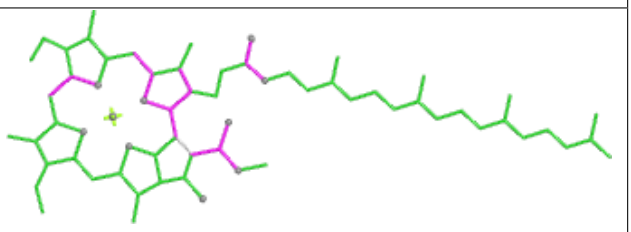
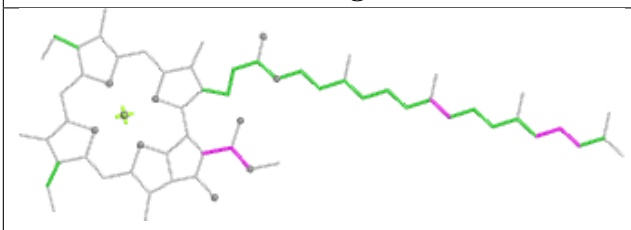


Bond angles



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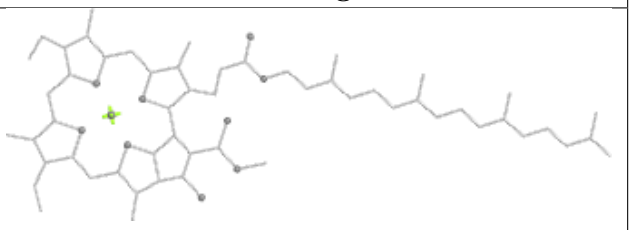
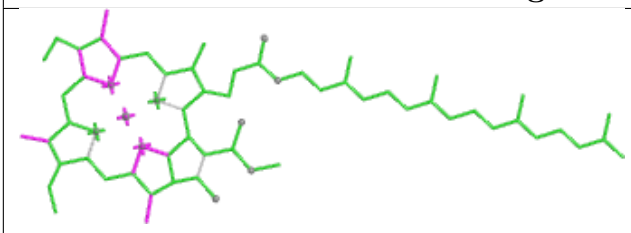


Rings

Ligand CLA b 601



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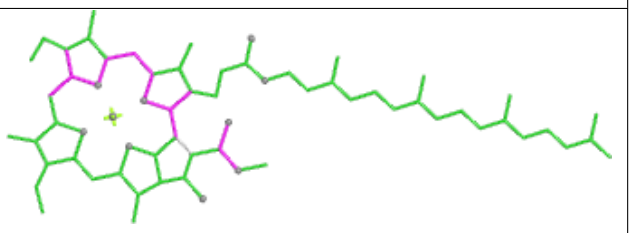
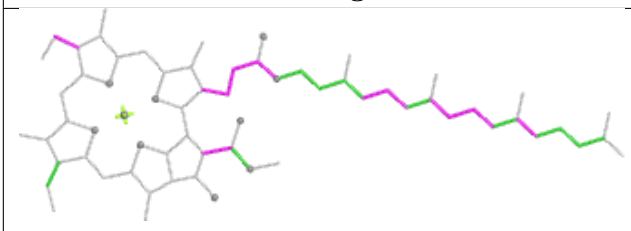


Bond angles



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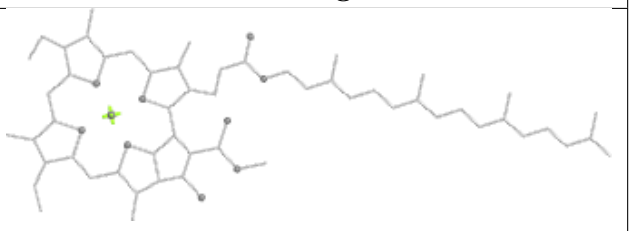
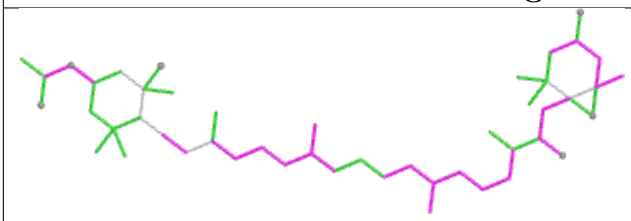


Rings

Ligand A86 12 318



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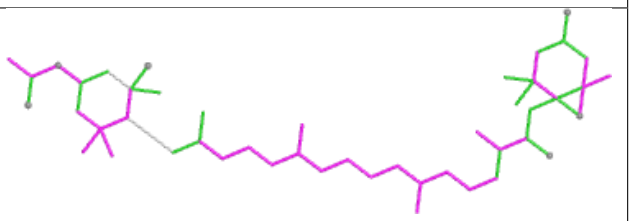
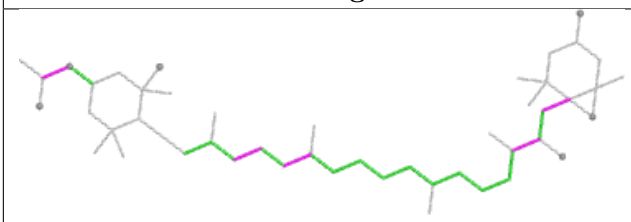
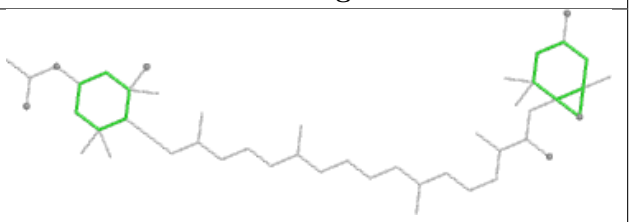


Bond angles

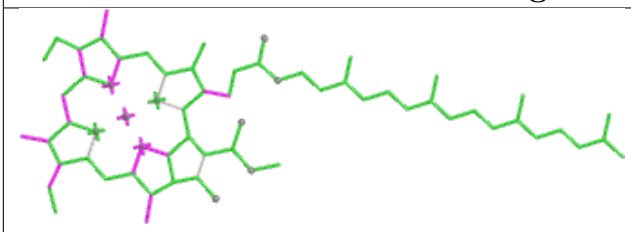


Torsions



Rings

Ligand CLA c 511



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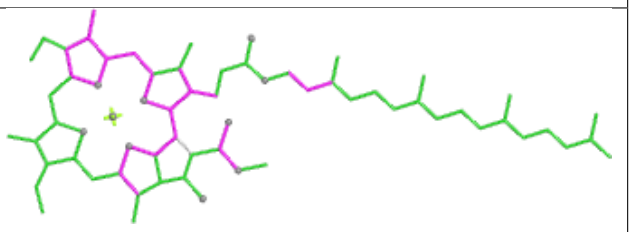
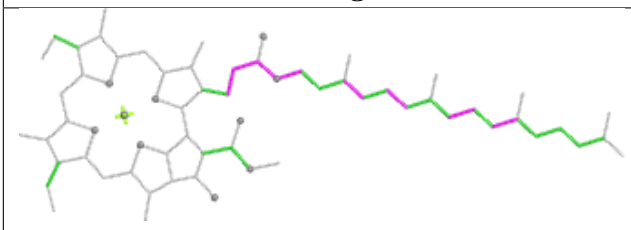


Bond angles



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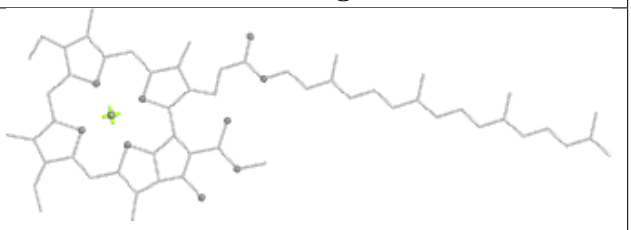
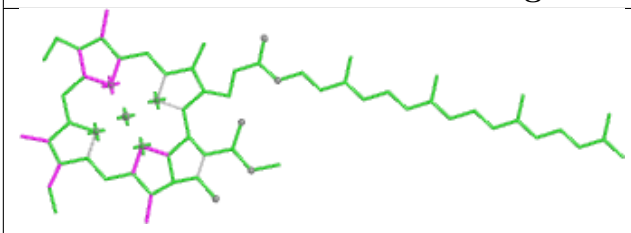


Rings

Ligand CLA B 605



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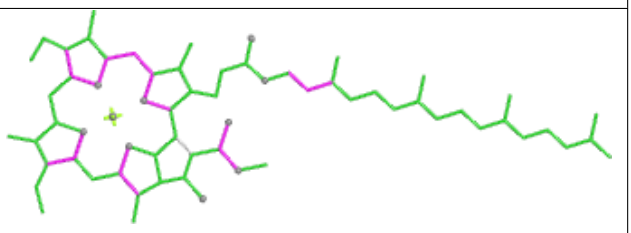

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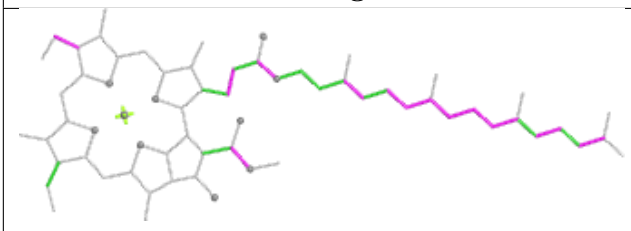

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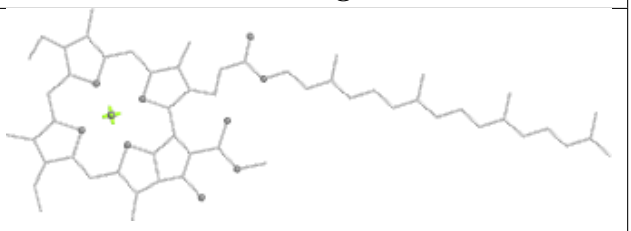
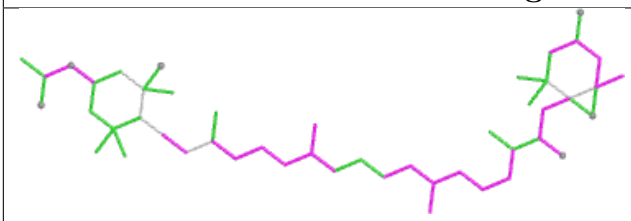


Rings

Ligand A86 15 311



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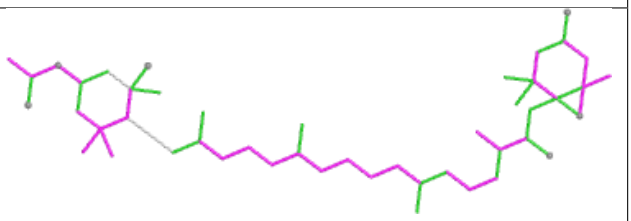

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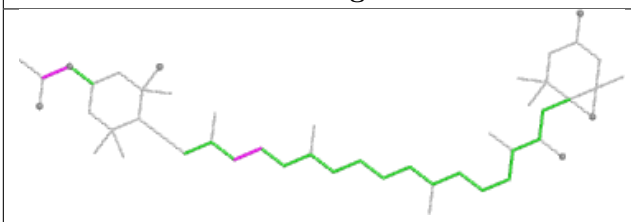

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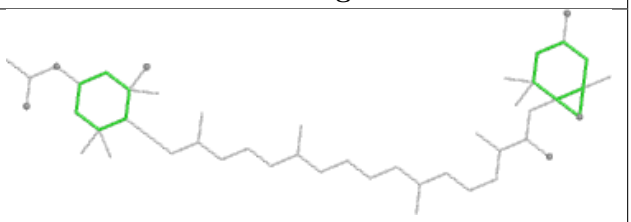
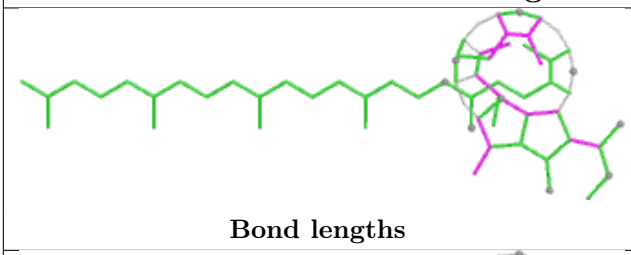


Rings

Ligand PHO d 404



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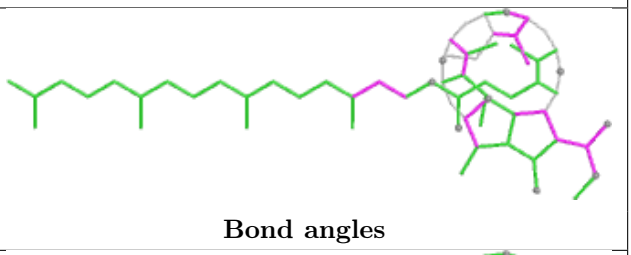

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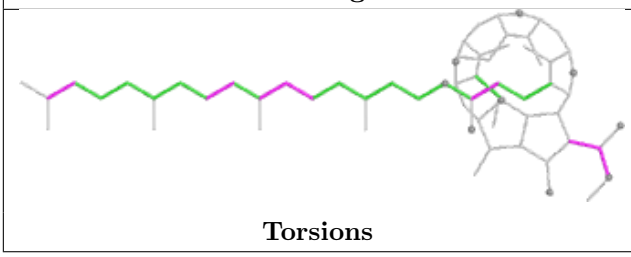

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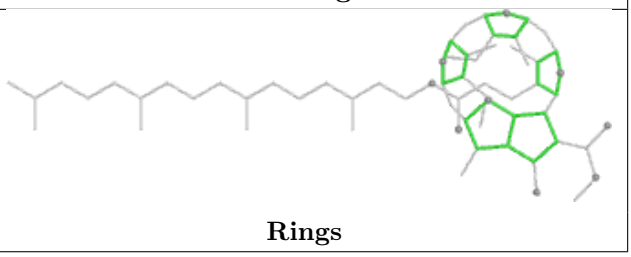

Rings

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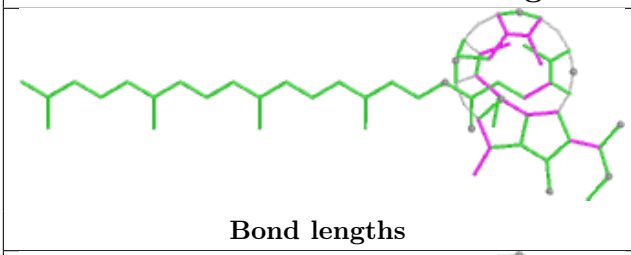

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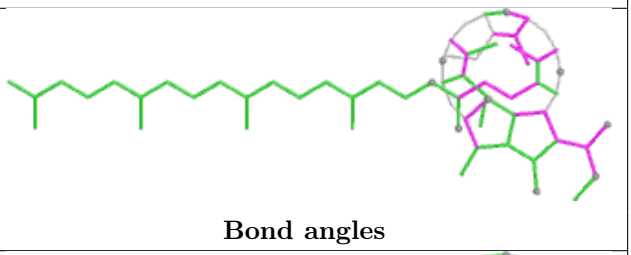

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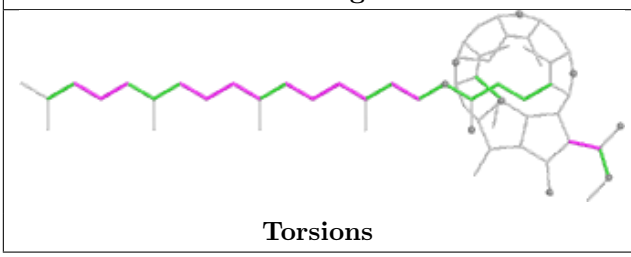
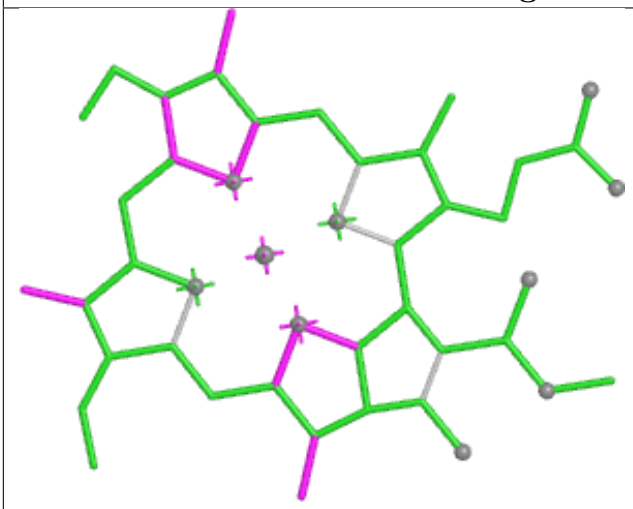


Torsions

Rings

Ligand CLA 11 304



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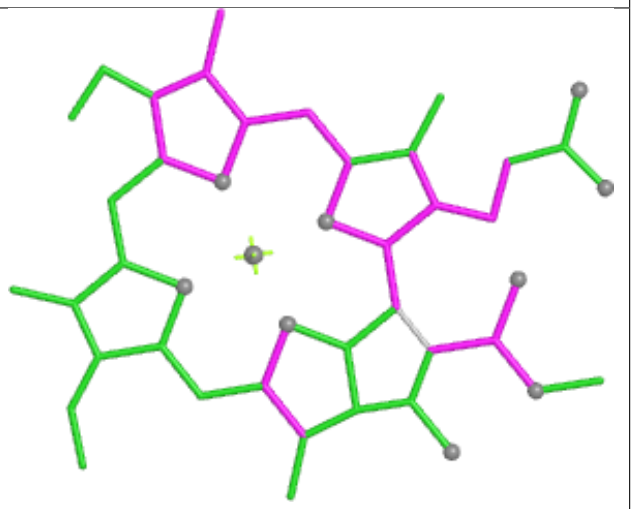

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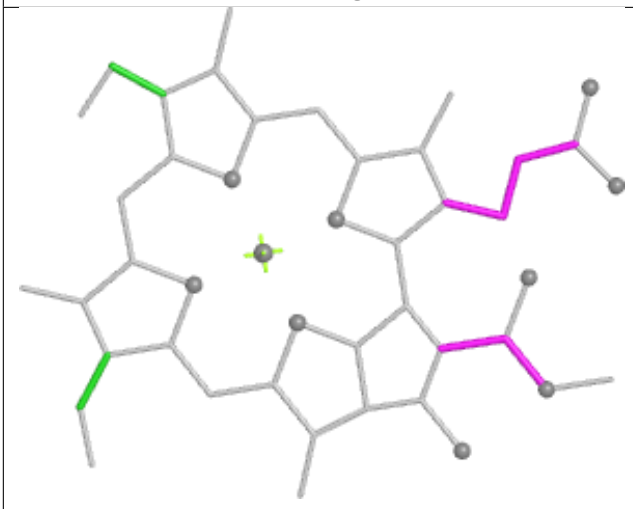
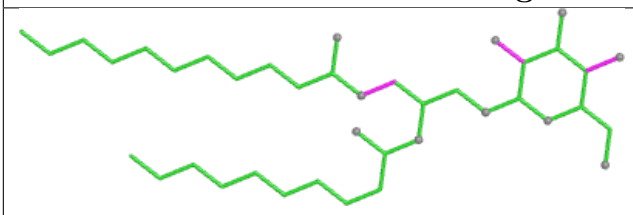


Torsions

Rings

Ligand LMG M 102



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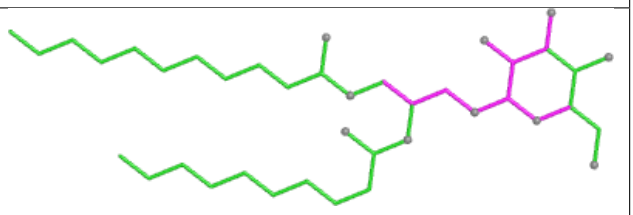

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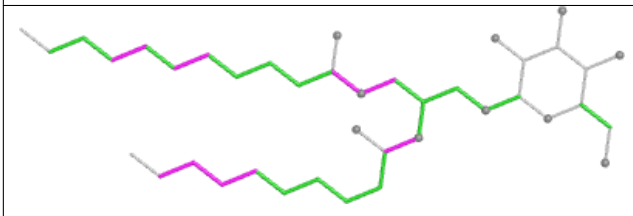

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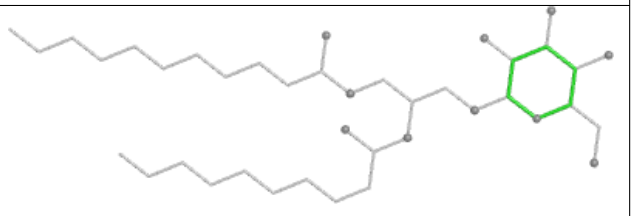
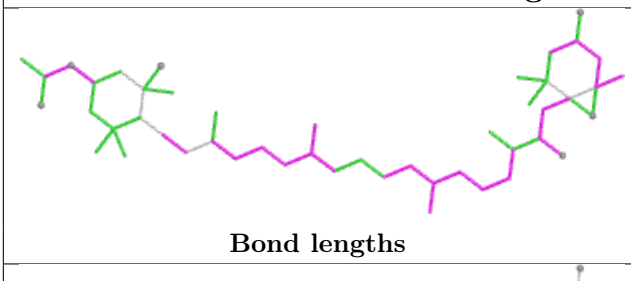


Rings

Ligand A86 14 313



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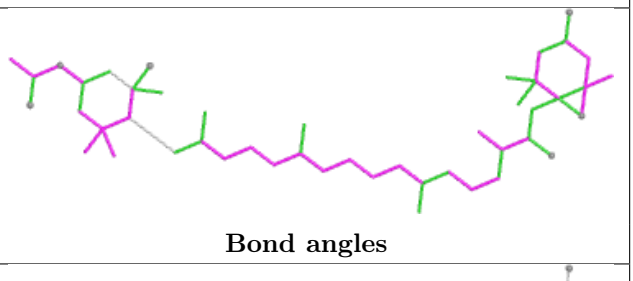

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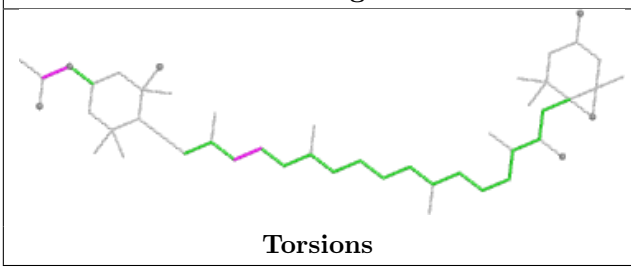

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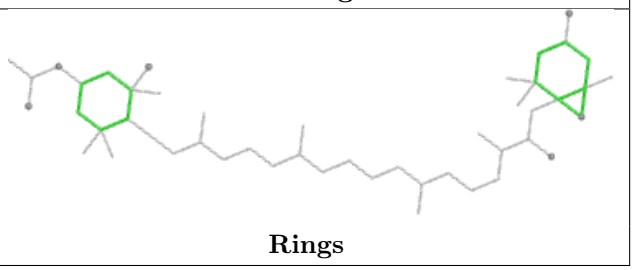
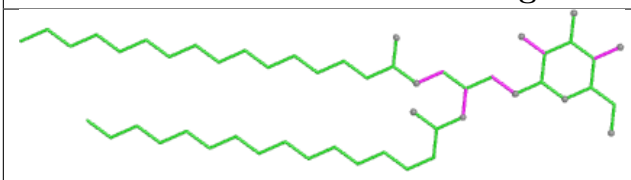


Rings

Ligand LMG Q 301



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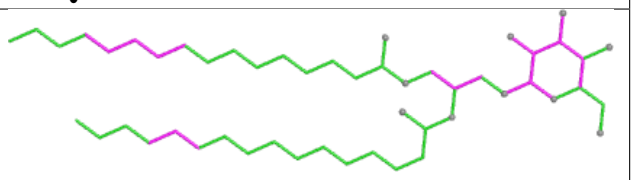

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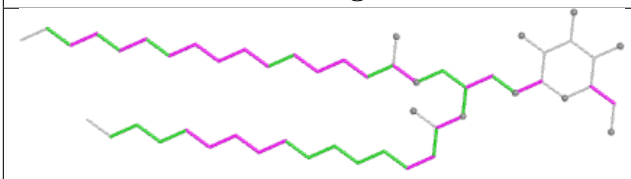

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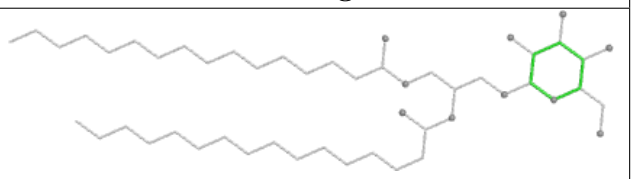
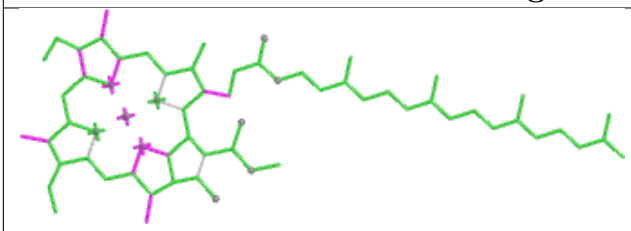


Rings

Ligand CLA b 613



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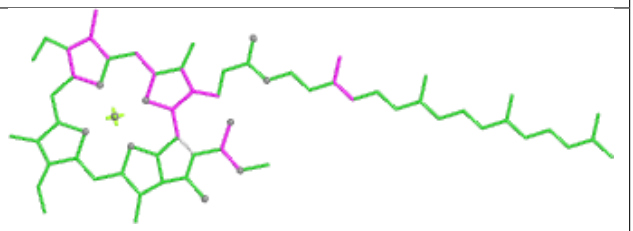

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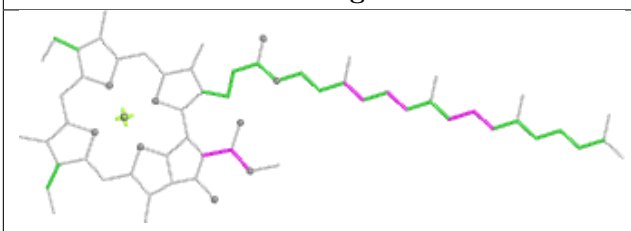

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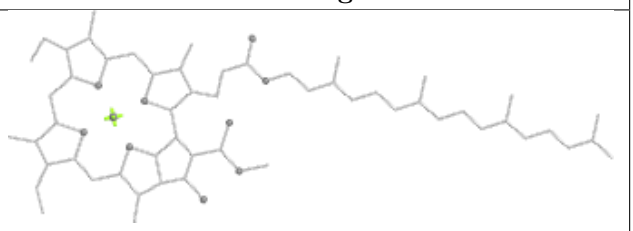
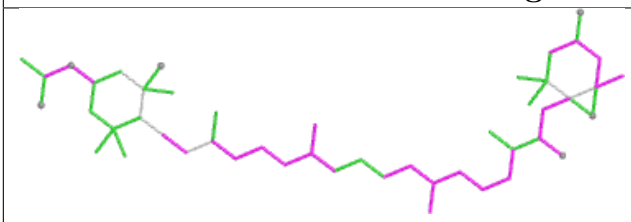


Rings

Ligand A86 19 310



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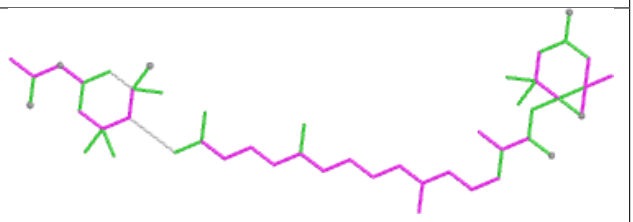

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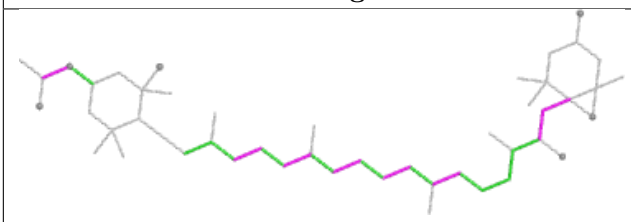

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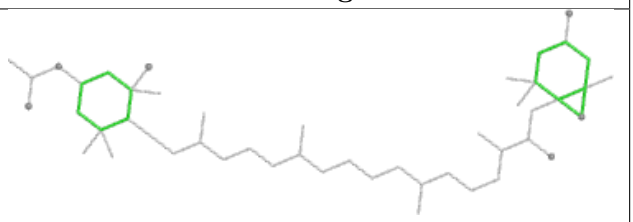
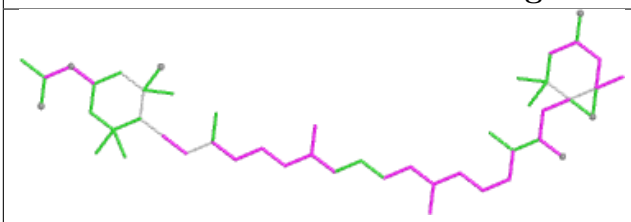


Rings

Ligand A86 13 315



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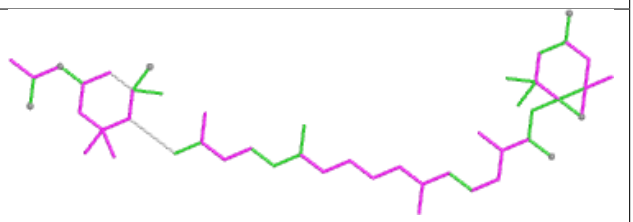

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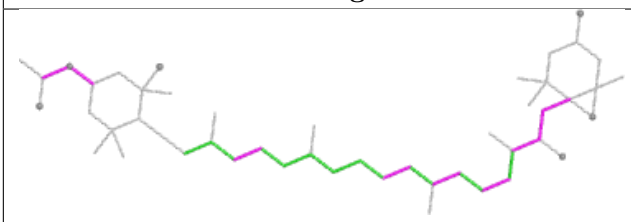

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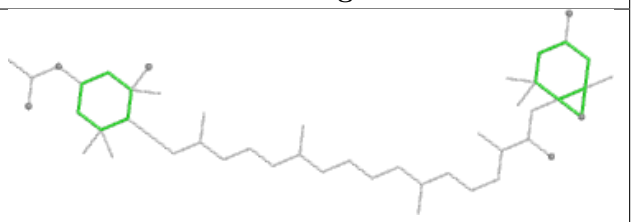
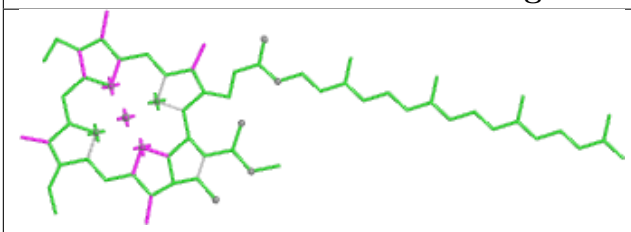


Rings

Ligand CLA C 510



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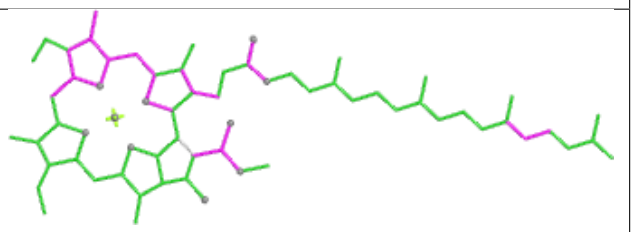
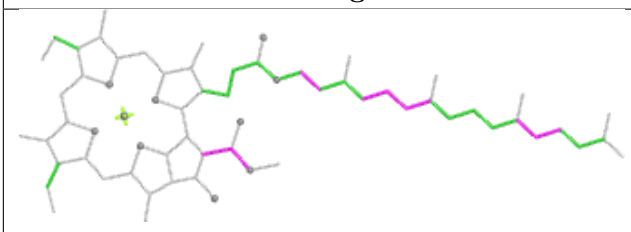


Bond angles



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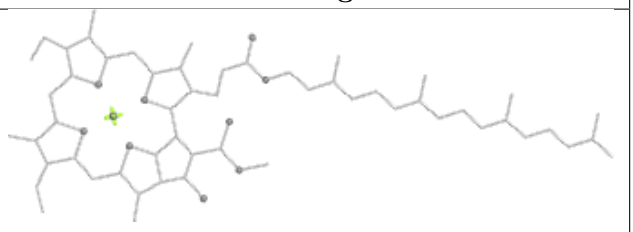
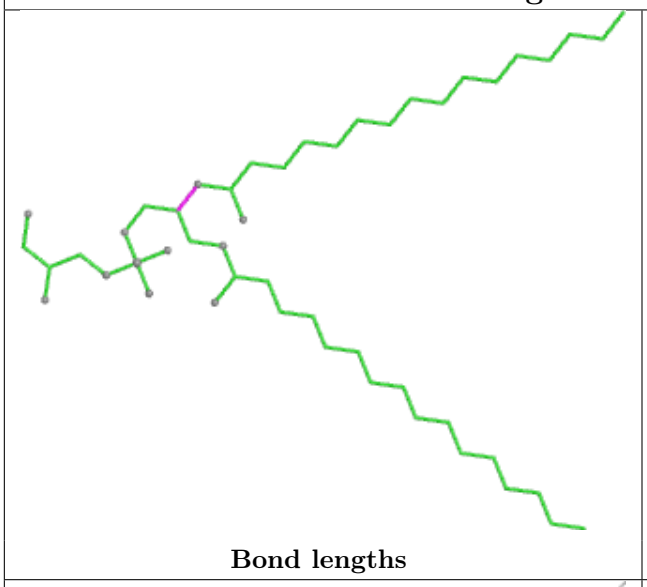


Rings

Ligand LHG L 101



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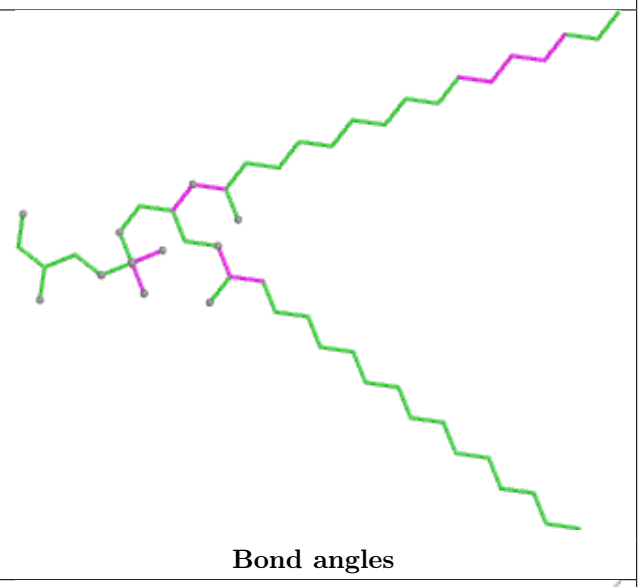
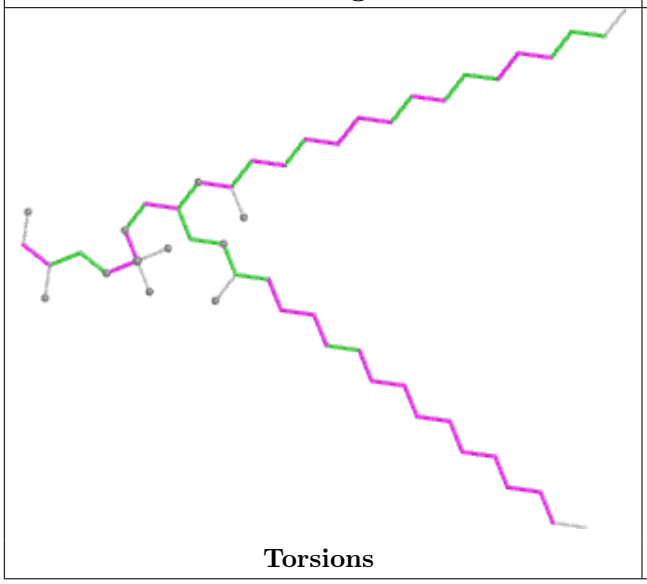


Bond angles



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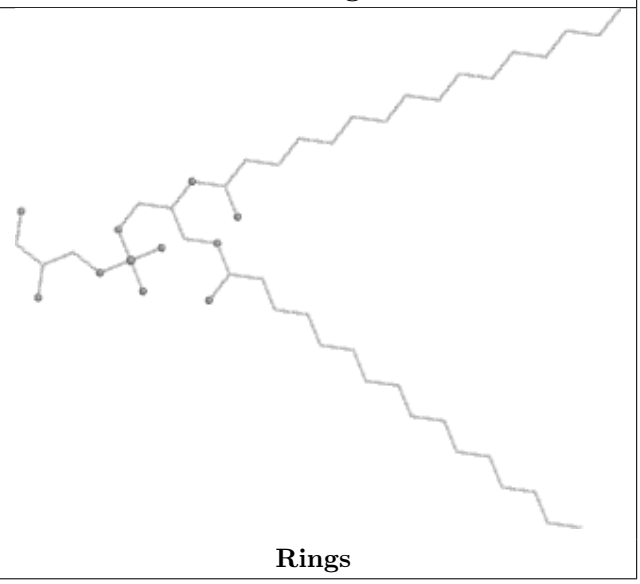
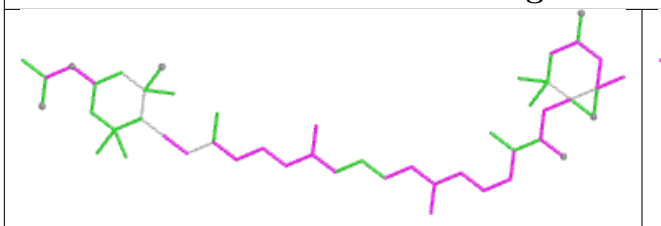


Rings

Ligand A86 11 313



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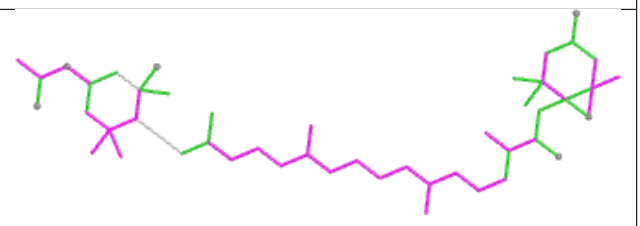

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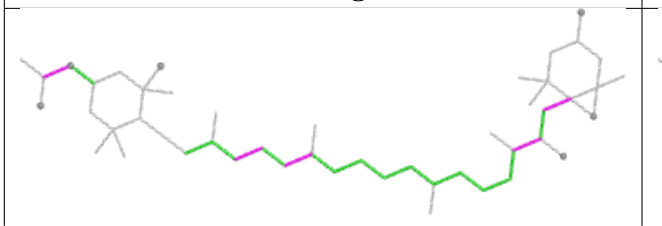

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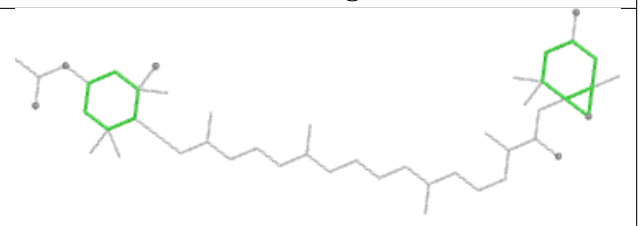
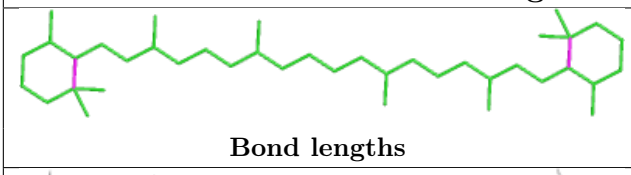


Rings

Ligand BCR a 408



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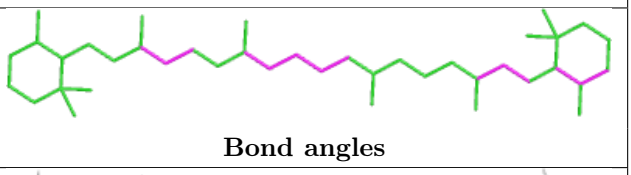

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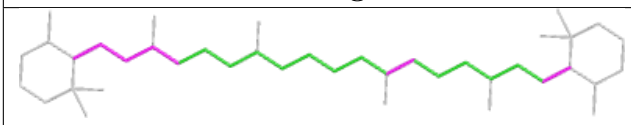

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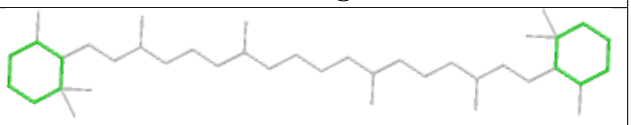
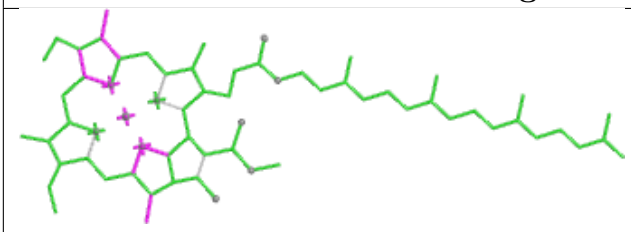


Rings

Ligand CLA 18 310



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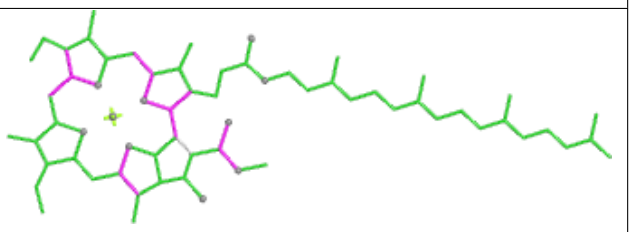

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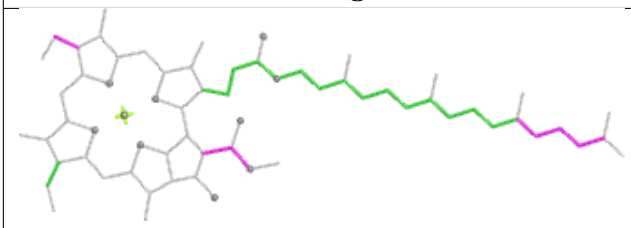

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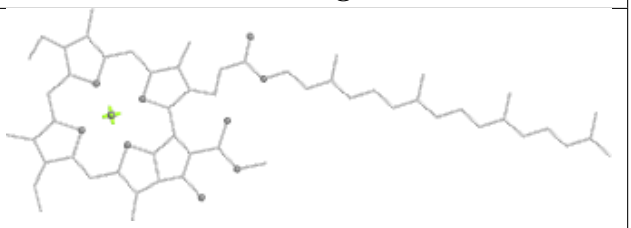
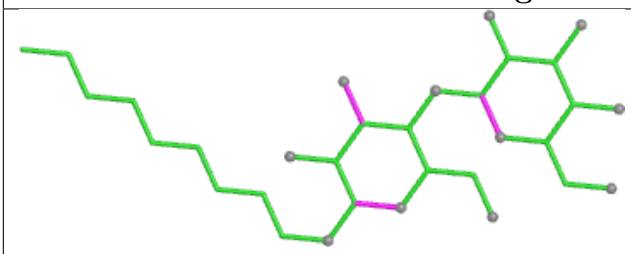


Rings

Ligand LMU 12 302



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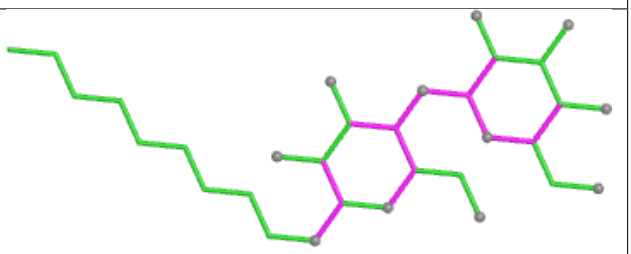

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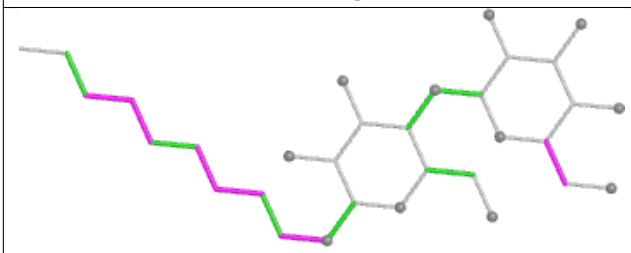

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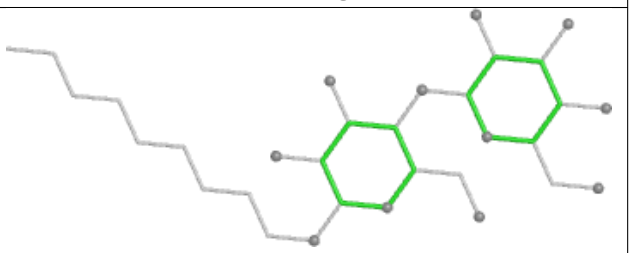

Rings

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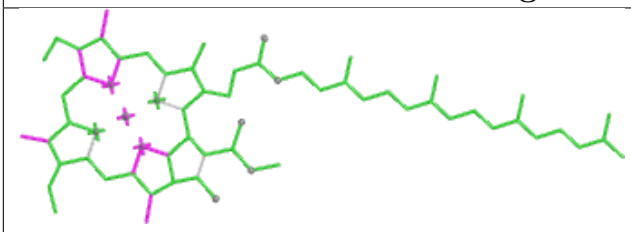

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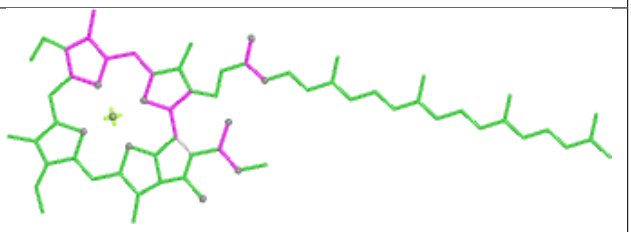

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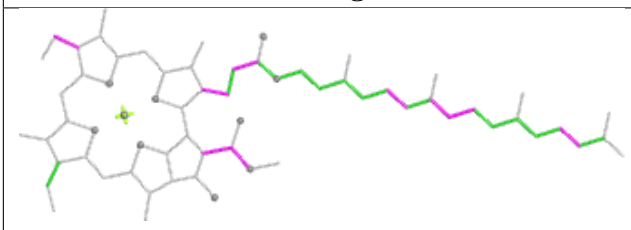

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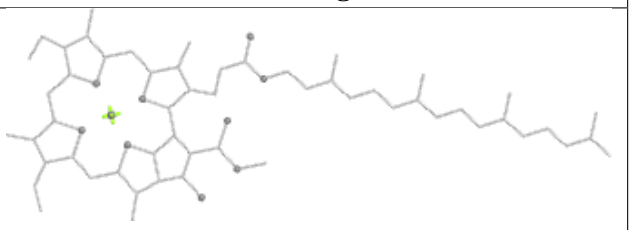

Rings

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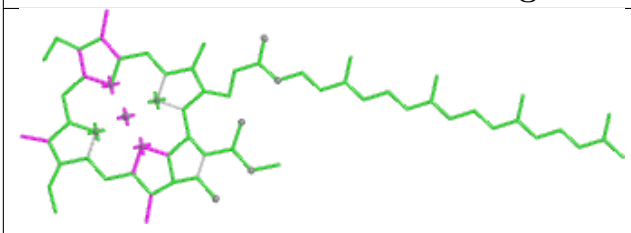

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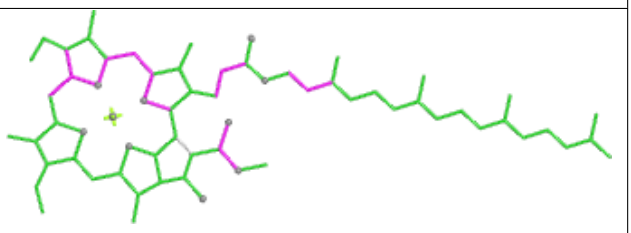

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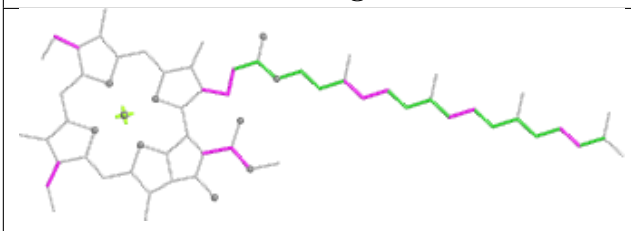

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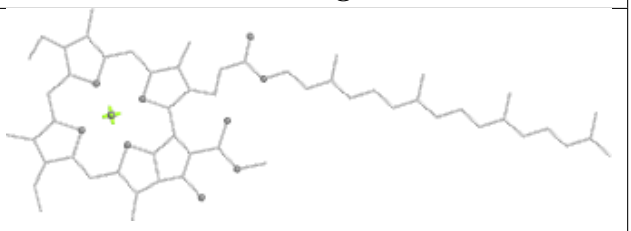

Rings

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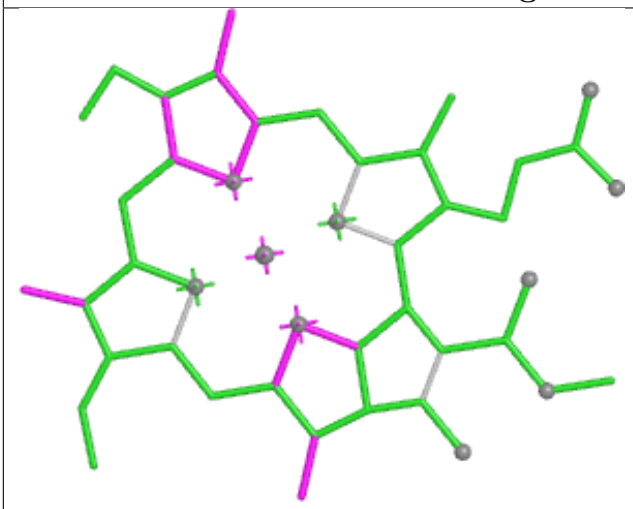

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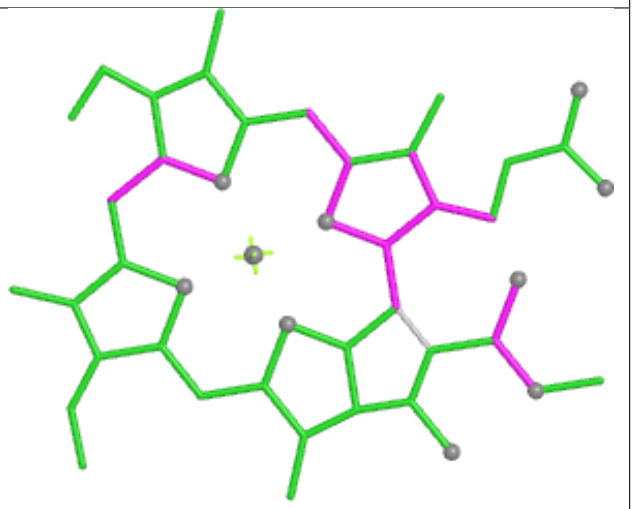

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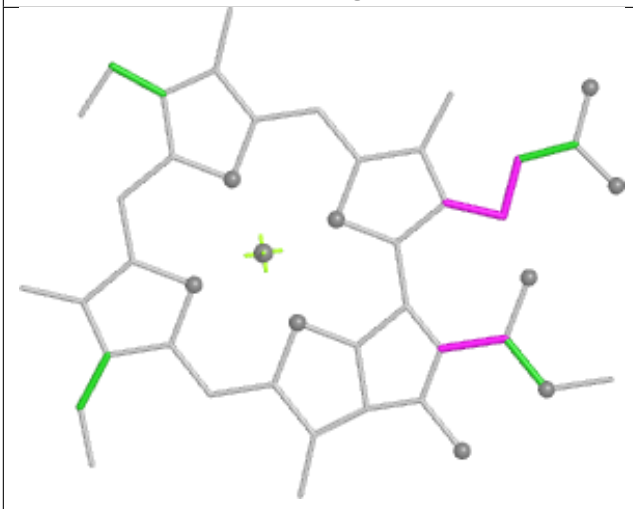

Torsions

Rings

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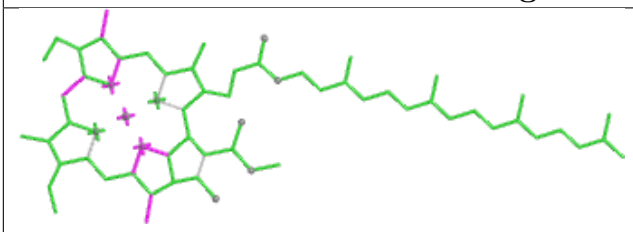

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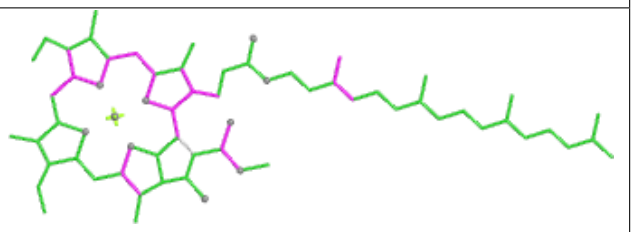

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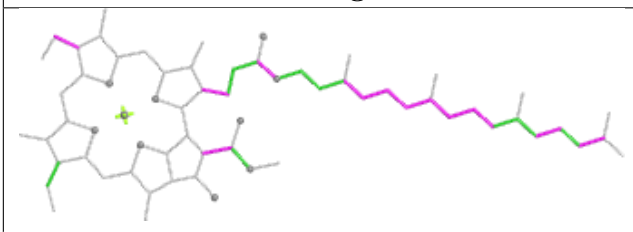

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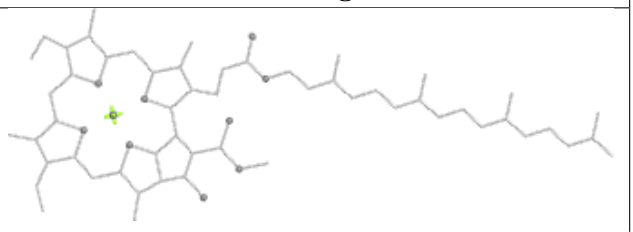
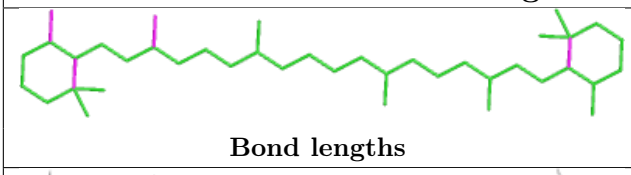


Rings

Ligand BCR Y 101



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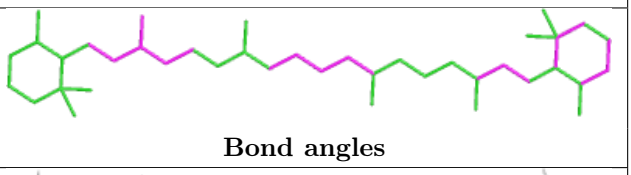

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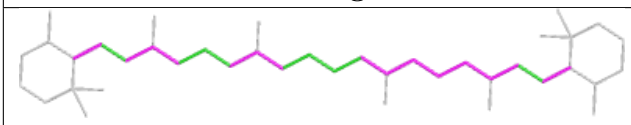

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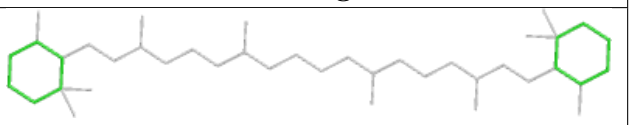

Rings

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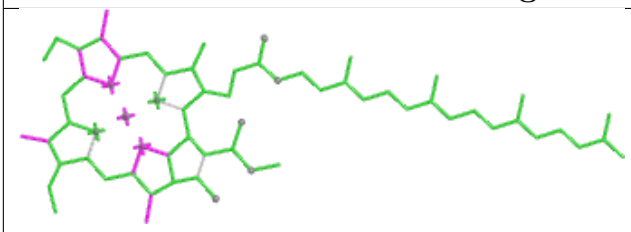

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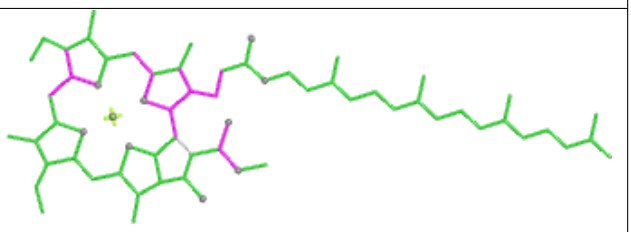

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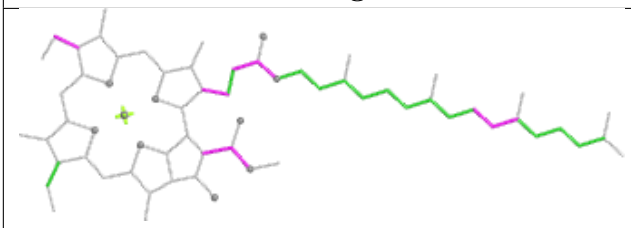

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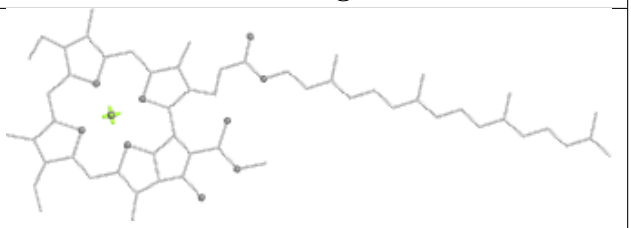
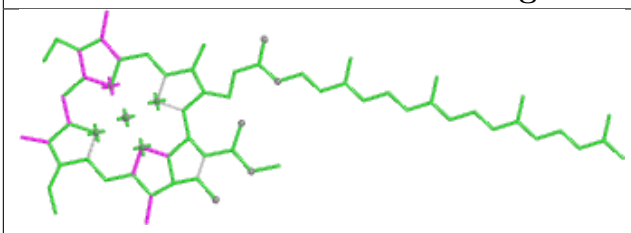


Rings

Ligand CLA 21 301



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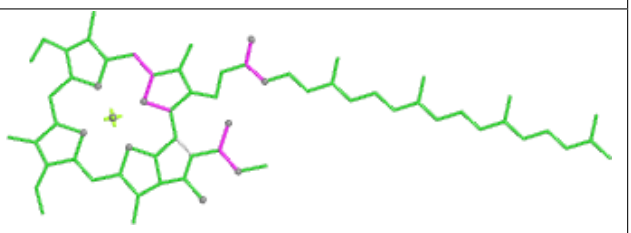

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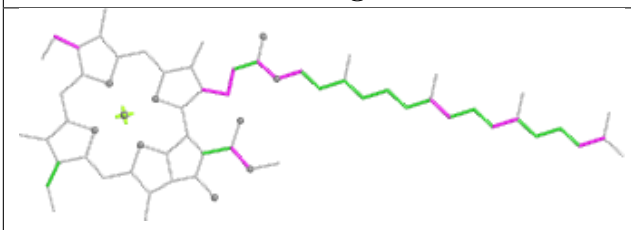

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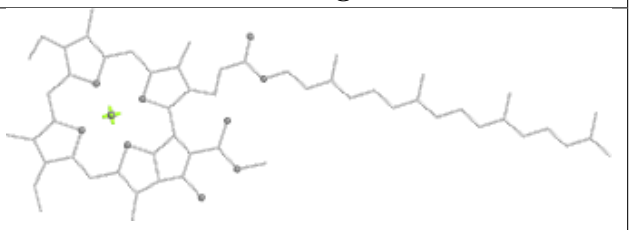
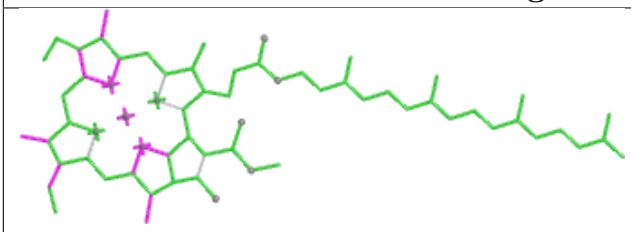


Rings

Ligand CLA b 610



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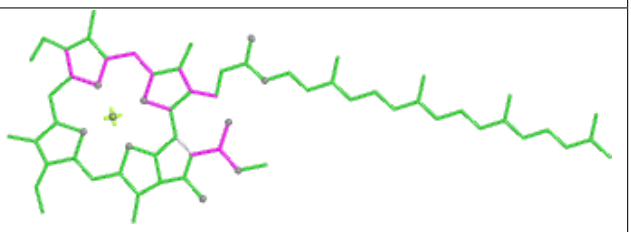
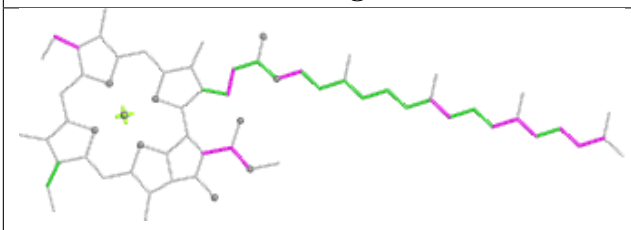


Bond angles



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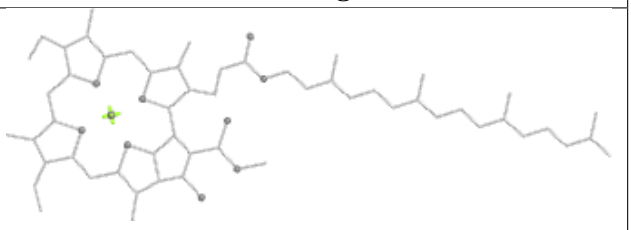
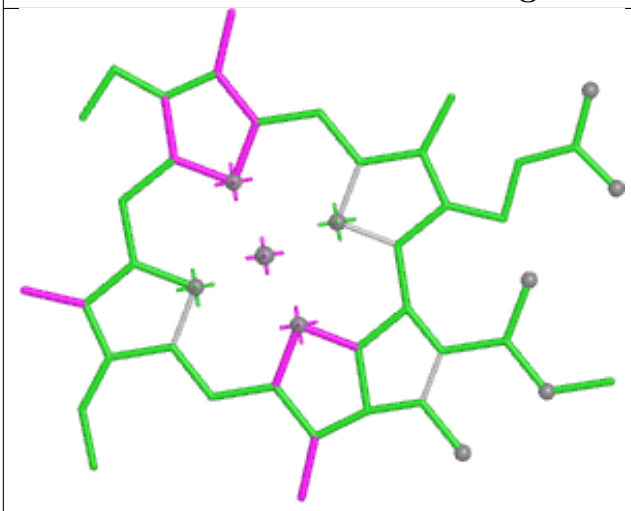


Rings

Ligand CLA 13 309



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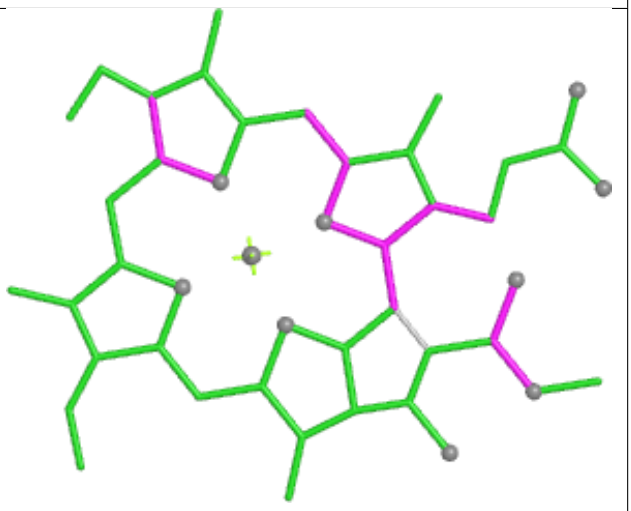
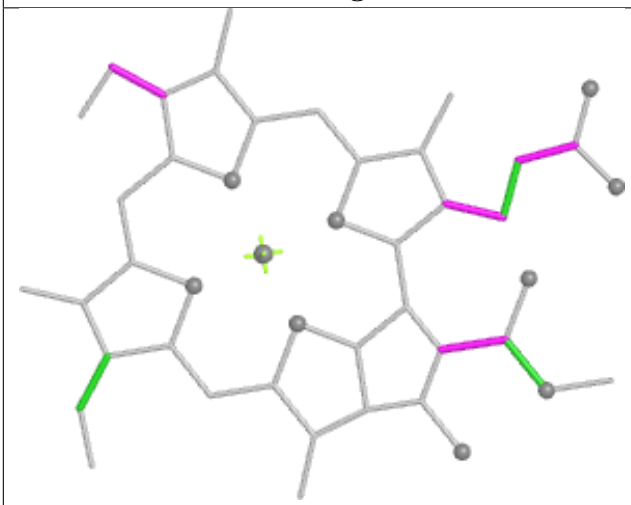


Bond angles



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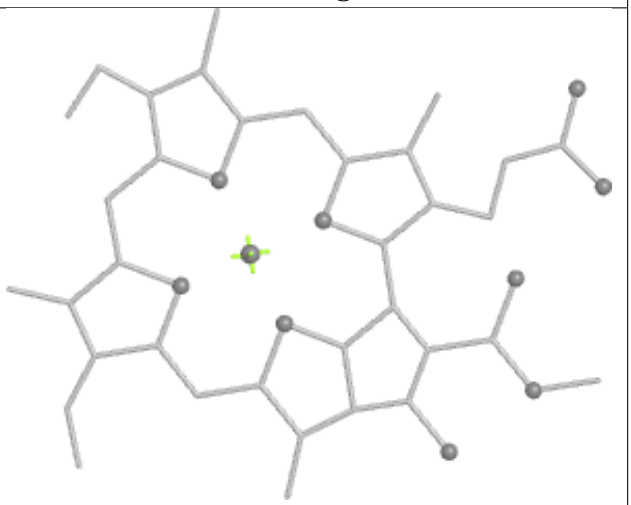

Rings

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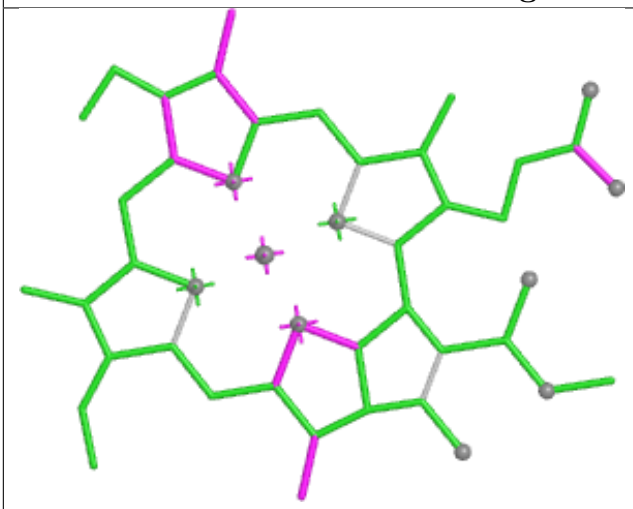

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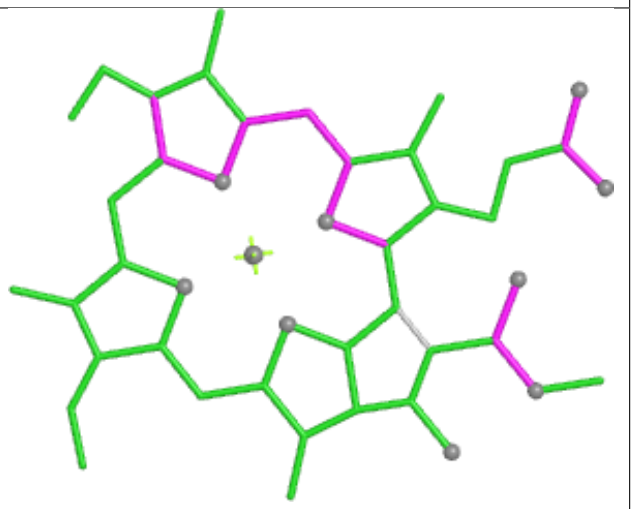
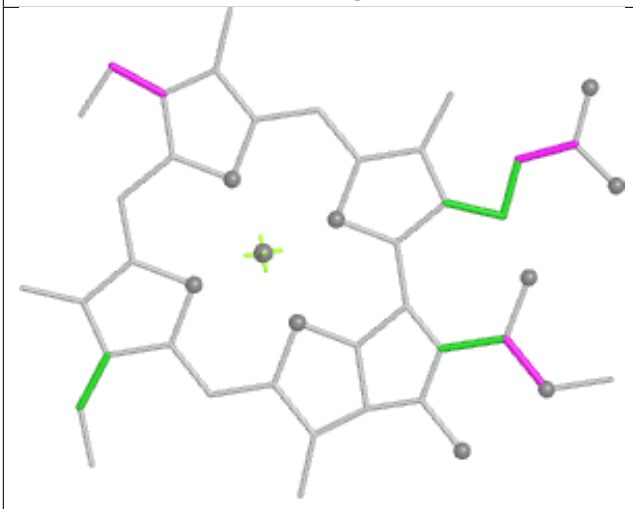


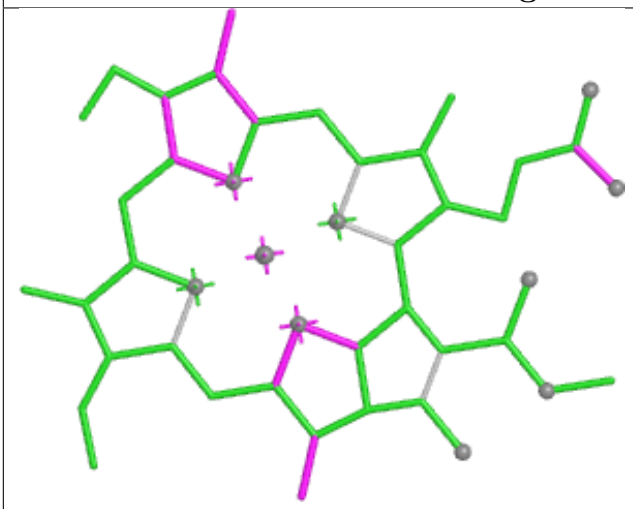
Bond angles



Torsions

Rings

Ligand CLA 15 309



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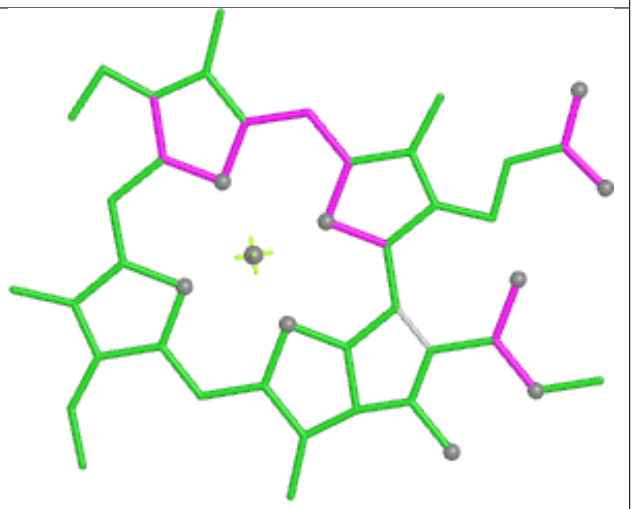
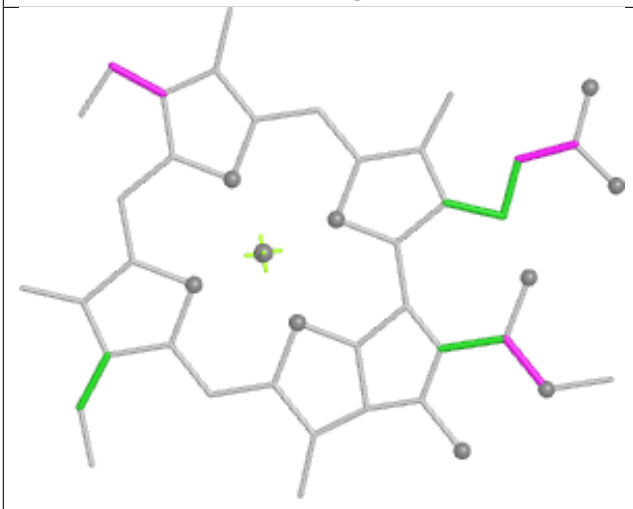


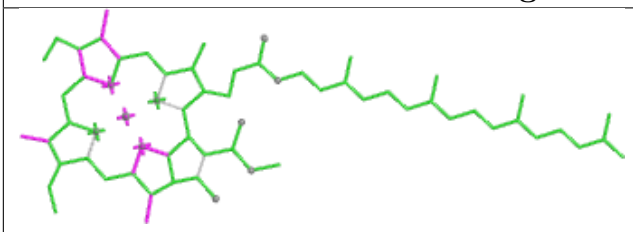
Bond angles



Torsions

Rings

Ligand CLA 18 303



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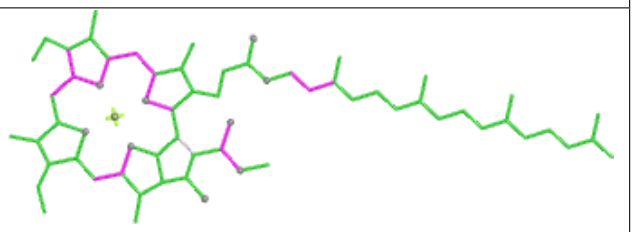

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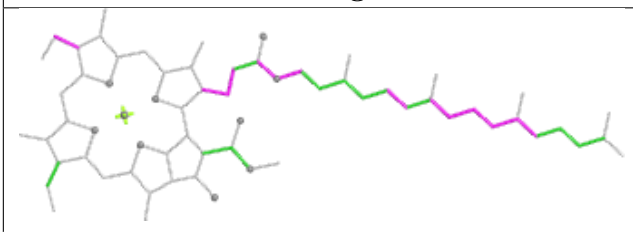

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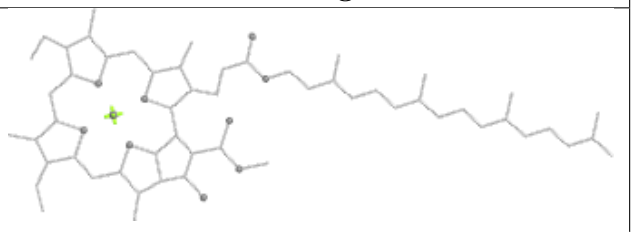
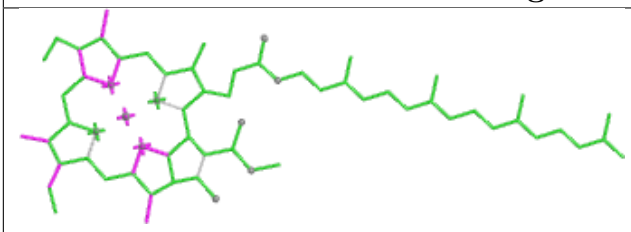


Rings

Ligand CLA b 615



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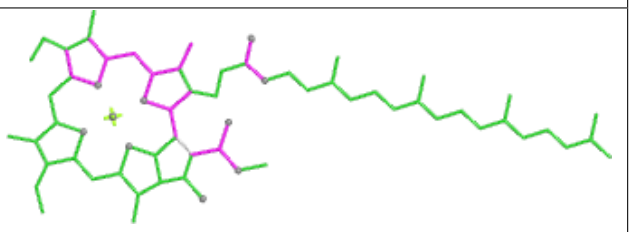

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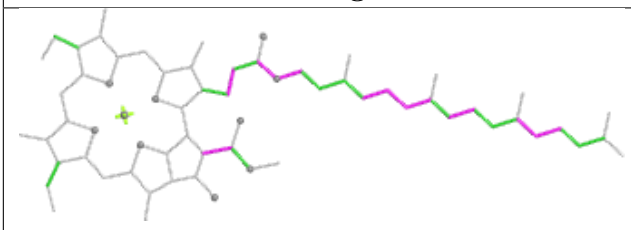

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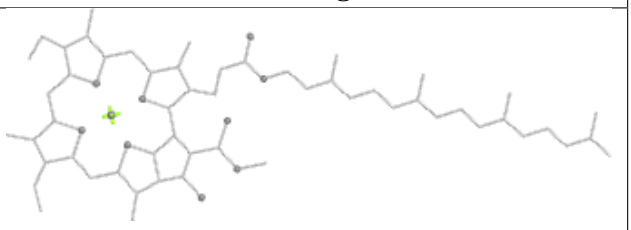
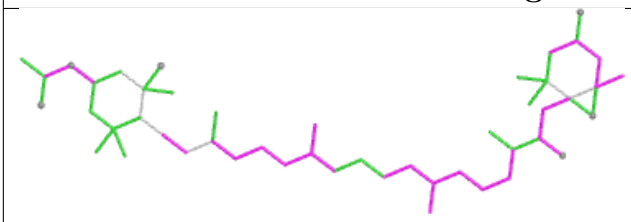


Rings

Ligand A86 13 301



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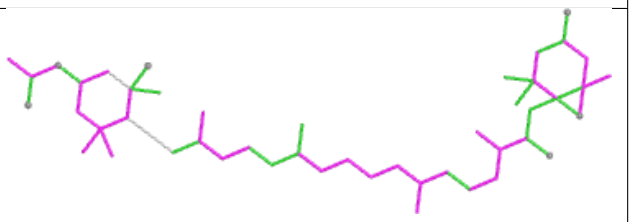

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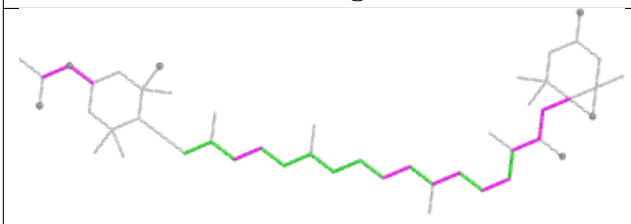

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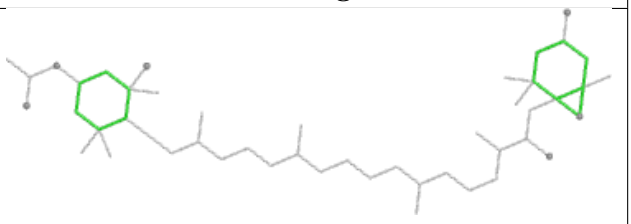
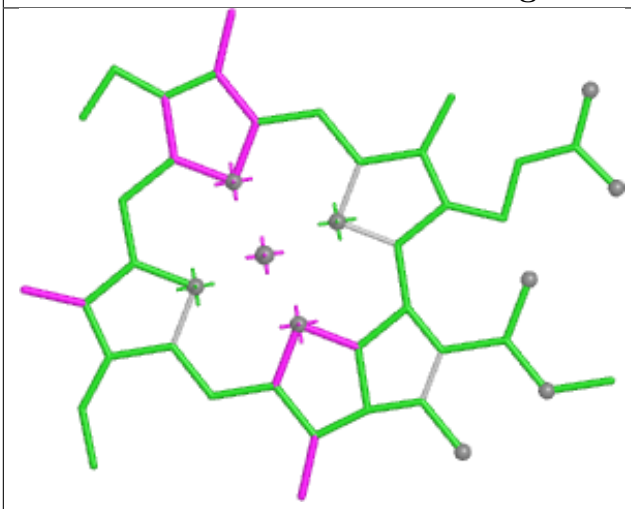


Rings

Ligand CLA 14 304



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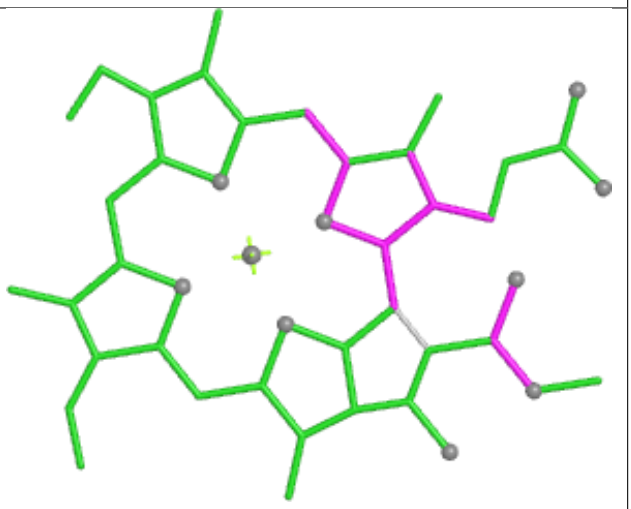

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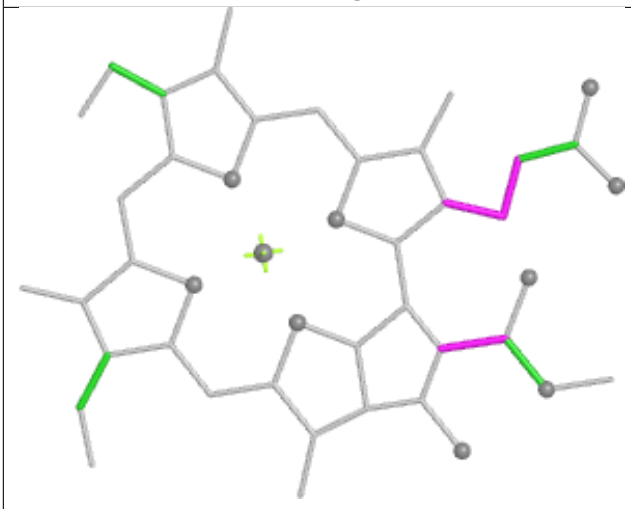
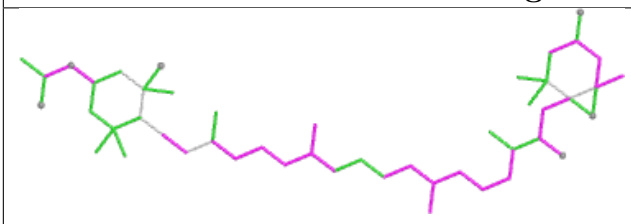


Torsions

Rings

Ligand A86 13 312



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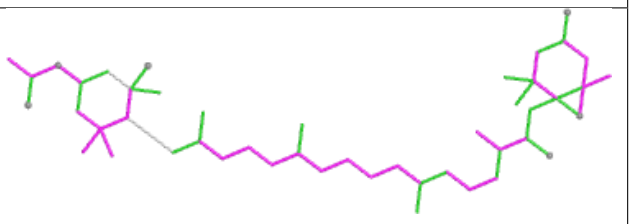

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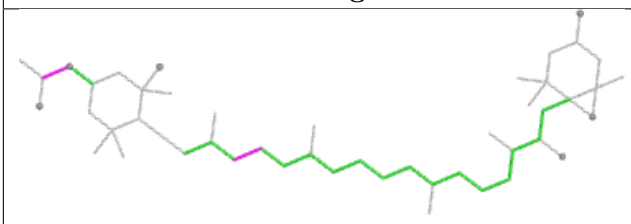

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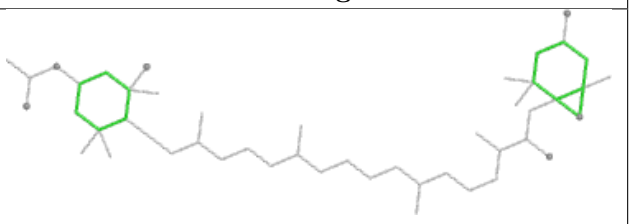
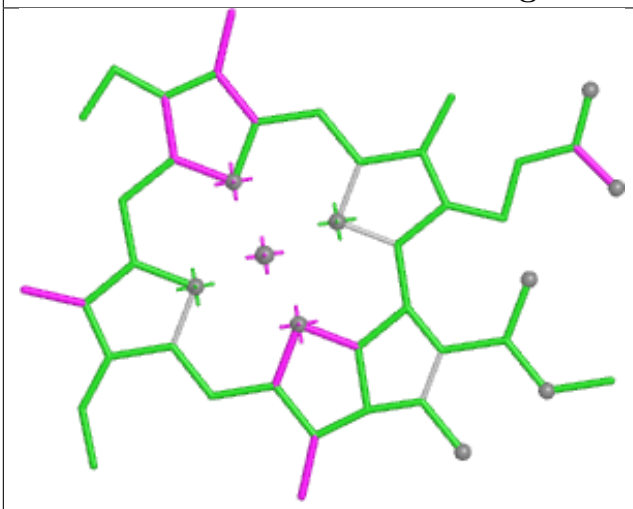


Rings

Ligand CLA 17 309



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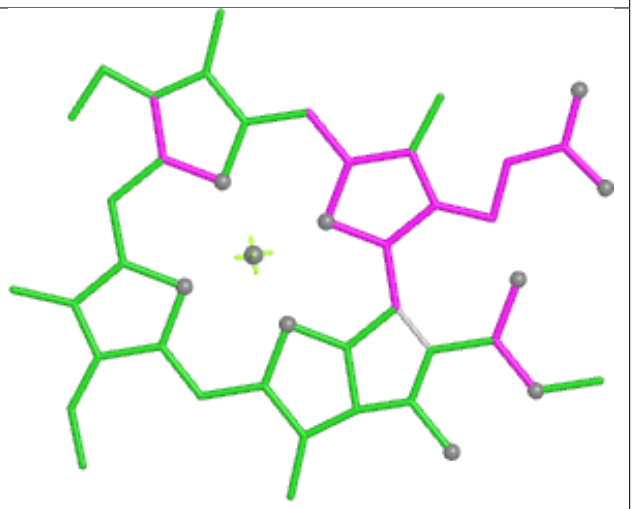

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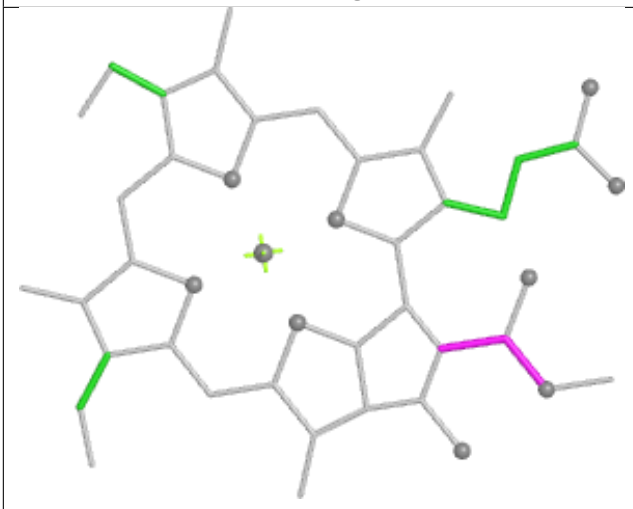

Torsions

Rings

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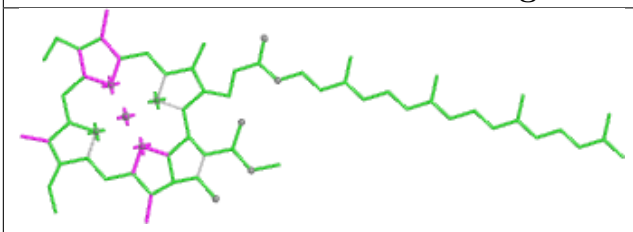

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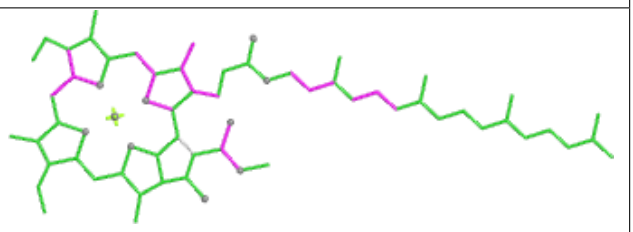

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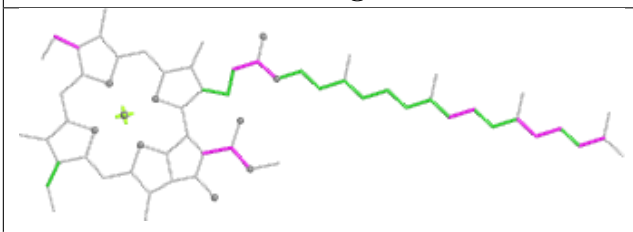

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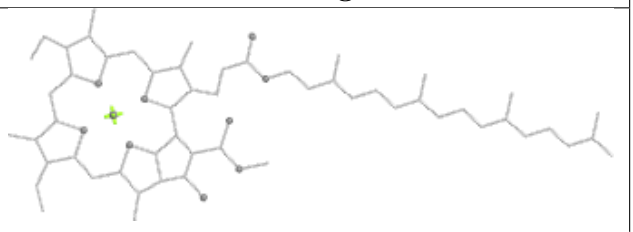

Rings

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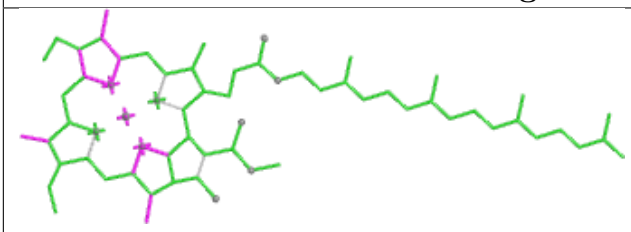

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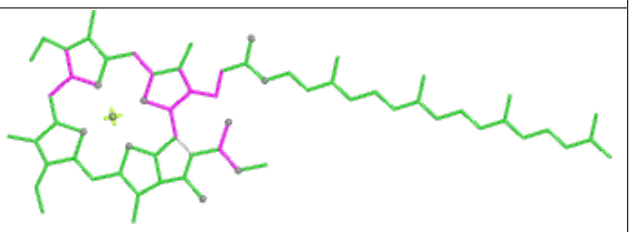

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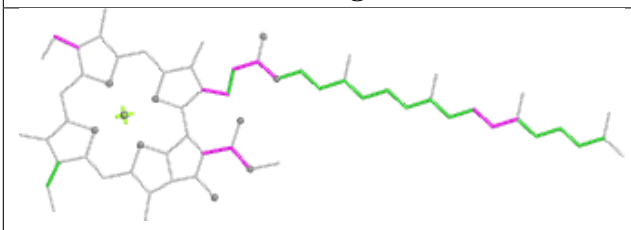

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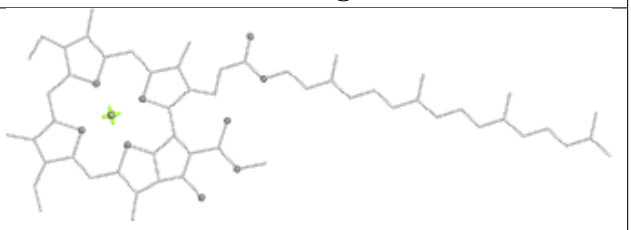

Rings

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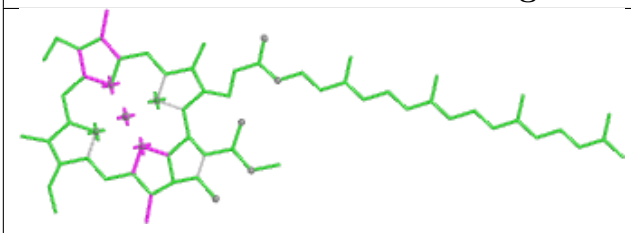

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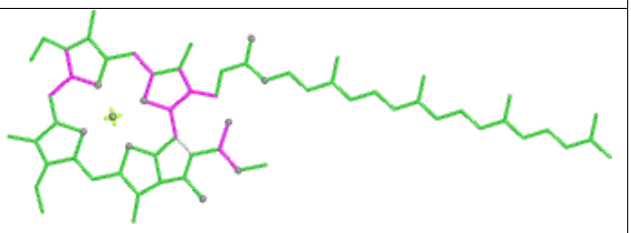

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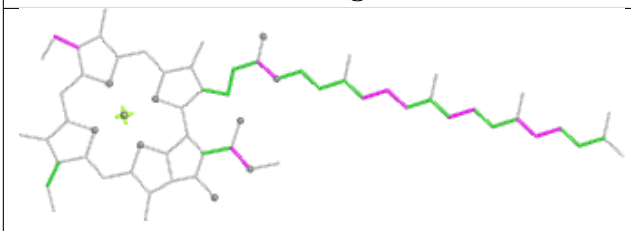

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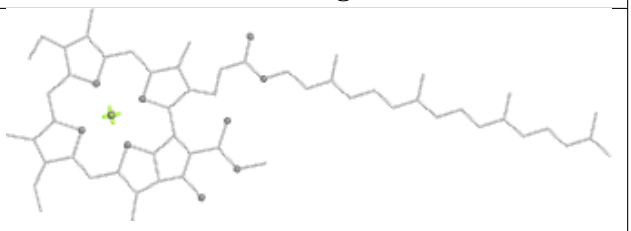
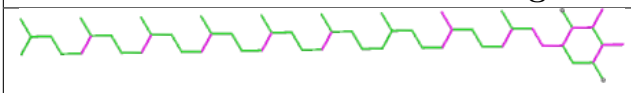


Rings

Ligand PL9 D 407



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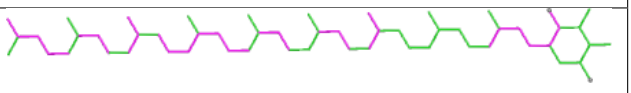

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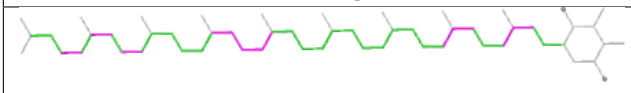

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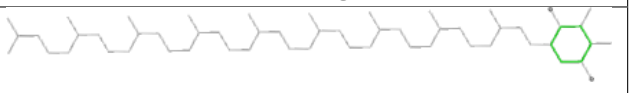
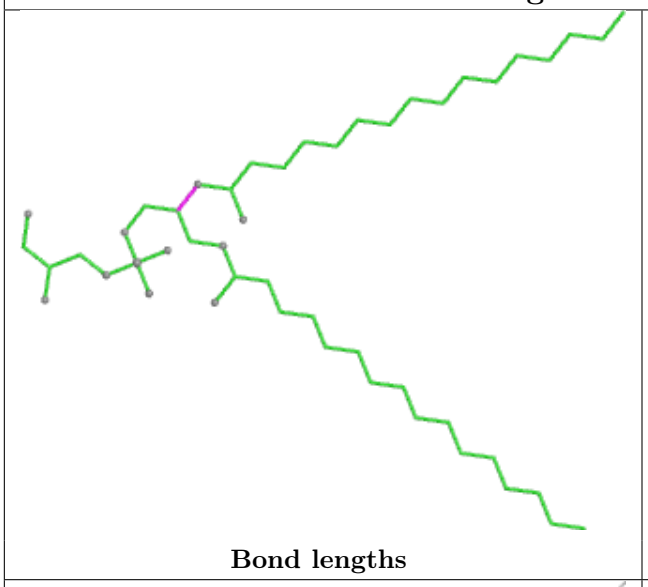


Rings

Ligand LHG b 621



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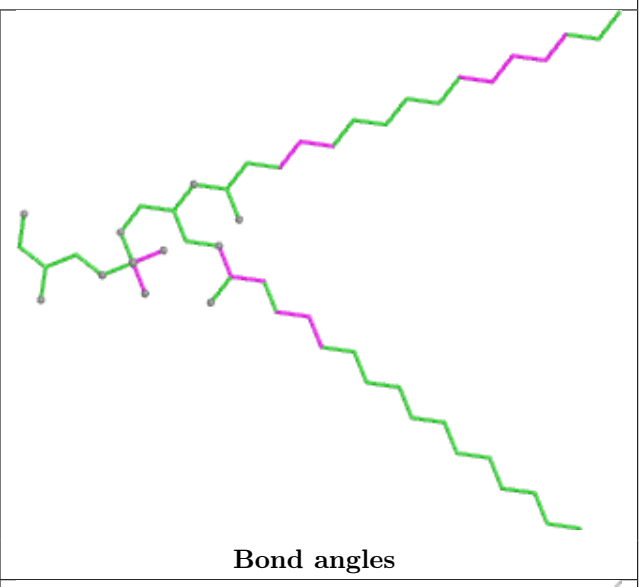

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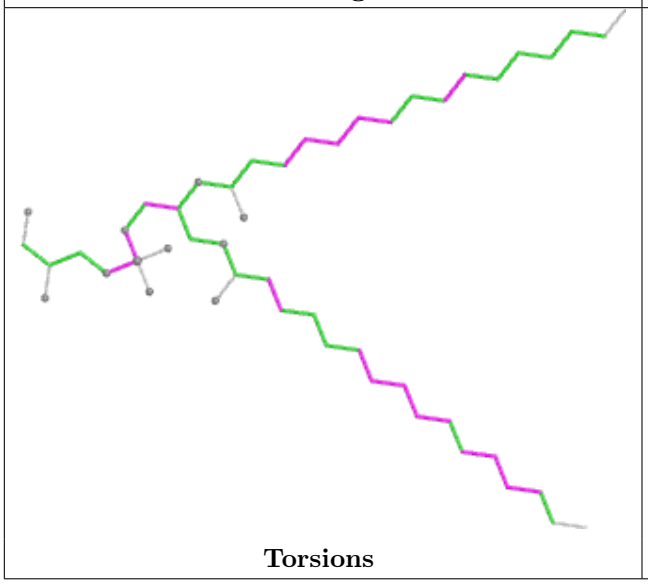

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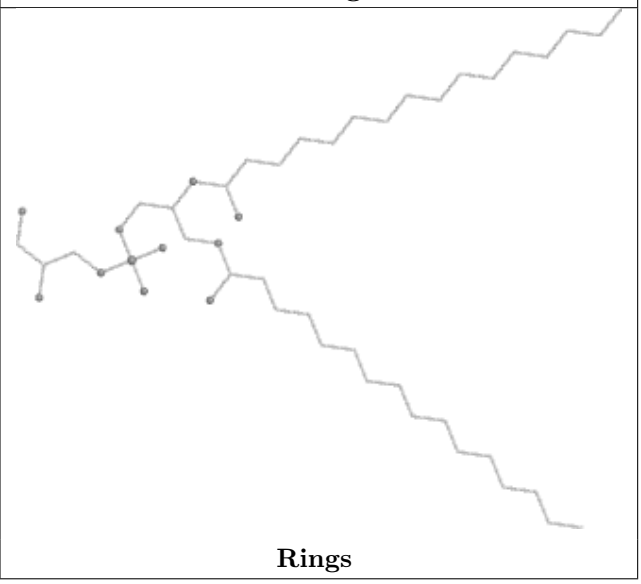
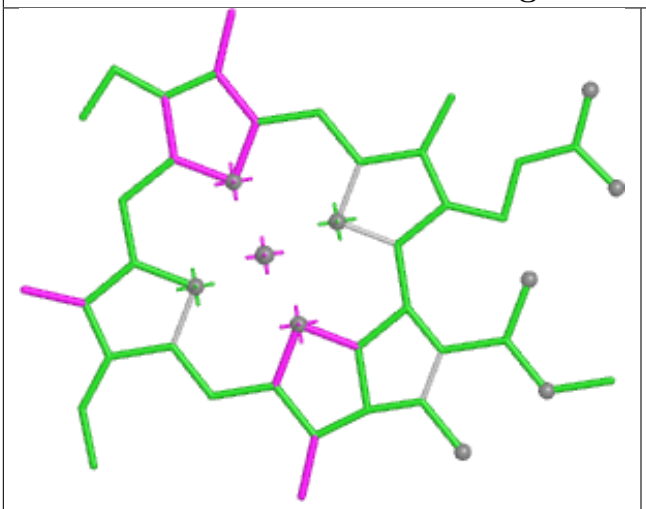


Rings

Ligand CLA 13 303



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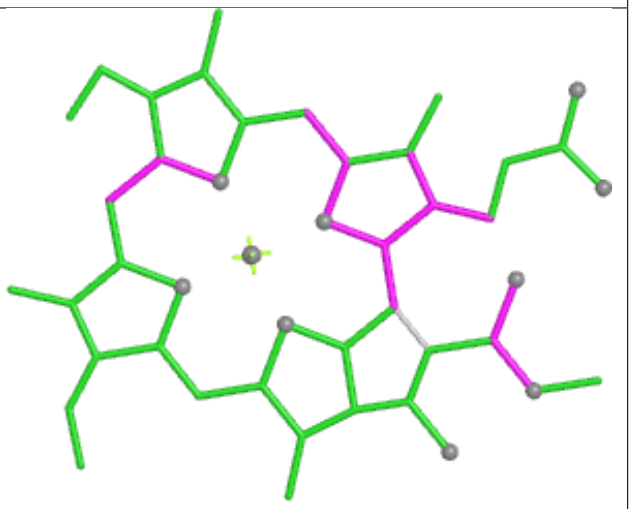
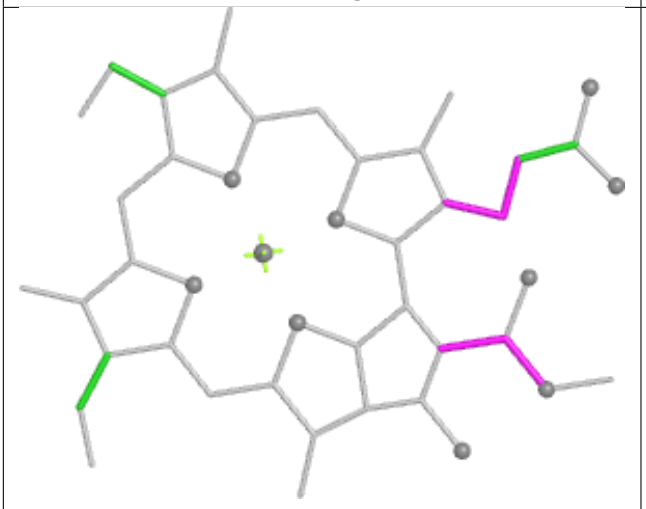


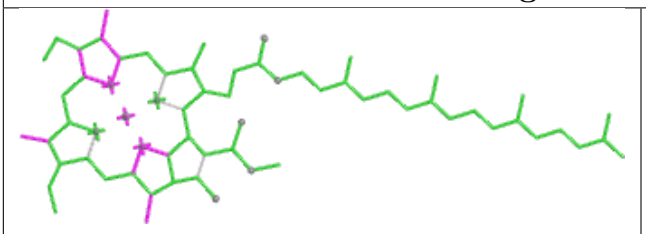
Bond angles



Torsions

Rings

Ligand CLA 19 301



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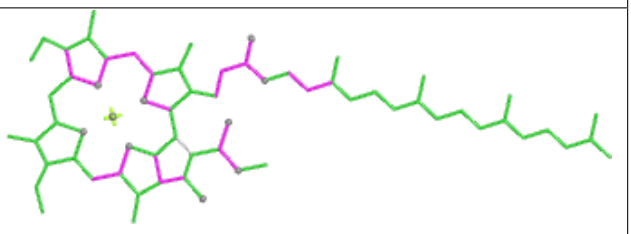

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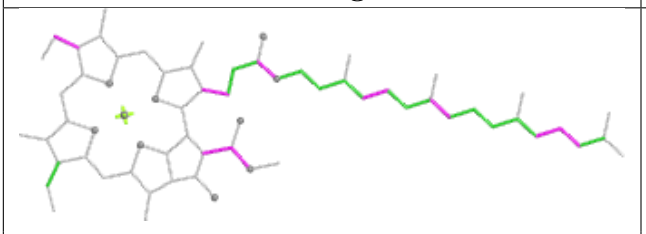

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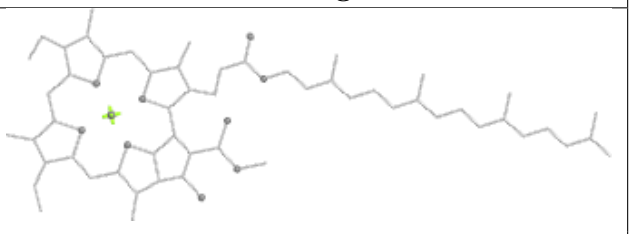
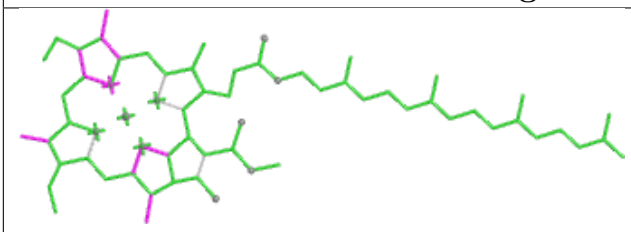


Rings

Ligand CLA 15 303



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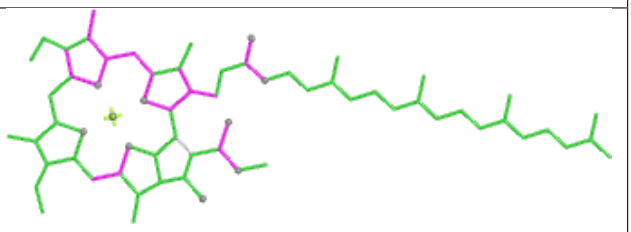
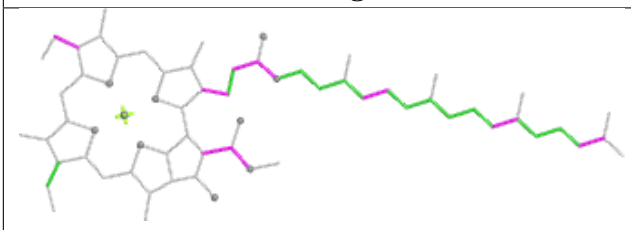


Bond angles



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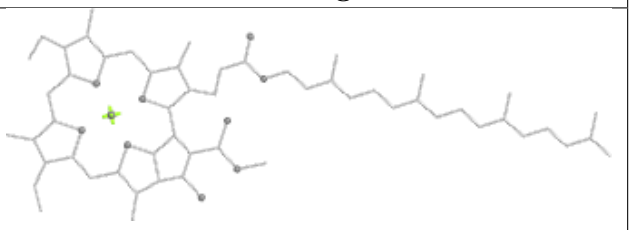
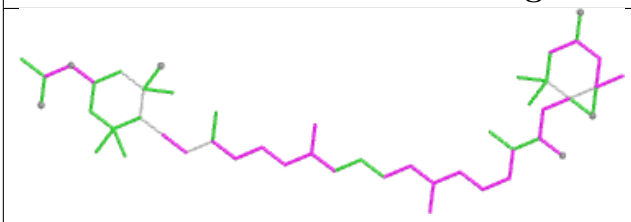
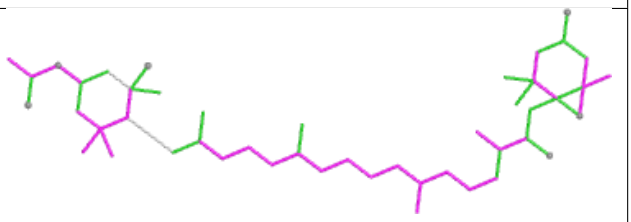


Rings

Ligand A86 20 213



Bond lengths



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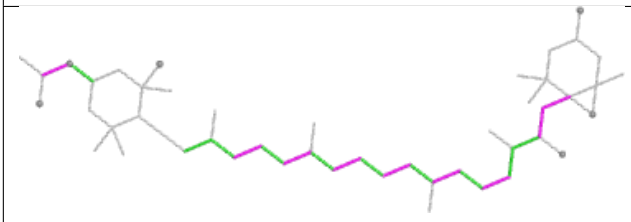

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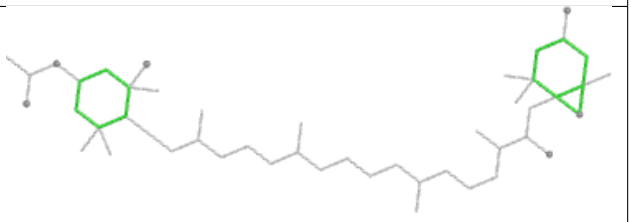
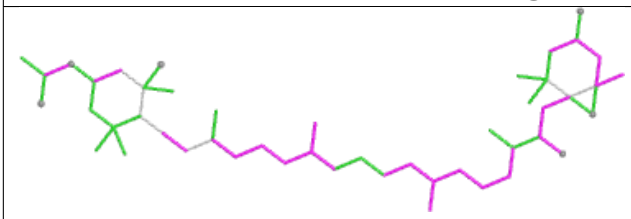


Rings

Ligand A86 13 313



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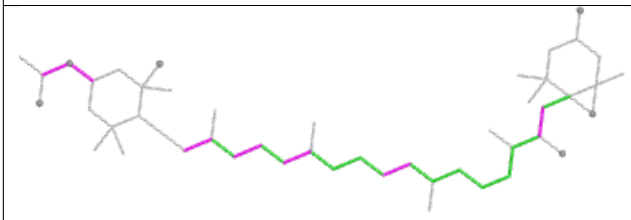

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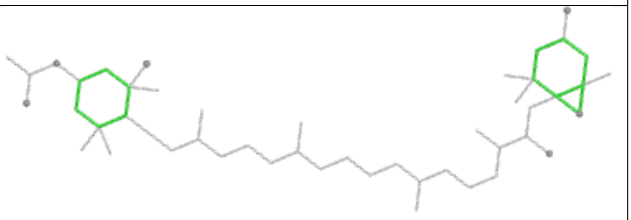
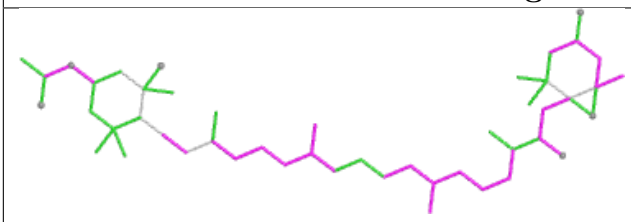


Rings

Ligand A86 17 312



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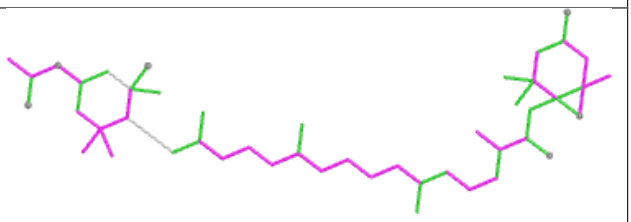

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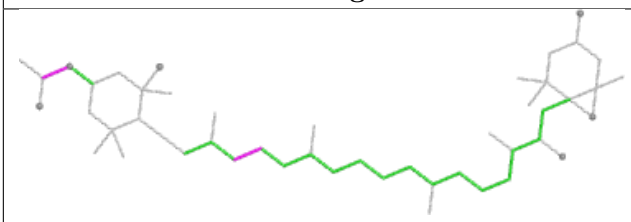

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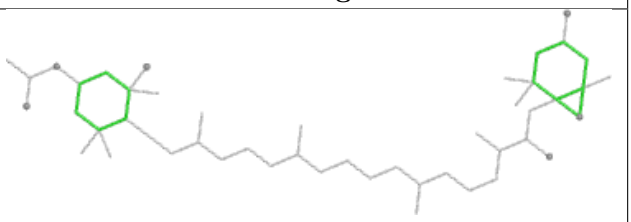
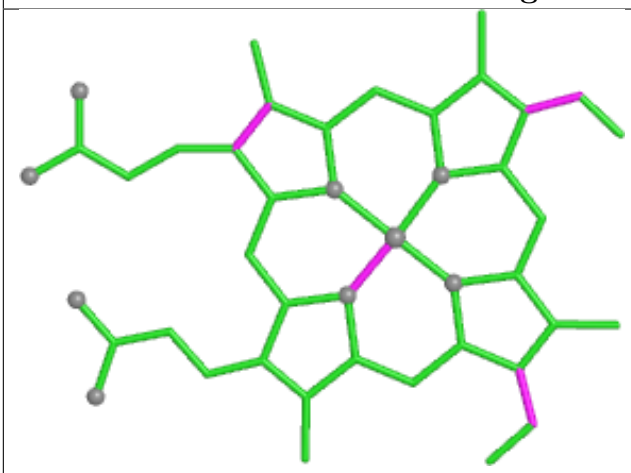


Rings

Ligand HEM F 102



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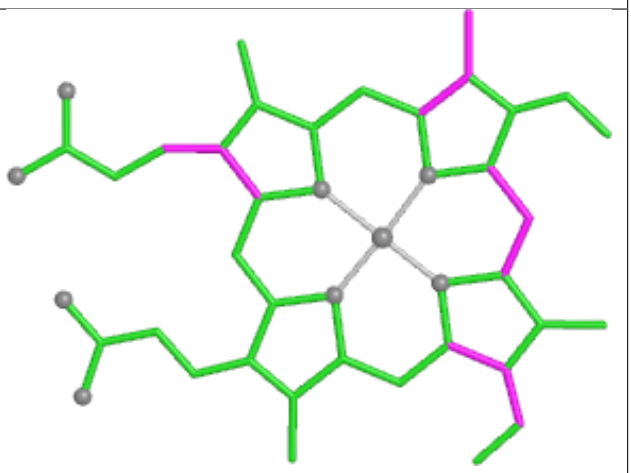

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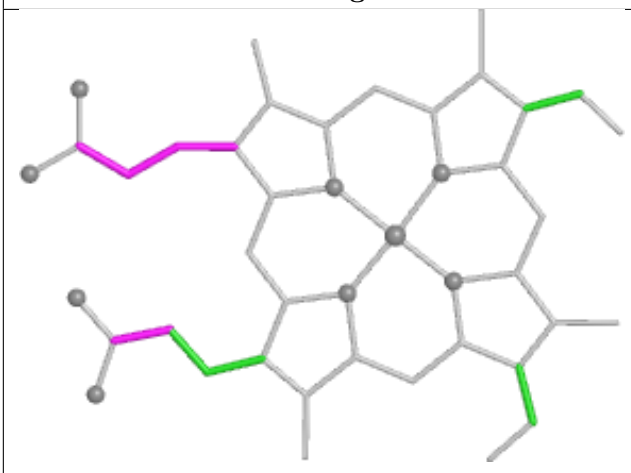

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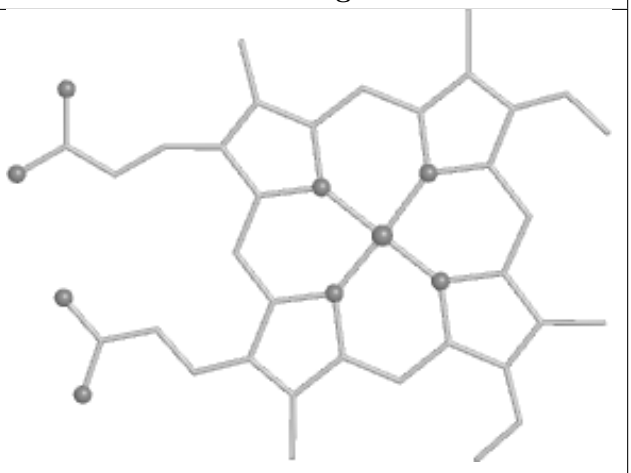
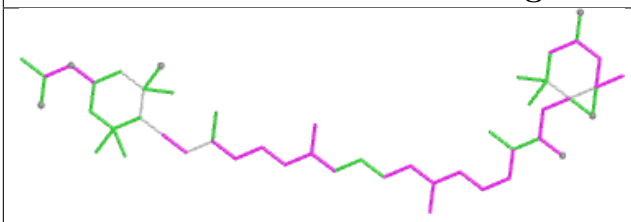


Rings

Ligand A86 15 313



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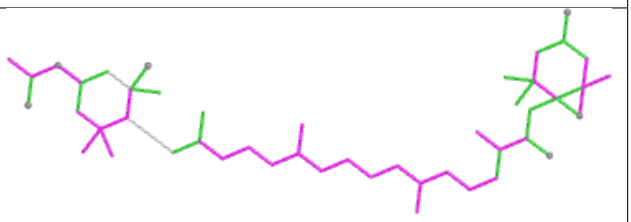

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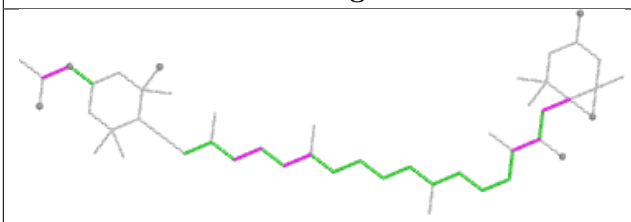

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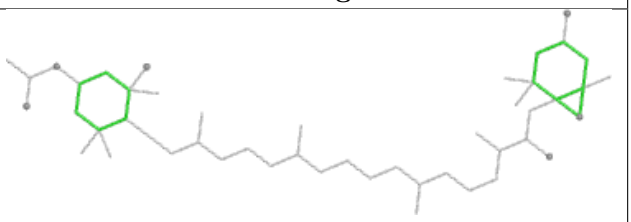
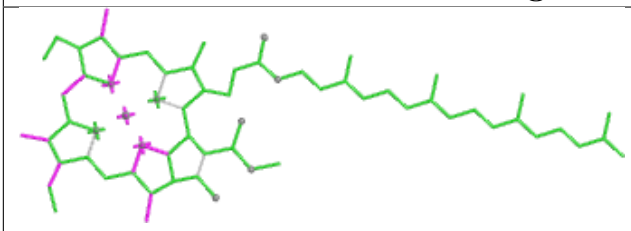


Rings

Ligand CLA b 604



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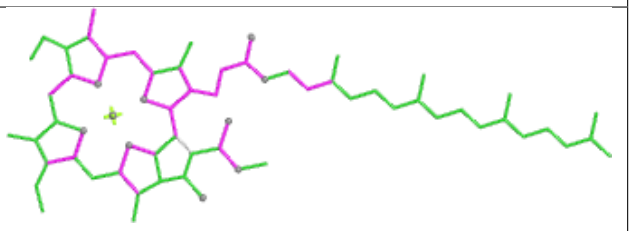

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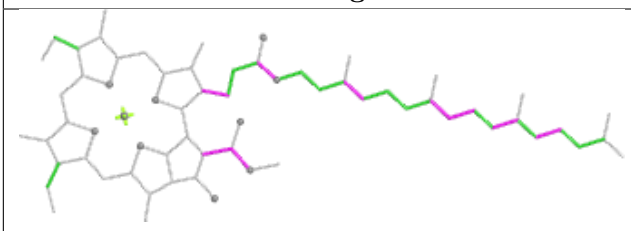

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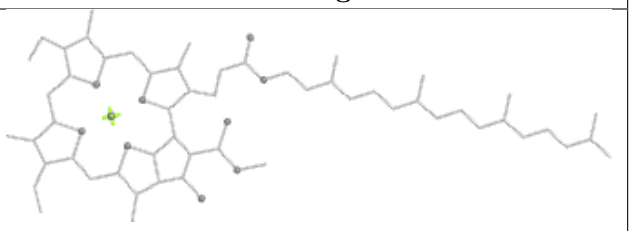
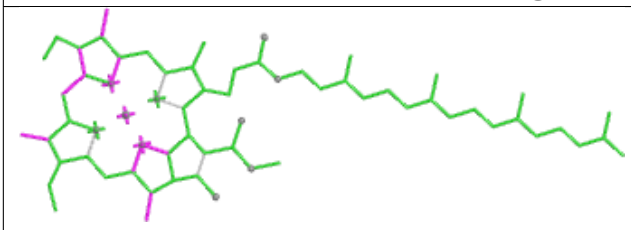


Rings

Ligand CLA c 509



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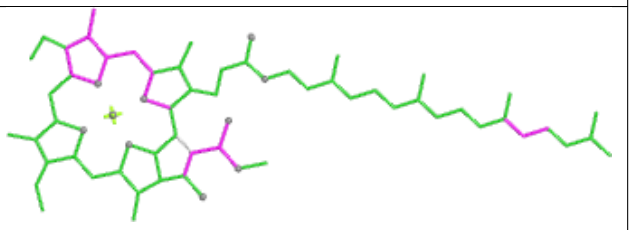

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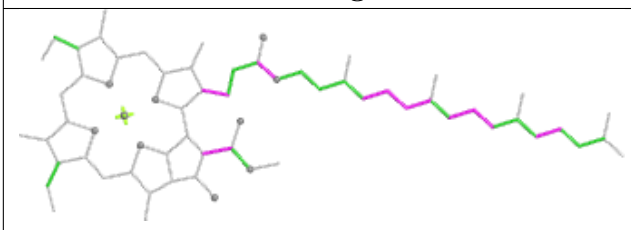

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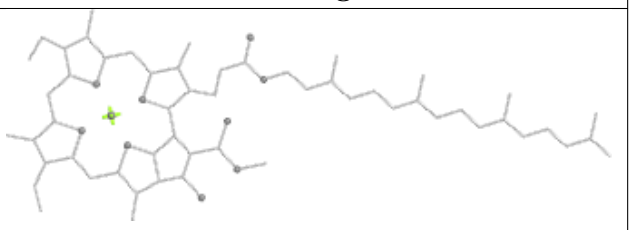
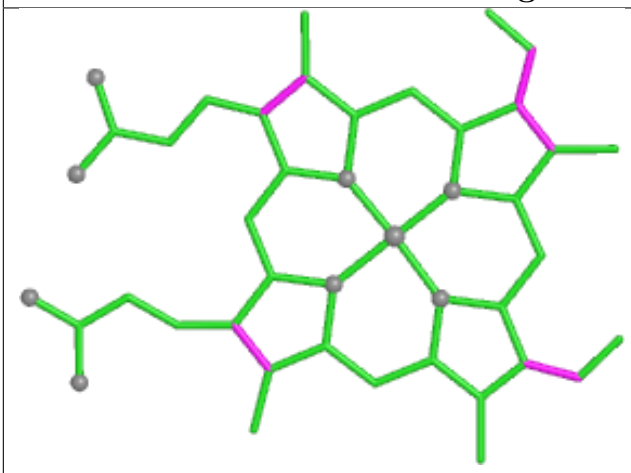


Rings

Ligand HEM V 201



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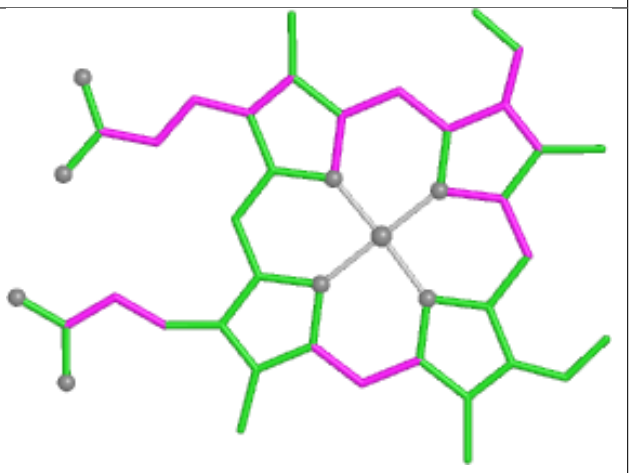

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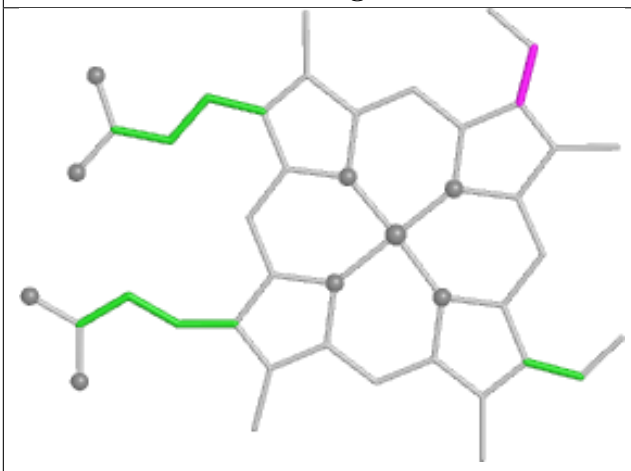

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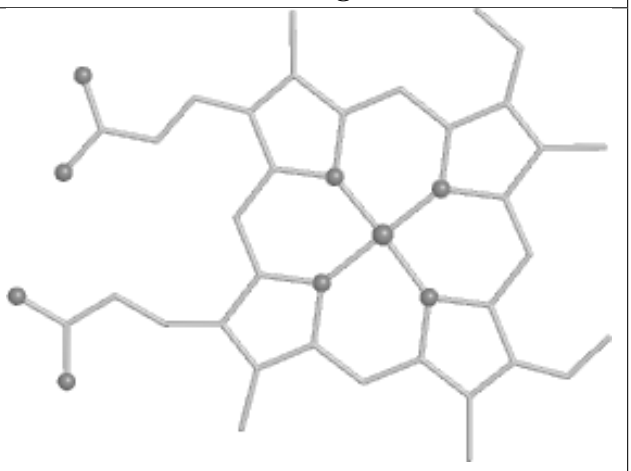
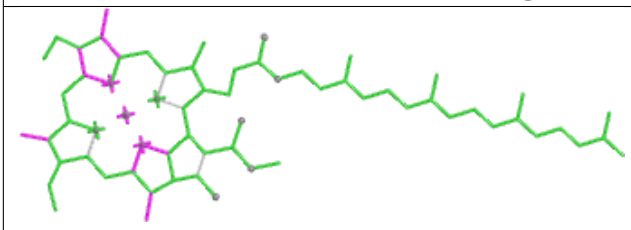


Rings

Ligand CLA 19 303



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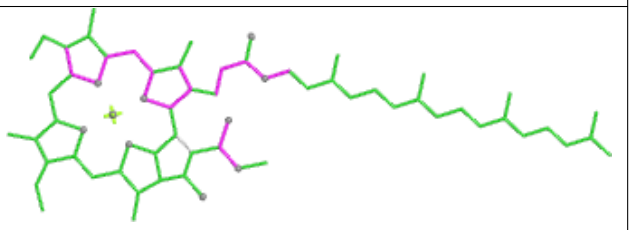

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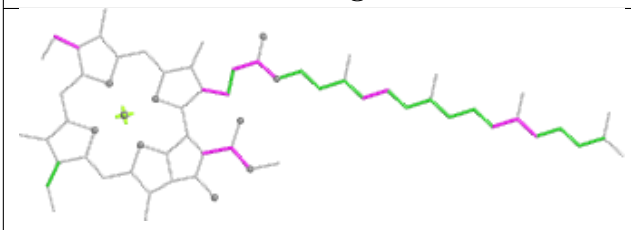

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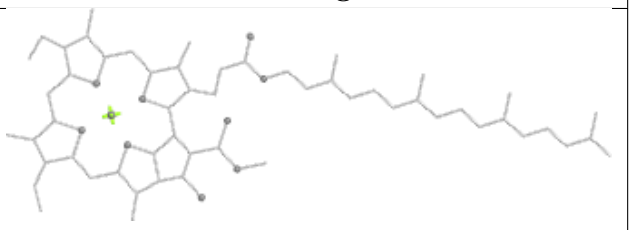
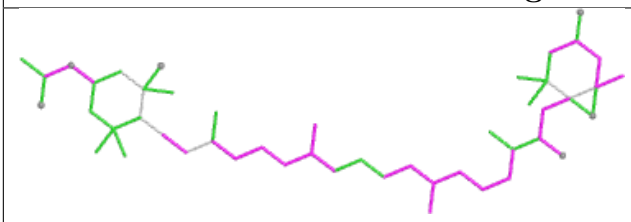


Rings

Ligand A86 16 310



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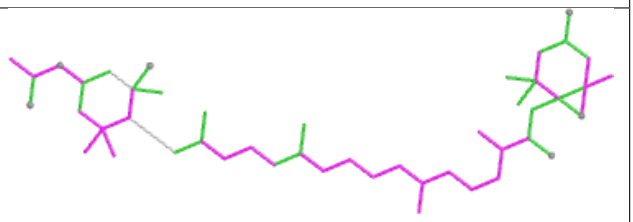

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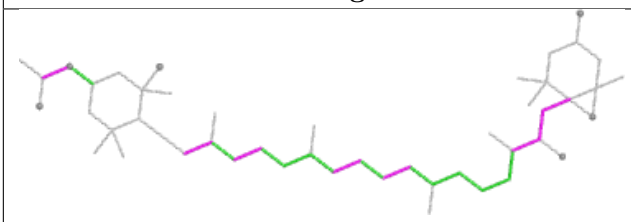

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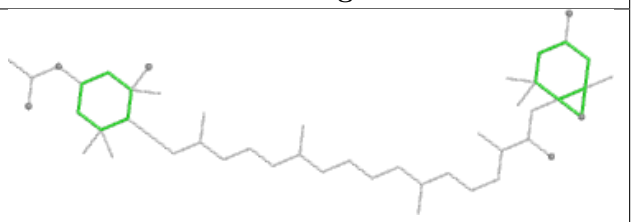
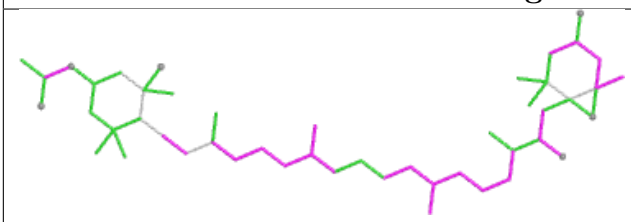


Rings

Ligand A86 19 312



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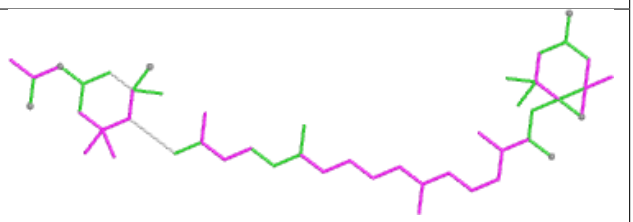

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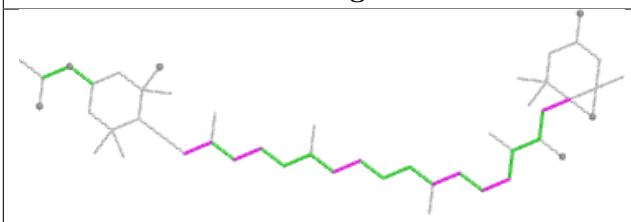

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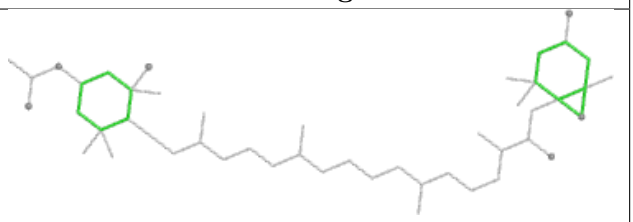
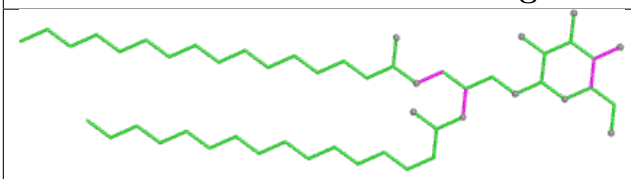


Rings

Ligand LMG w 101



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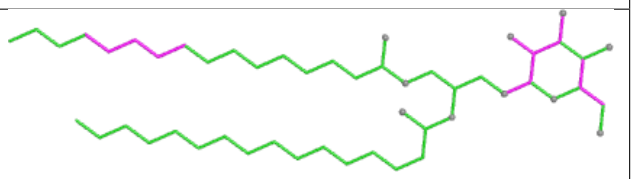

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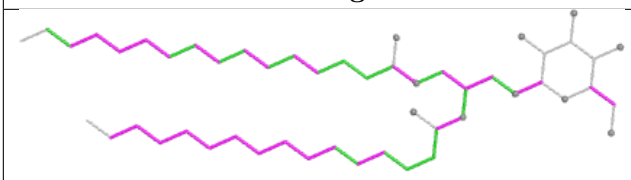

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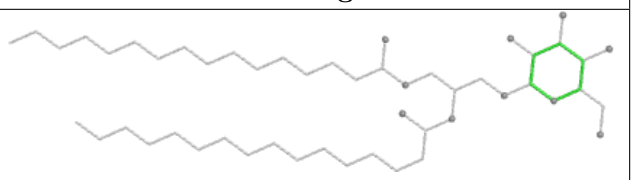
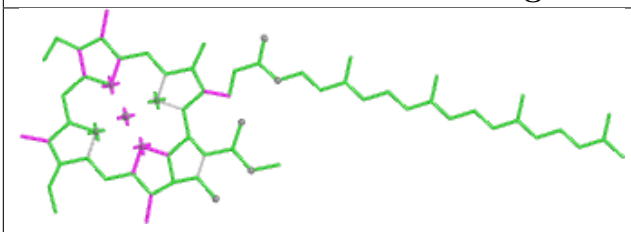


Rings

Ligand CLA B 613



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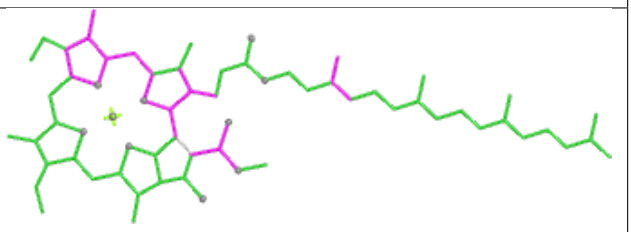
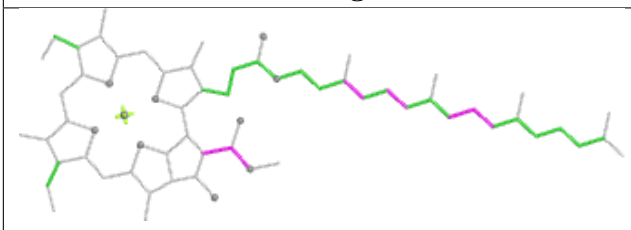


Bond angles



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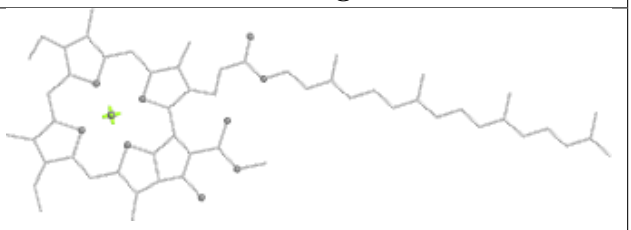
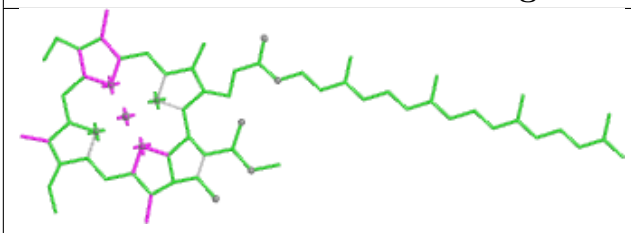


Rings

Ligand CLA 17 305



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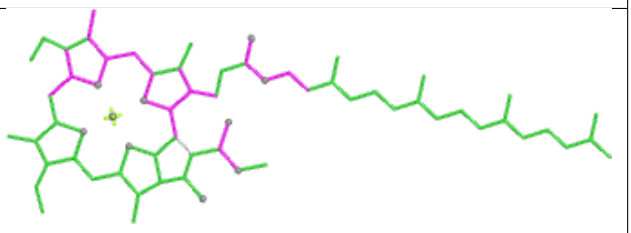
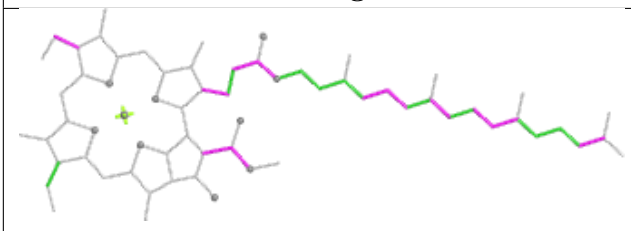


Bond angles



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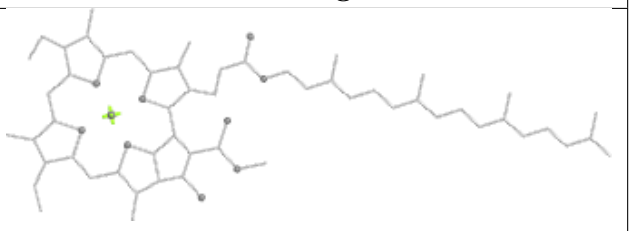
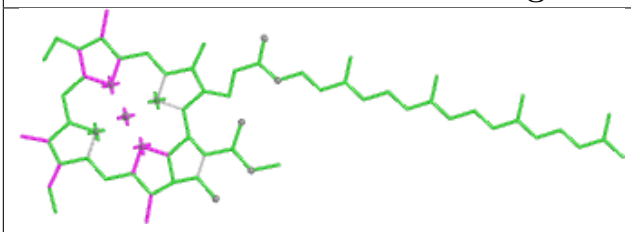
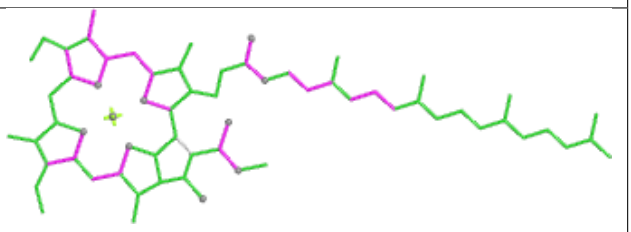


Rings

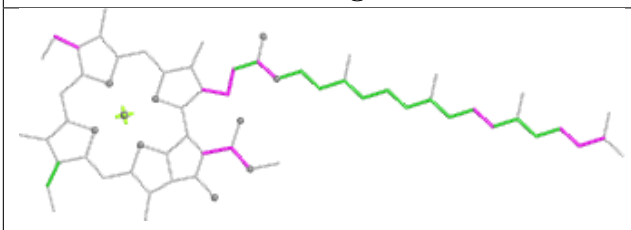
Ligand CLA b 611



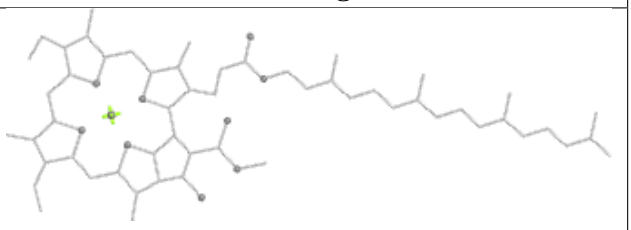
Bond lengths



Bond angles

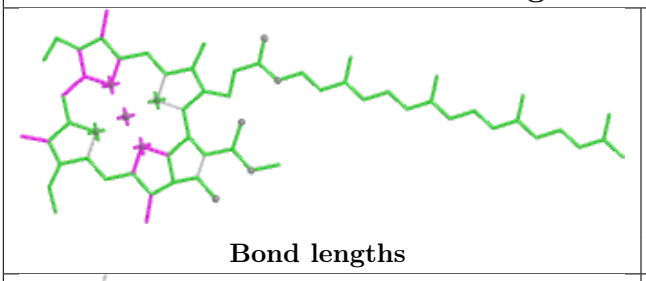


Torsions



Rings

Ligand CLA b 603



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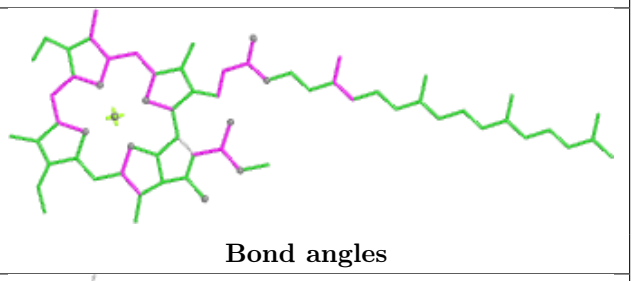

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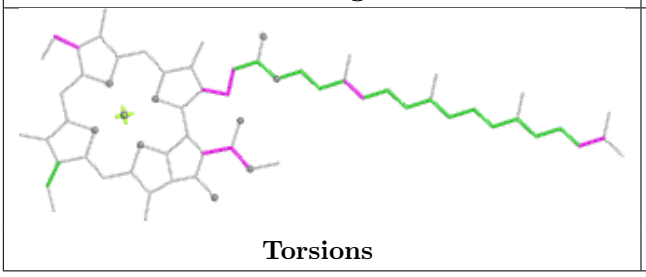

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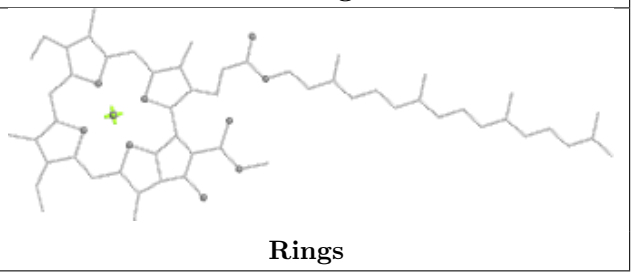
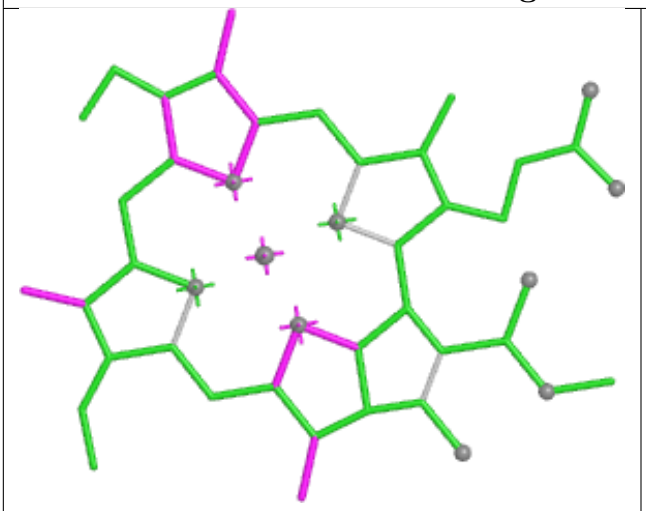


Rings

Ligand CLA 11 308



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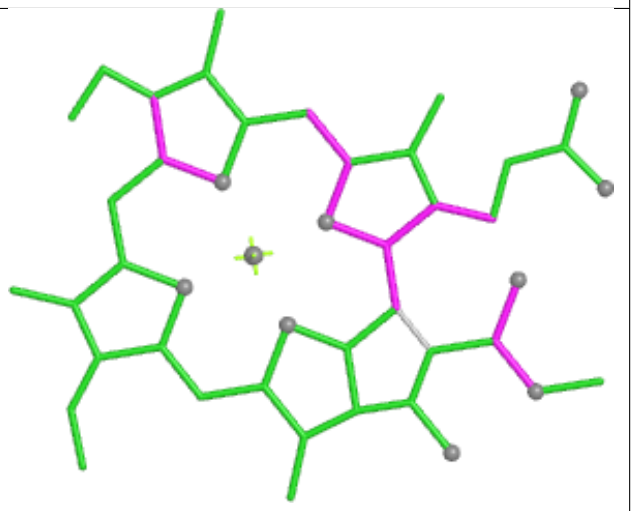

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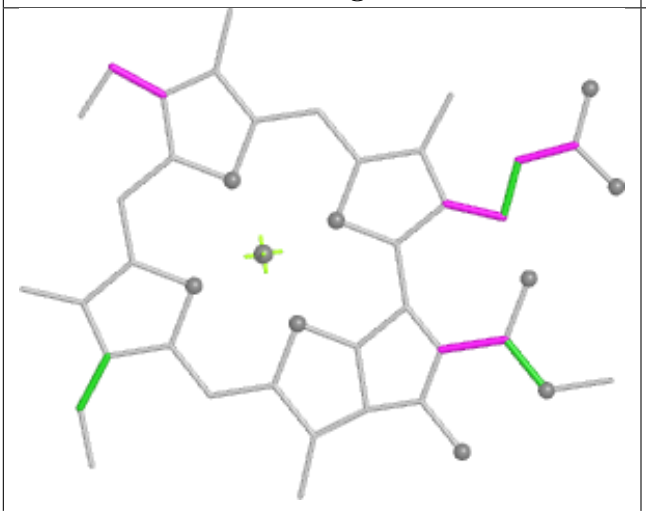
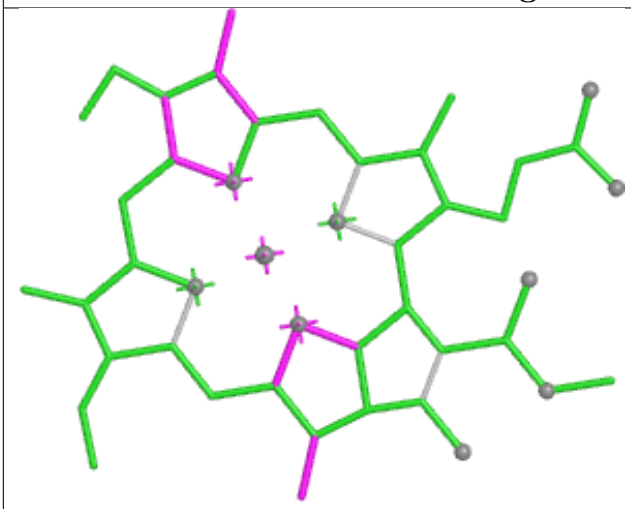


Torsions

Rings

Ligand CLA 19 309



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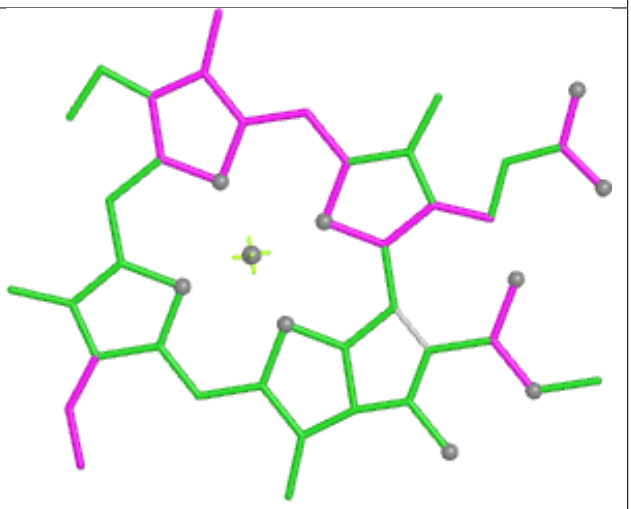

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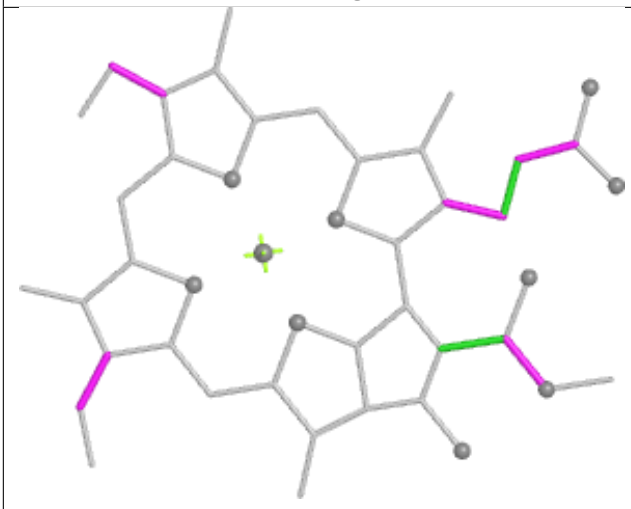
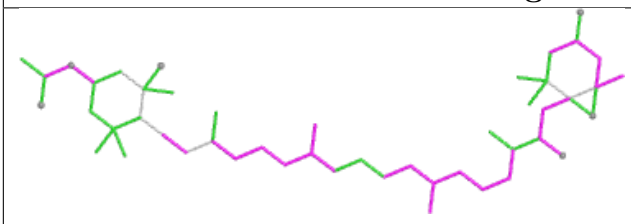


Torsions

Rings

Ligand A86 15 310



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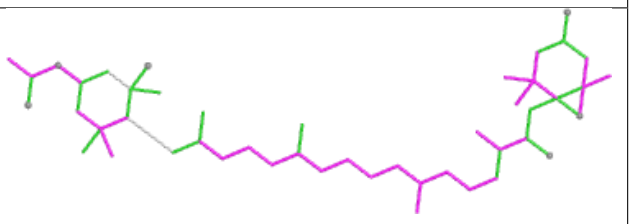

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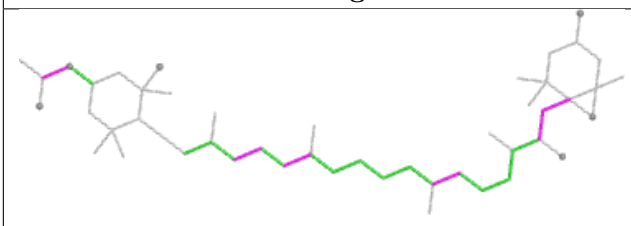

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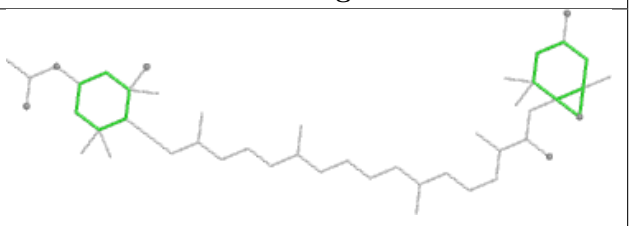
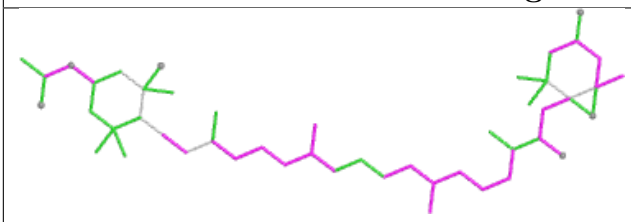


Rings

Ligand A86 12 316



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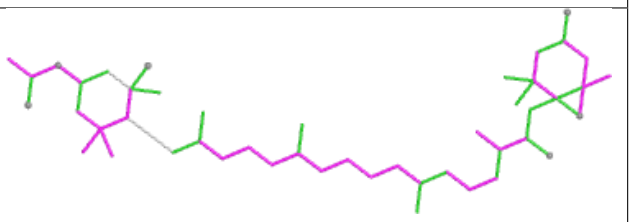

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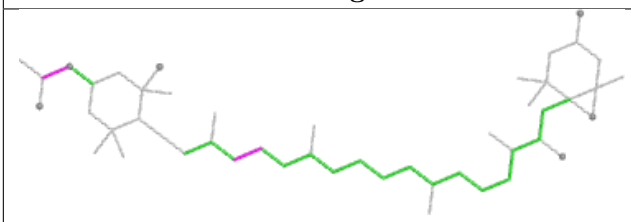

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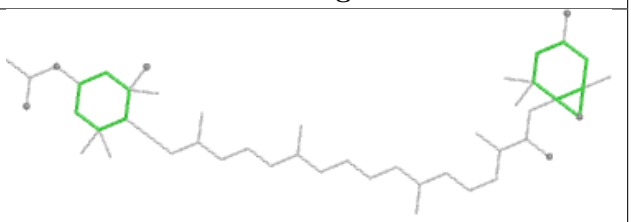
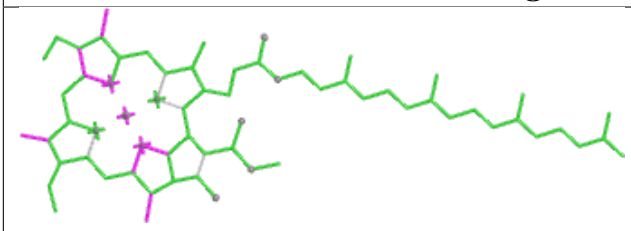


Rings

Ligand CLA B 608



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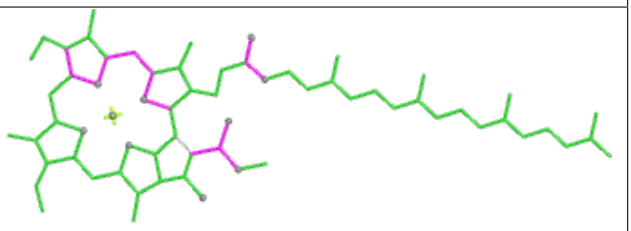

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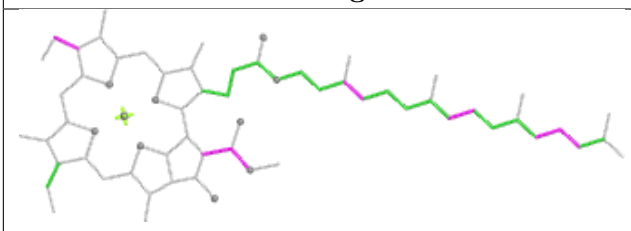

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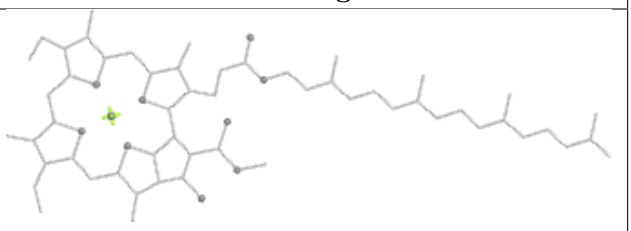

Rings

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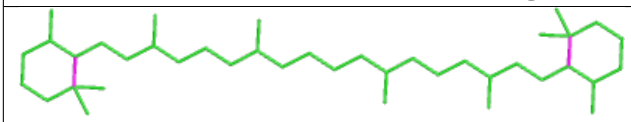

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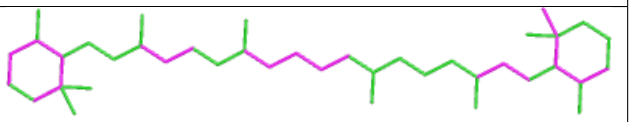

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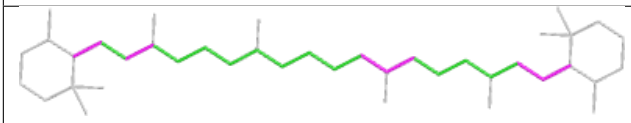

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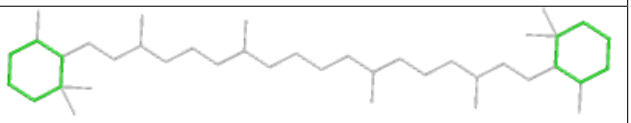

Rings

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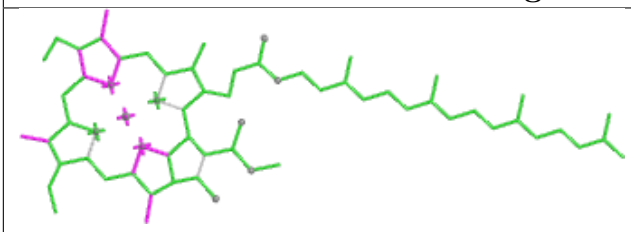

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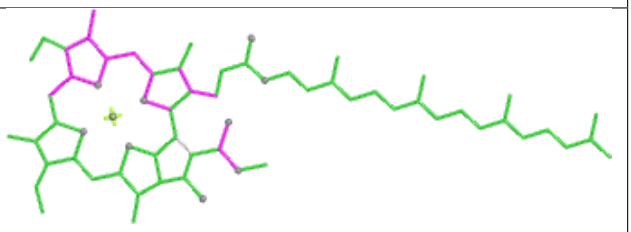

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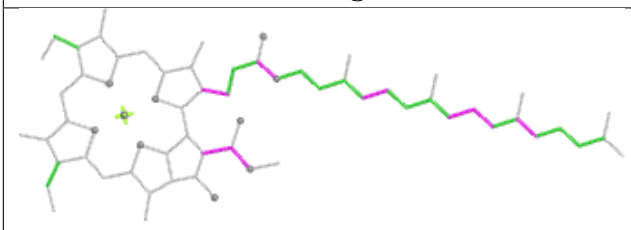

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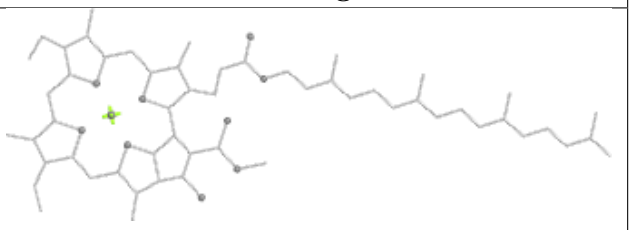
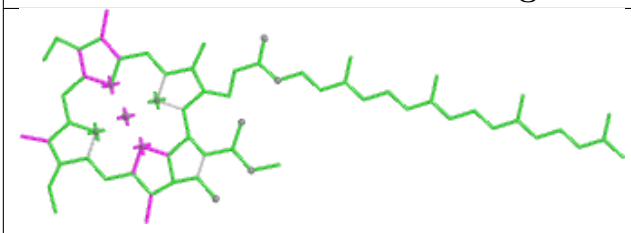


Rings

Ligand CLA 16 304



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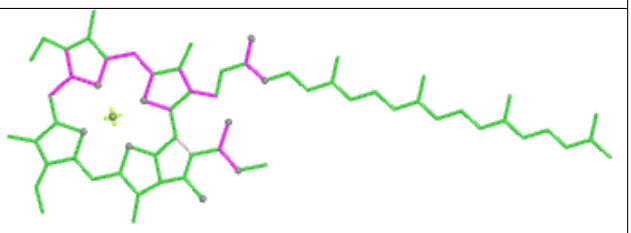
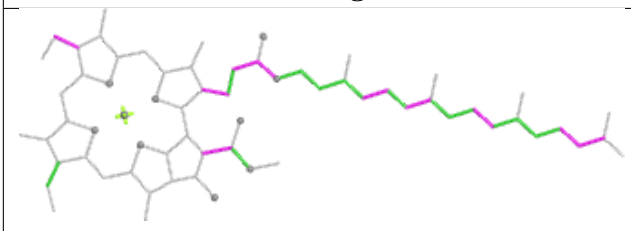


Bond angles



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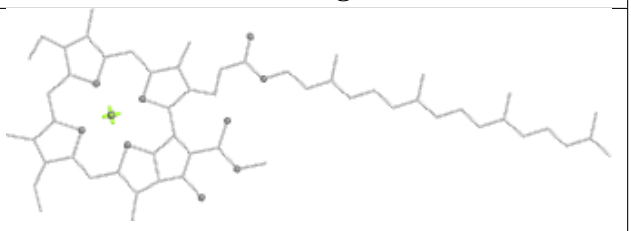
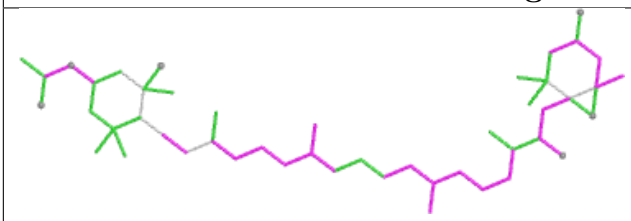


Rings

Ligand A86 14 312



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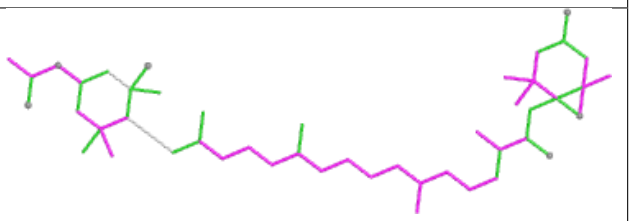
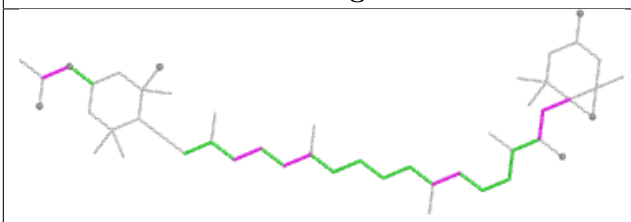


Bond angles



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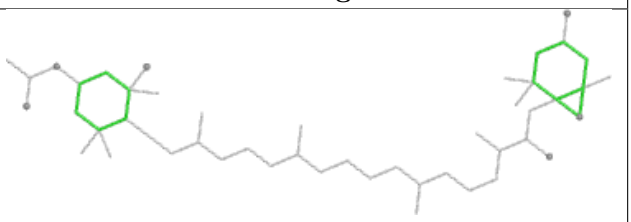
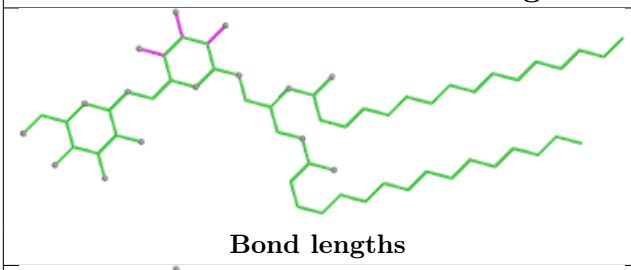


Rings

Ligand DGD h 102



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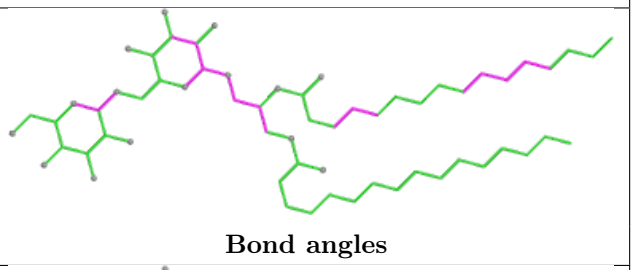

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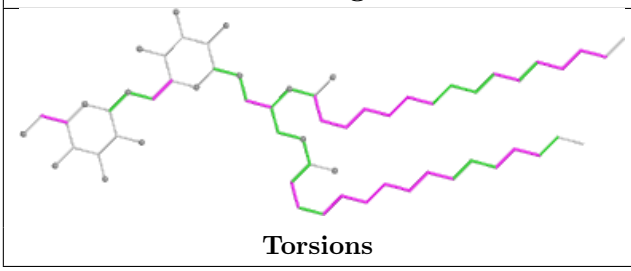

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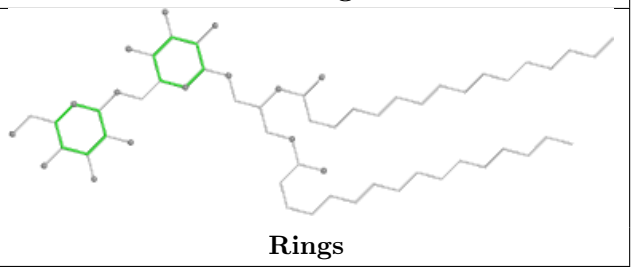
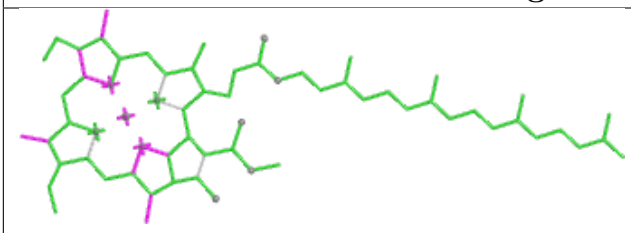


Rings

Ligand CLA b 608



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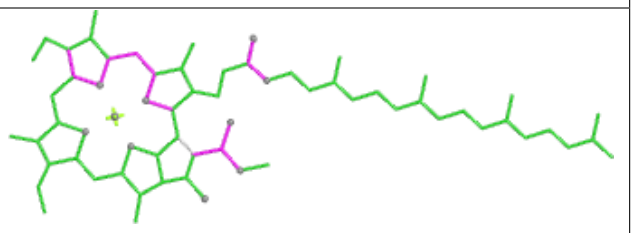

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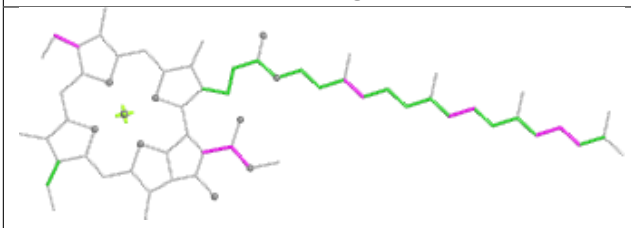

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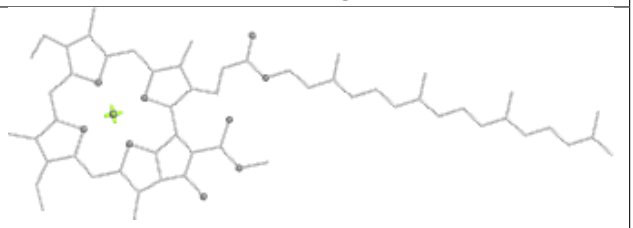
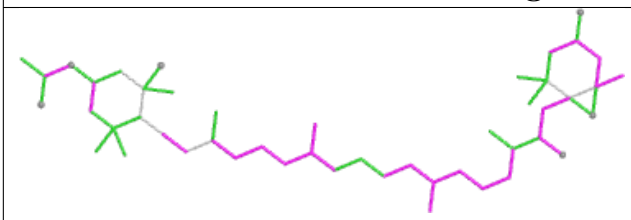


Rings

Ligand A86 11 312



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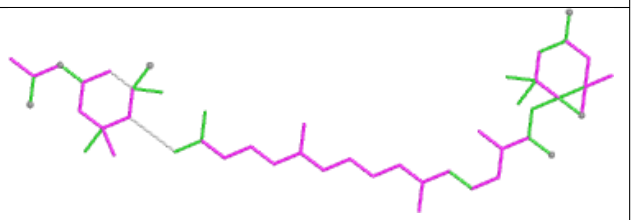
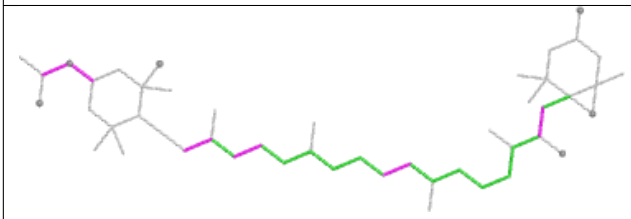


Bond angles



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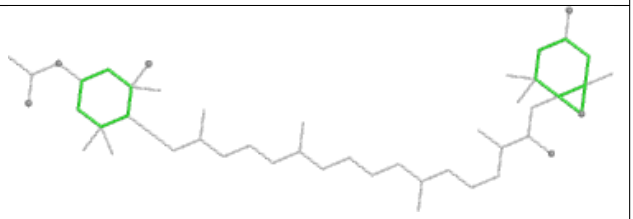
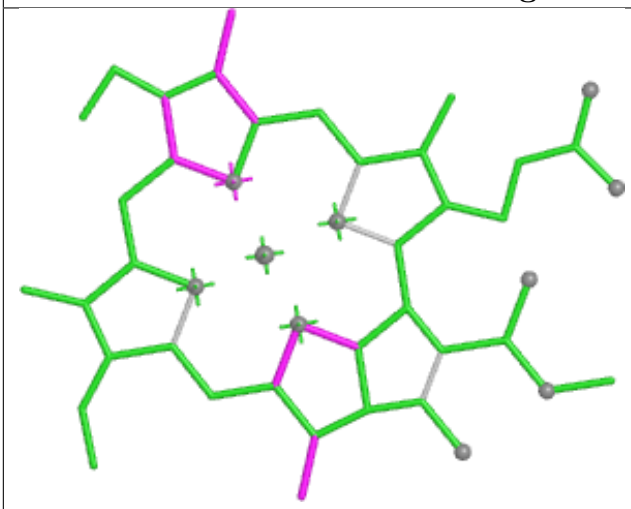


Rings

Ligand CLA 14 308



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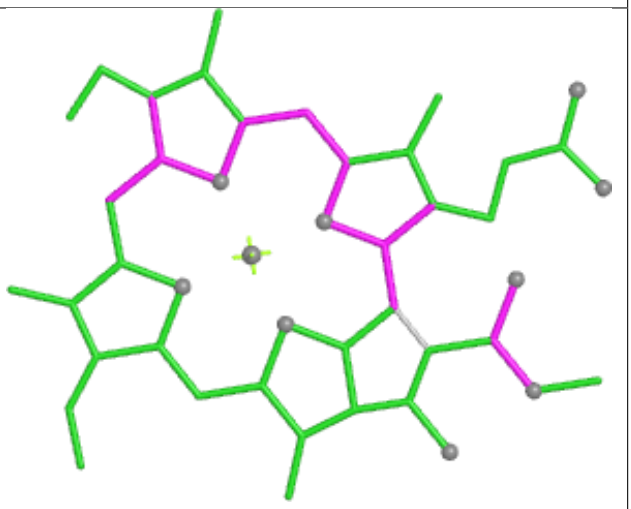
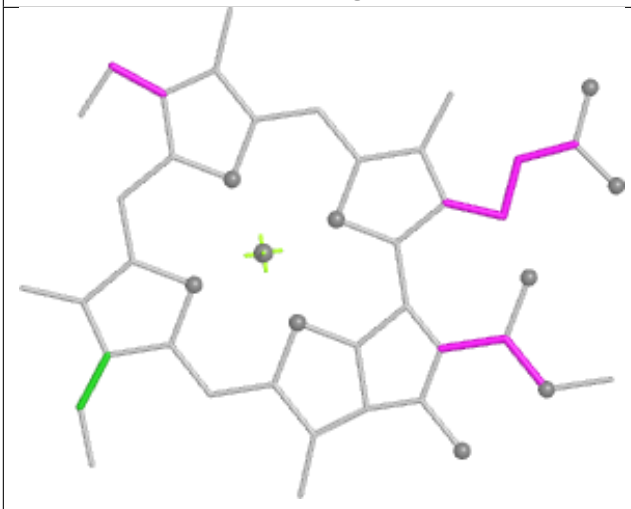


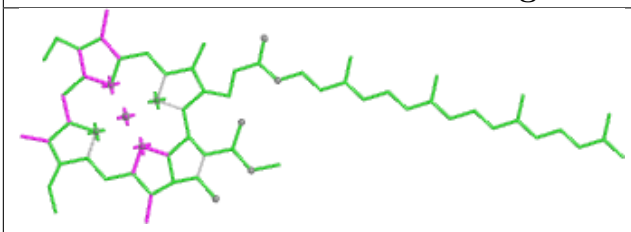
Bond angles



Torsions

Rings

Ligand CLA 15 301



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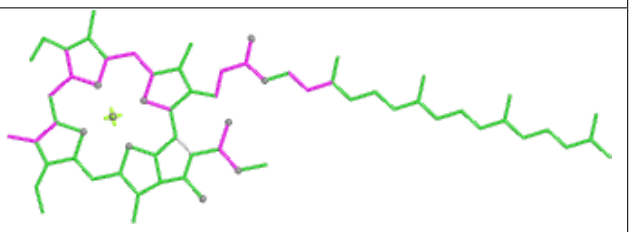
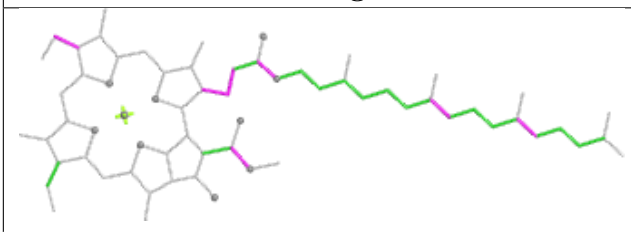


Bond angles



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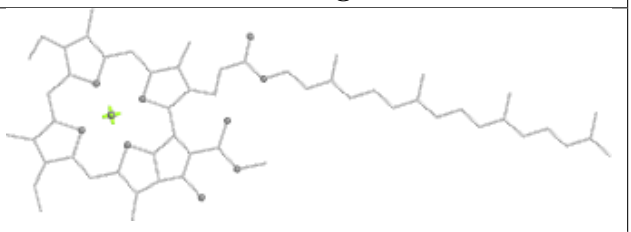
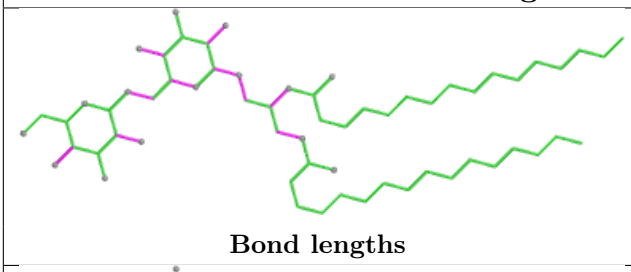


Rings

Ligand DGD C 517



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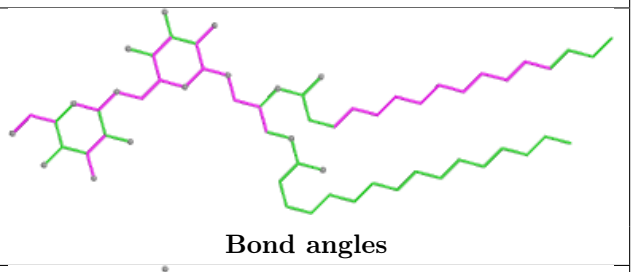
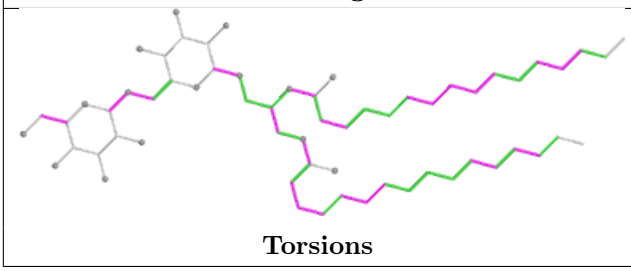


Bond angles



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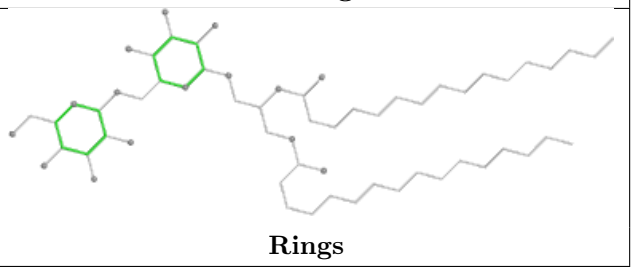
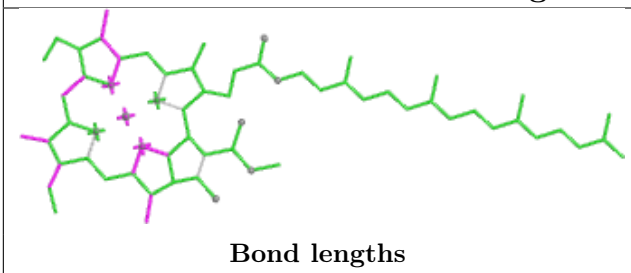


Rings

Ligand CLA c 502



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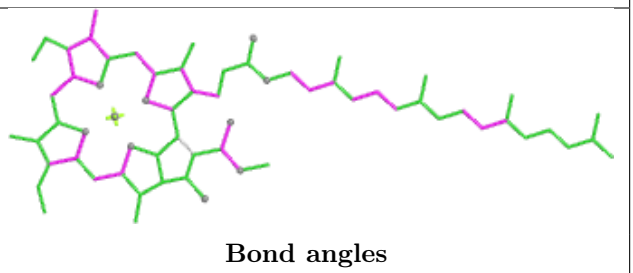

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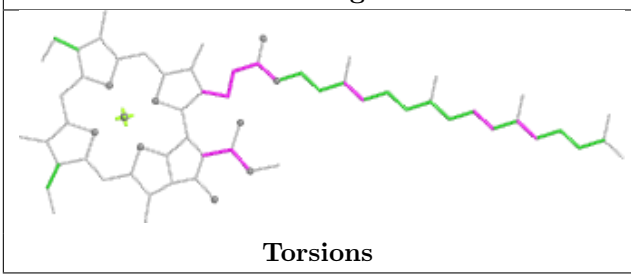

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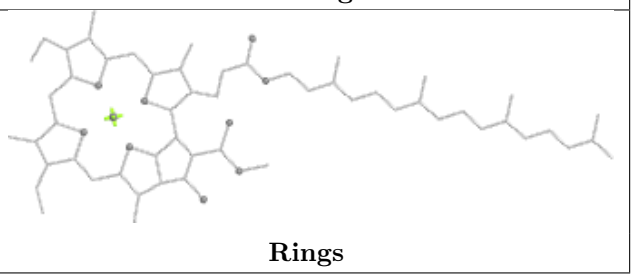
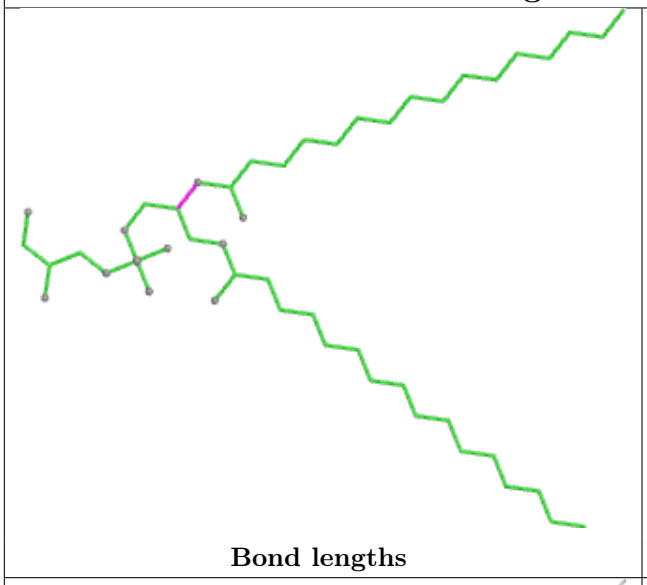


Rings

Ligand LHG B 622



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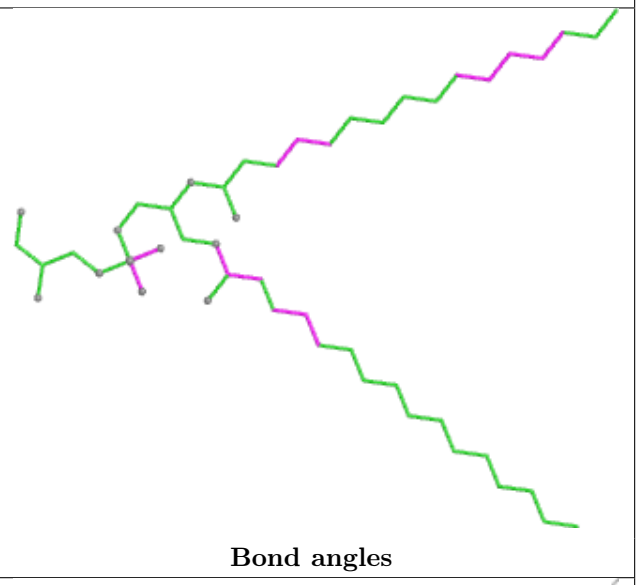
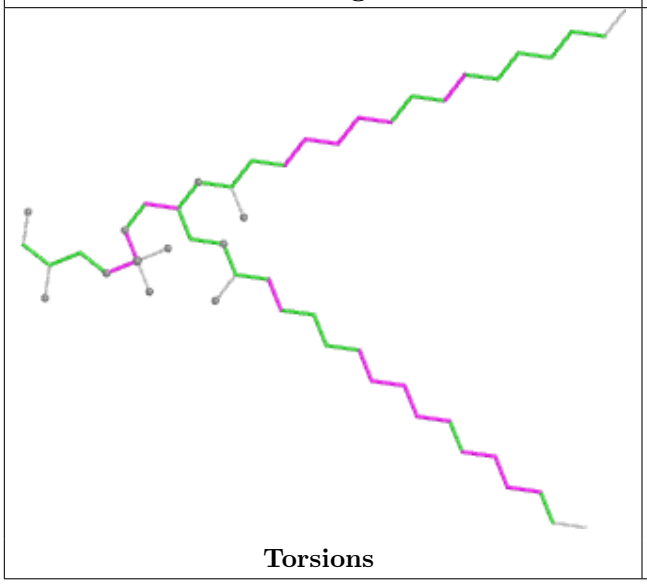


Bond angles



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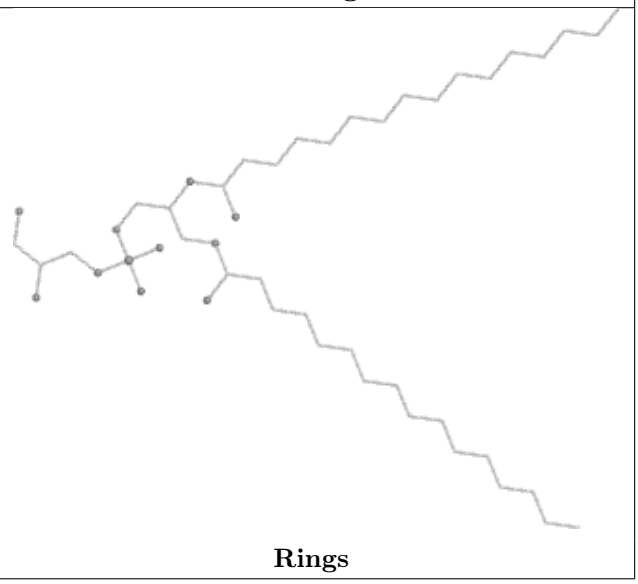
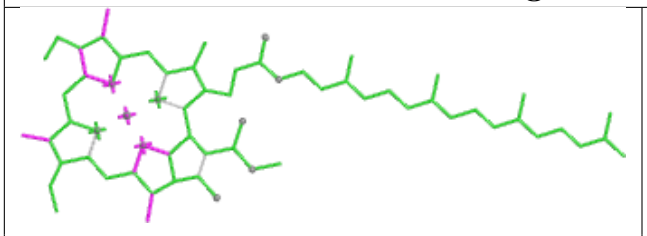


Rings

Ligand CLA C 506



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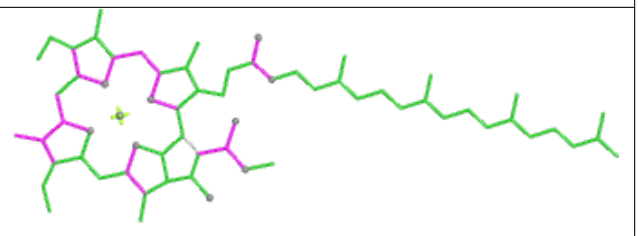
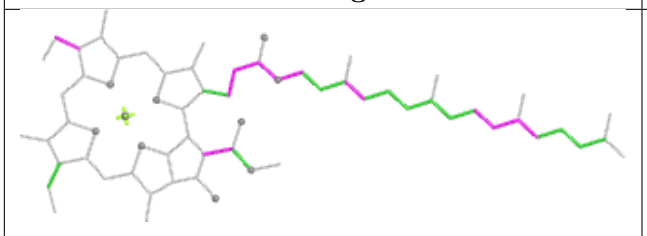


Bond angles



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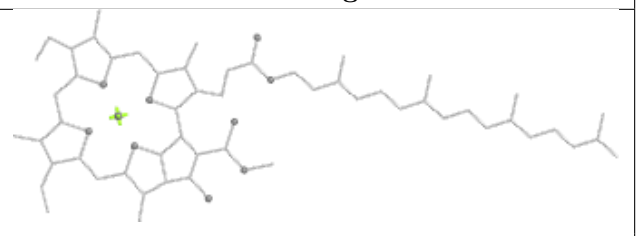
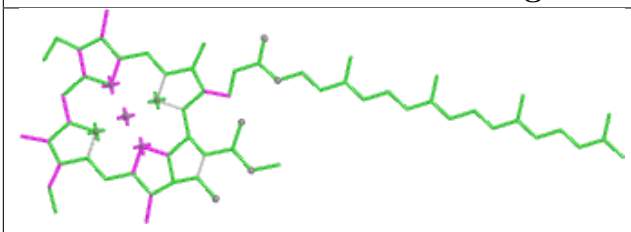


Rings

Ligand CLA C 511



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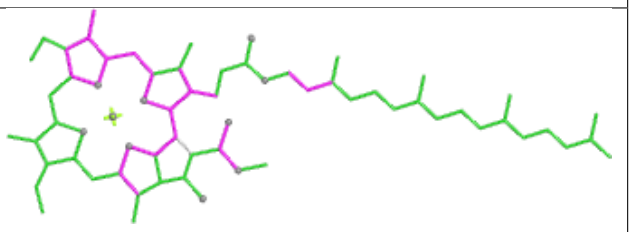
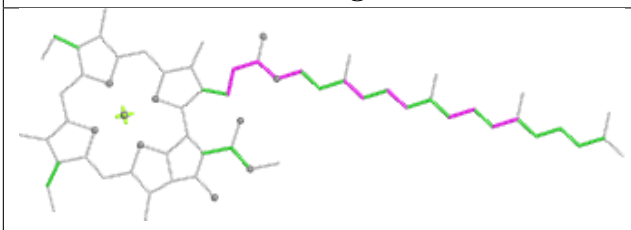


Bond angles



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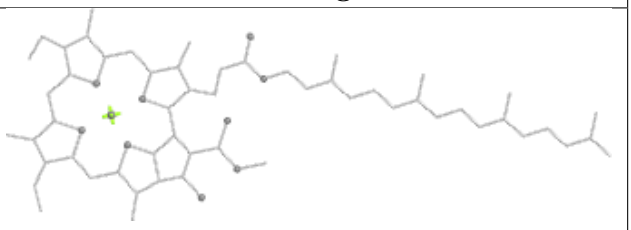
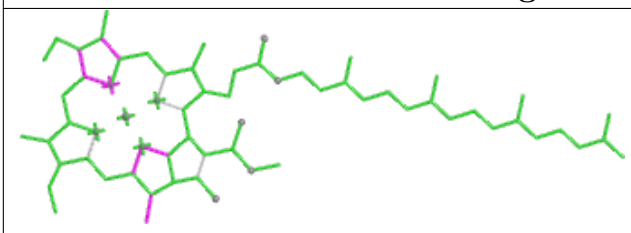


Rings

Ligand CLA W 103



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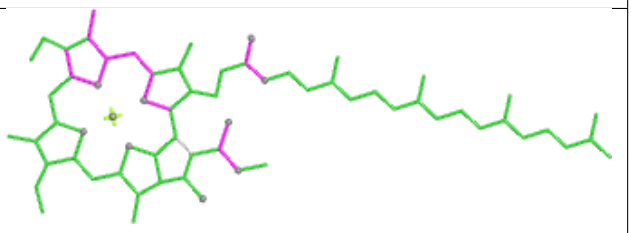

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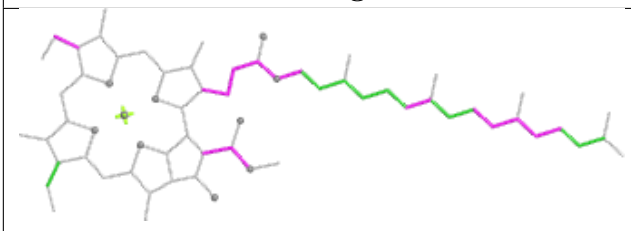

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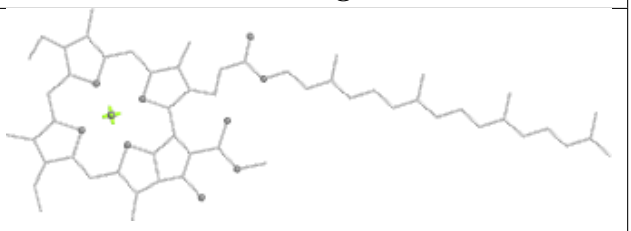
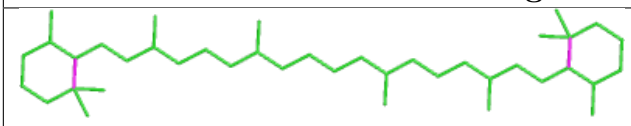


Rings

Ligand BCR b 617



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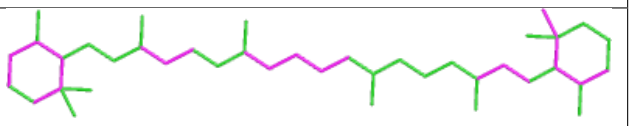

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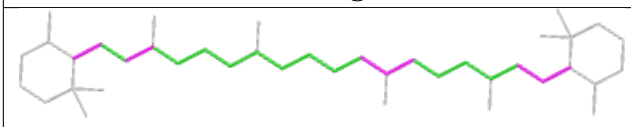

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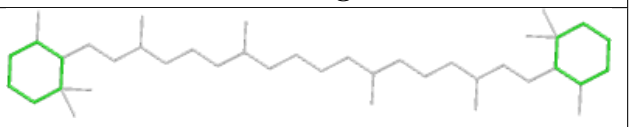
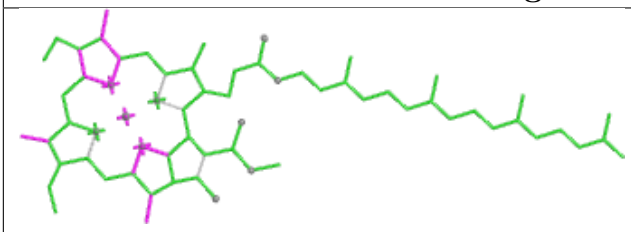


Rings

Ligand CLA C 504



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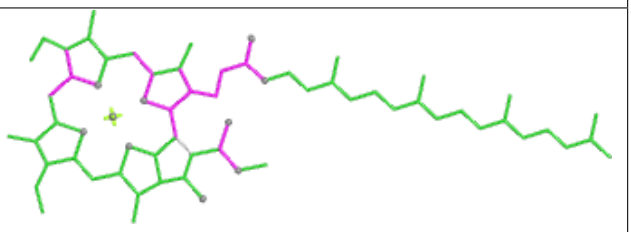

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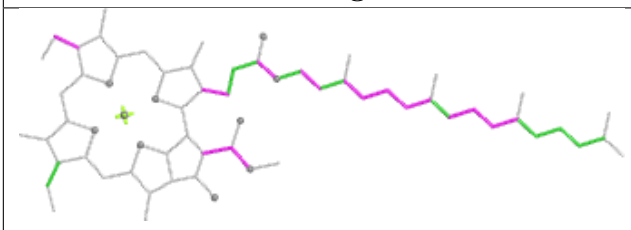

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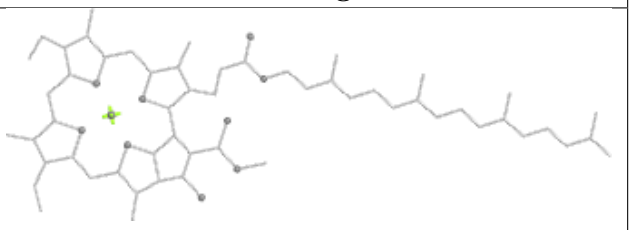
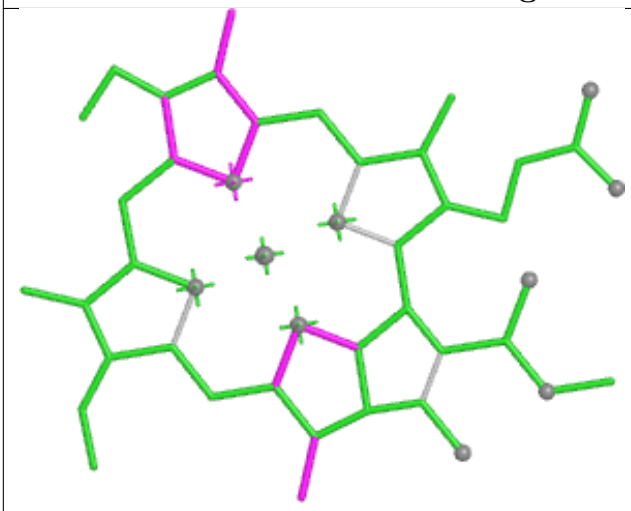


Rings

Ligand CLA 12 310



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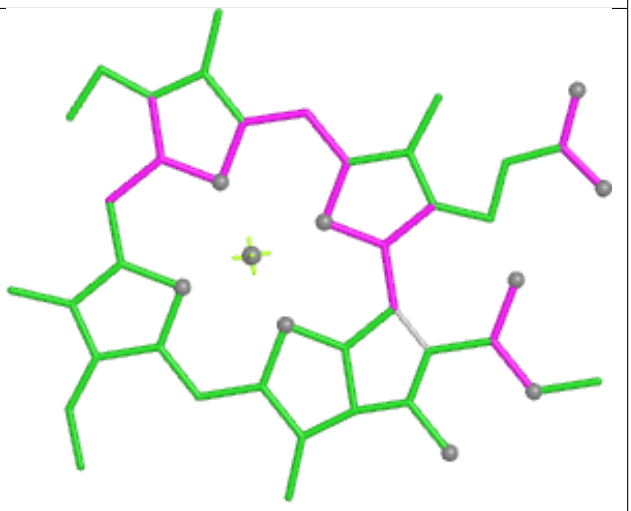
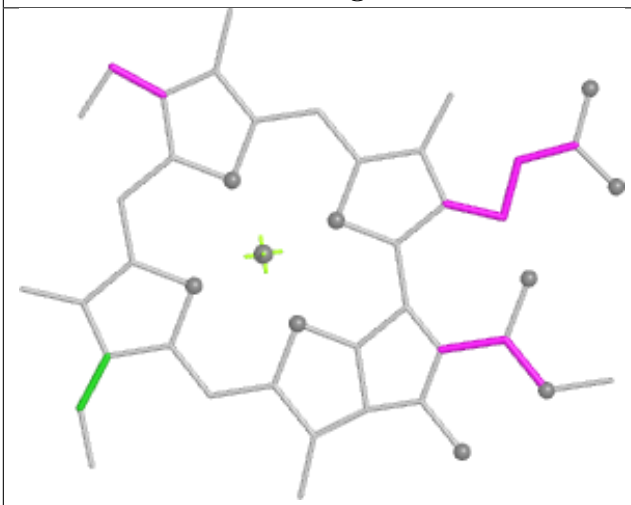


Bond angles



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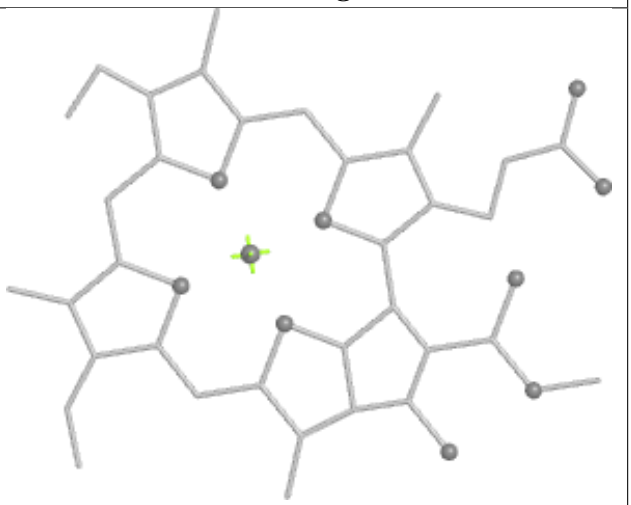
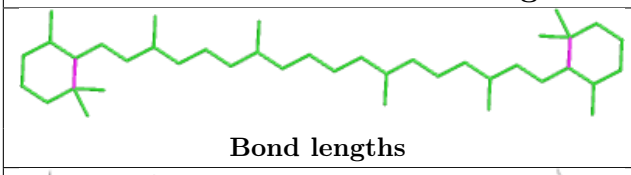


Rings

Ligand BCR m 103



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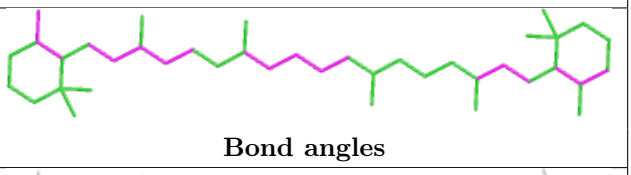
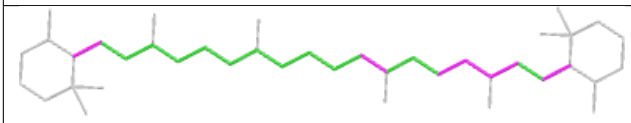


Bond angles



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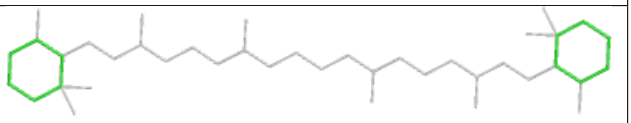
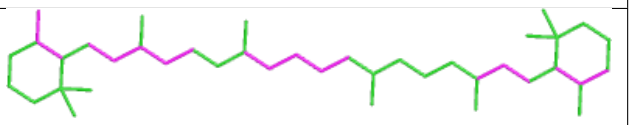


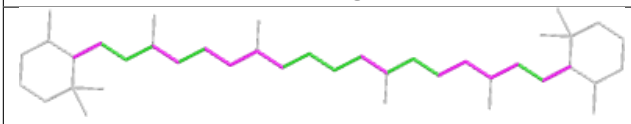
Rings

Ligand BCR Z 101

Bond lengths



Bond angles



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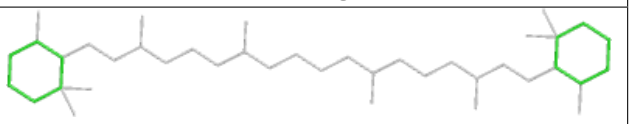
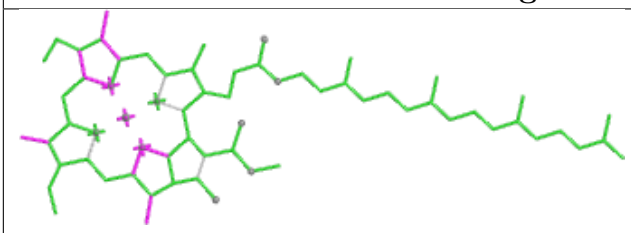


Rings

Ligand CLA 12 312



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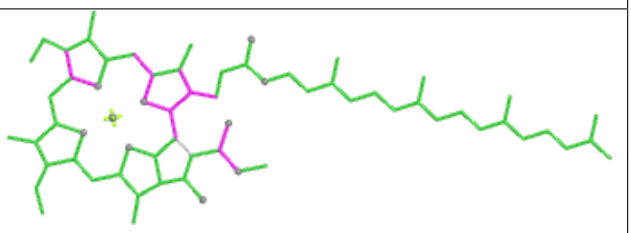
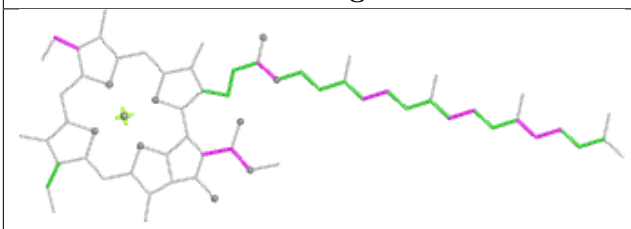


Bond angles



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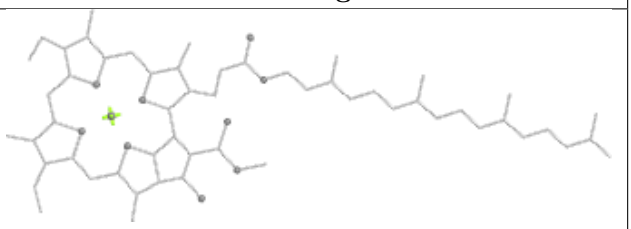
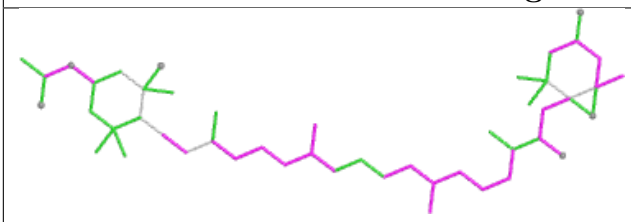


Rings

Ligand A86 11 316



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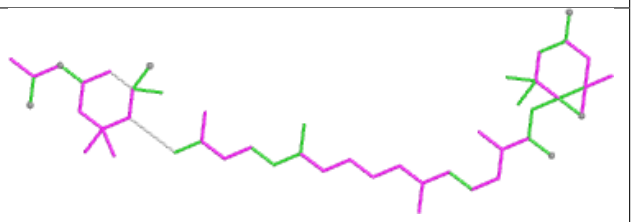
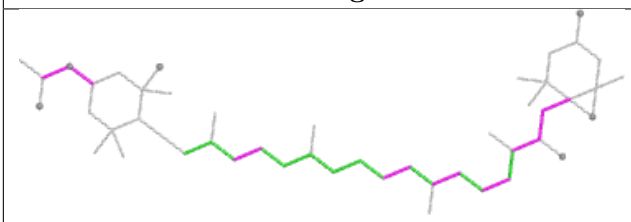
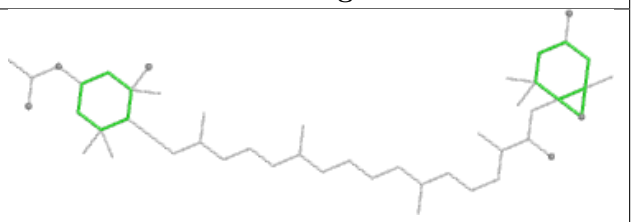


Bond angles

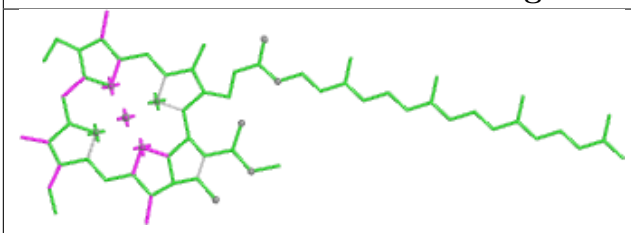


Torsions



Rings

Ligand CLA B 604



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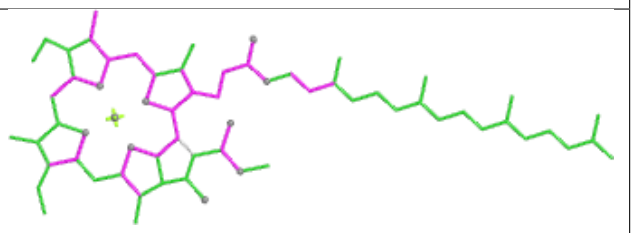
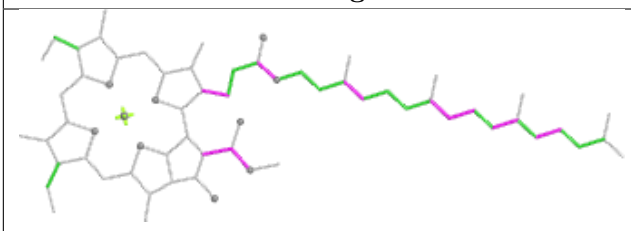


Bond angles



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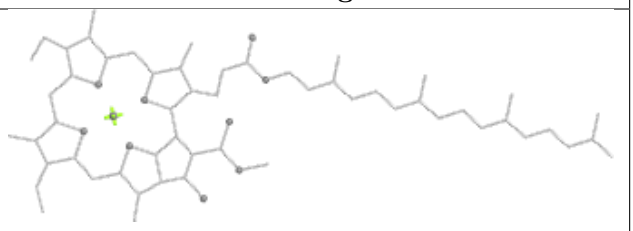
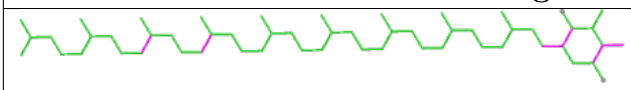


Rings

Ligand PL9 d 405



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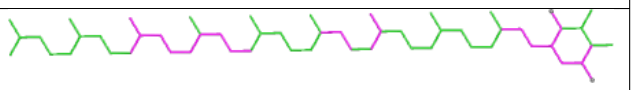

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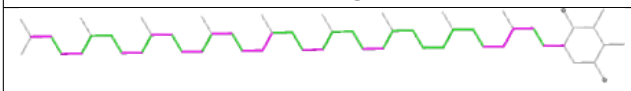

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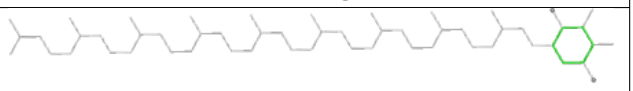
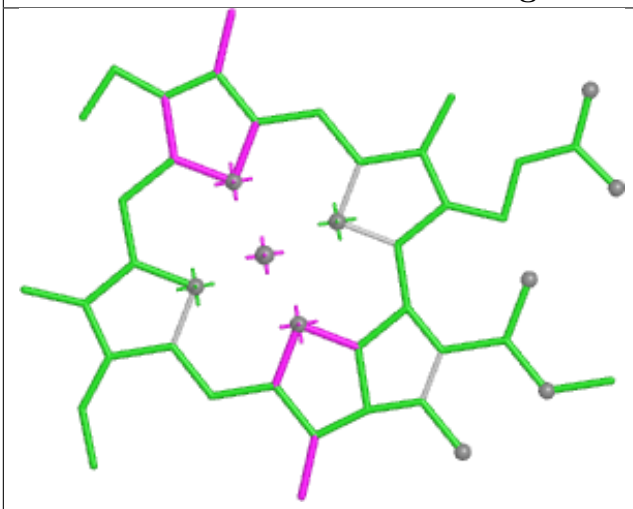


Rings

Ligand CLA 17 306



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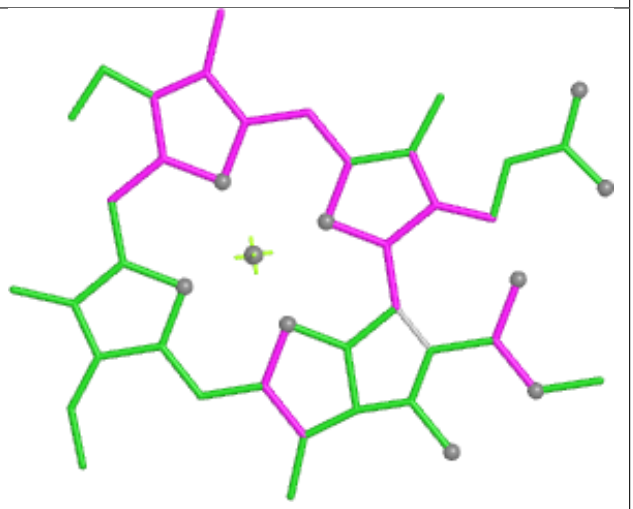

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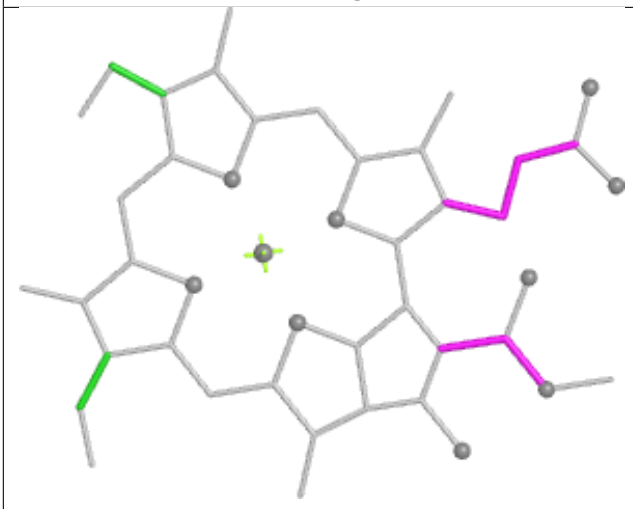
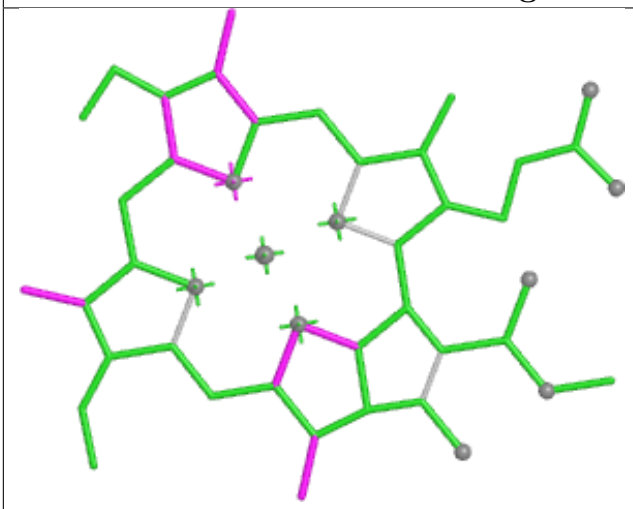


Torsions

Rings

Ligand CLA 21 302



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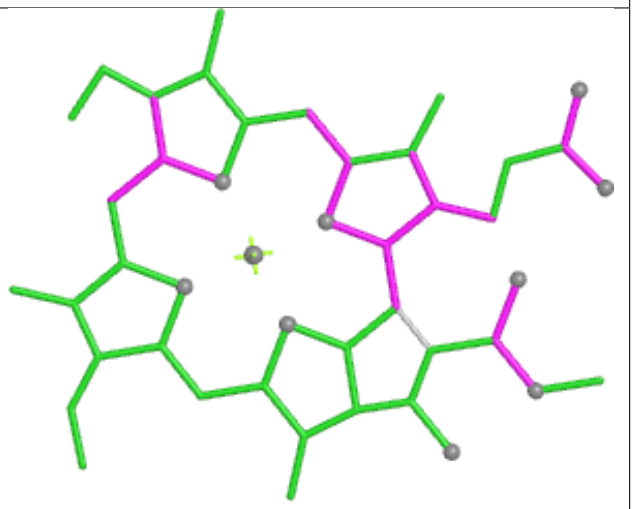

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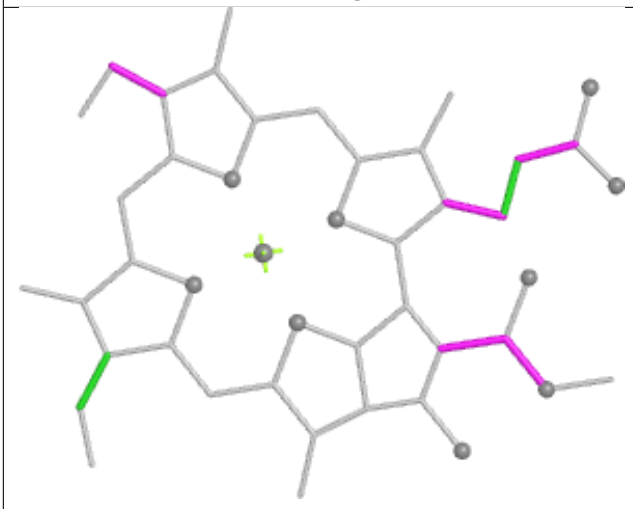

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Rings

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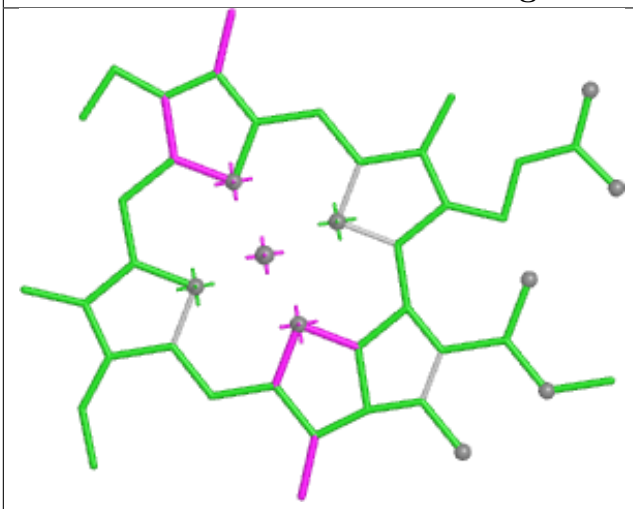

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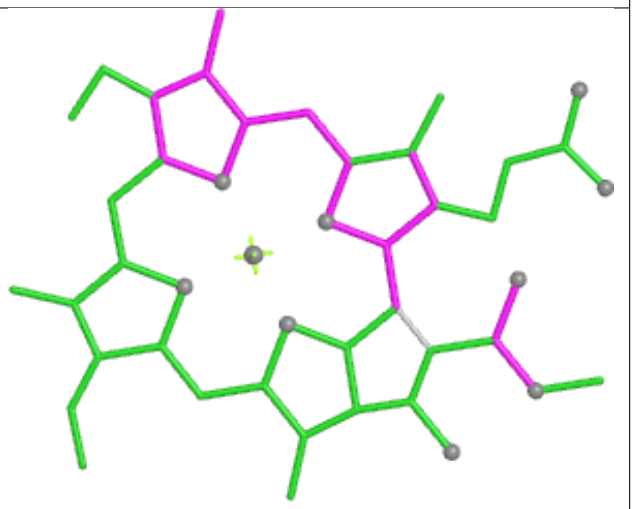

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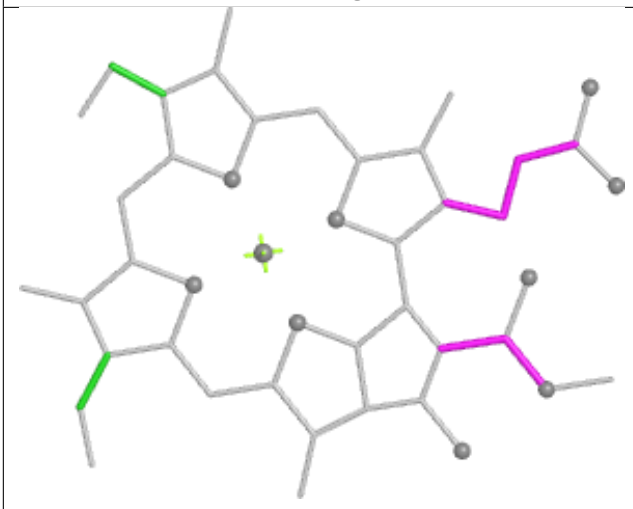

Torsions

Rings

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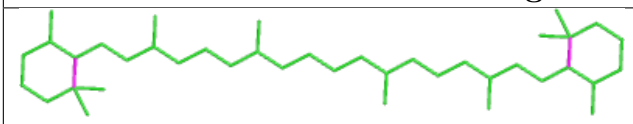

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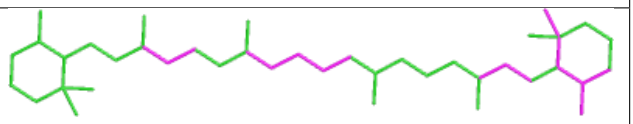

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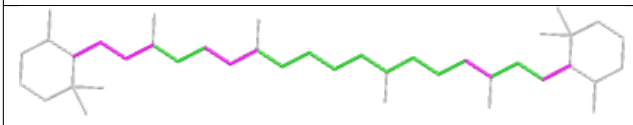

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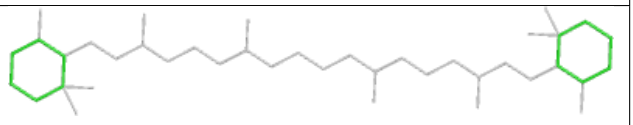
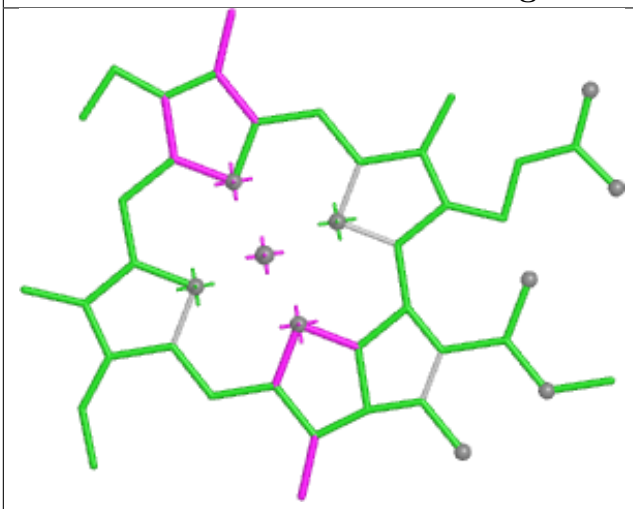


Rings

Ligand CLA 16 305



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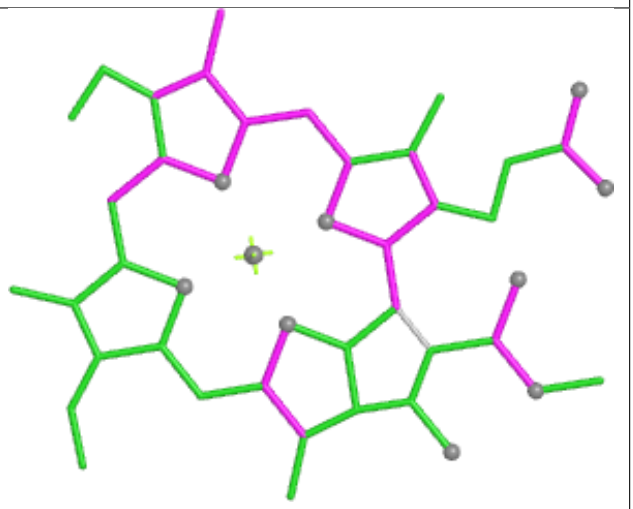

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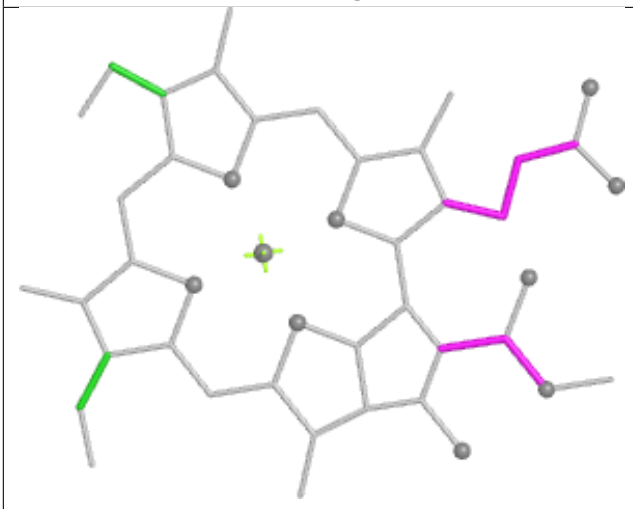

Torsions

Rings

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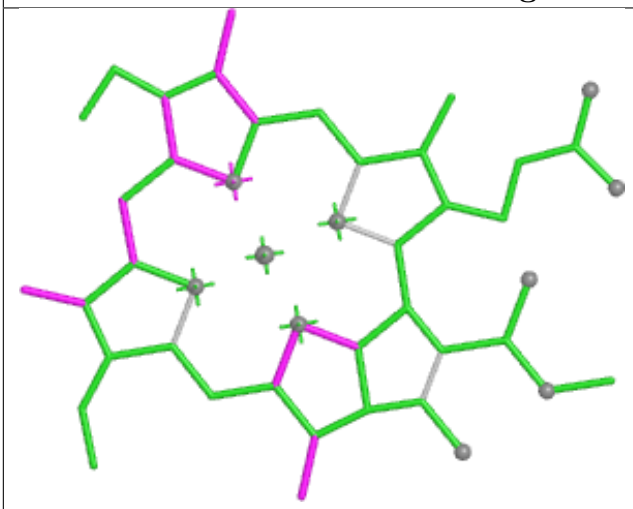

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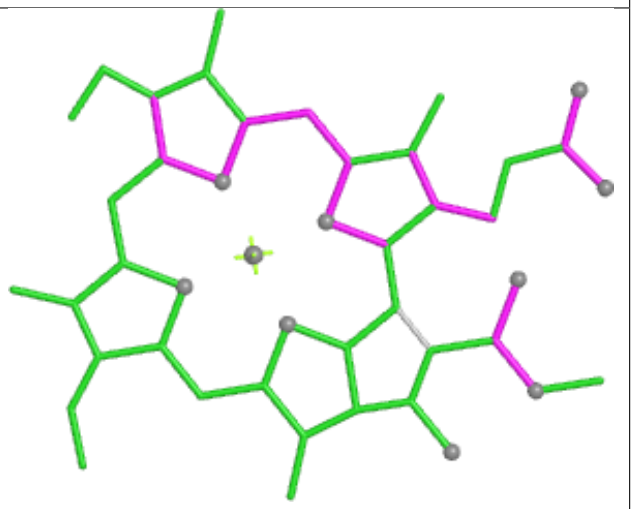

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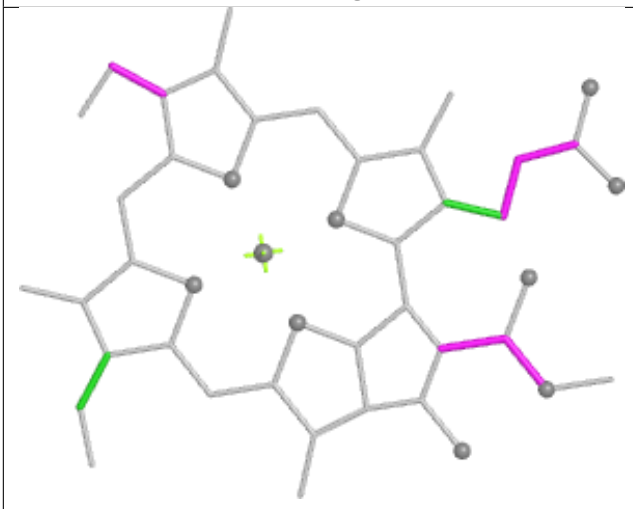

Torsions

Rings

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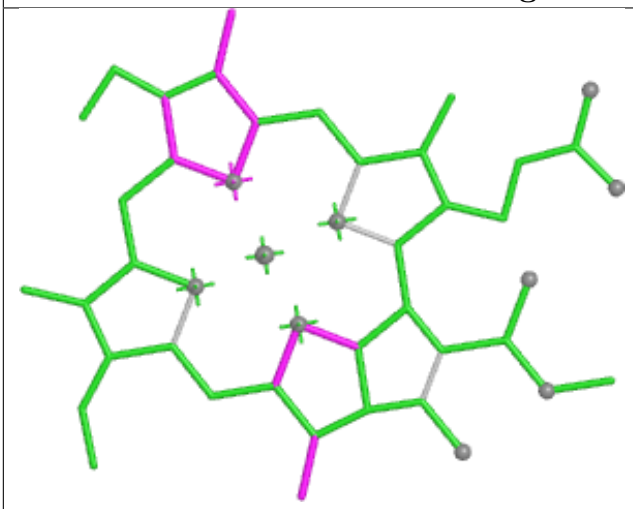

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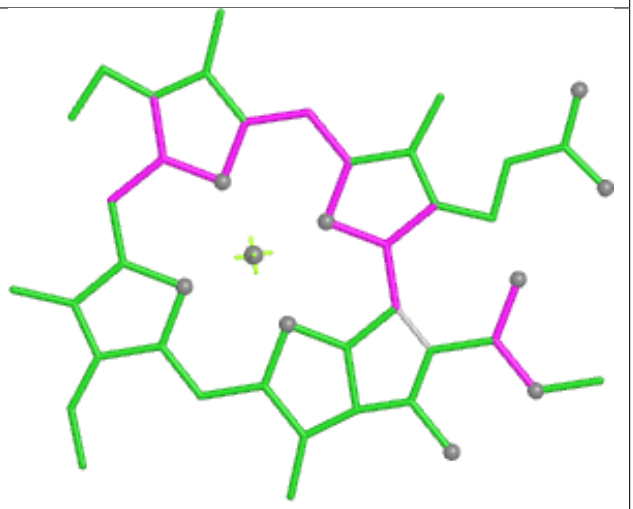

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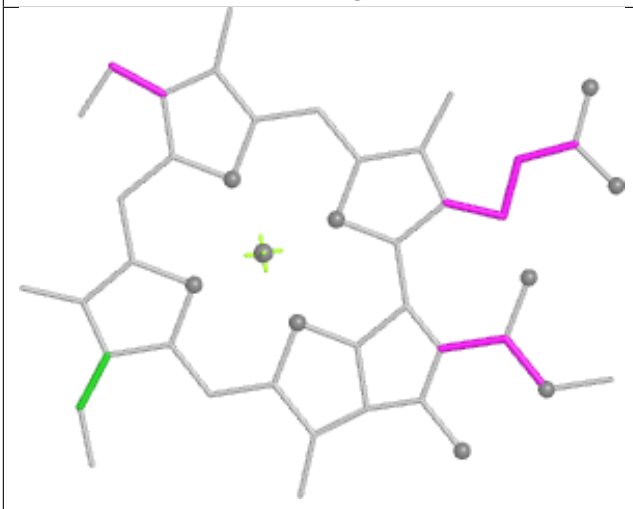

Torsions

Rings

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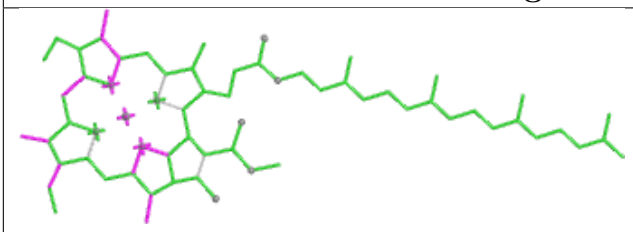

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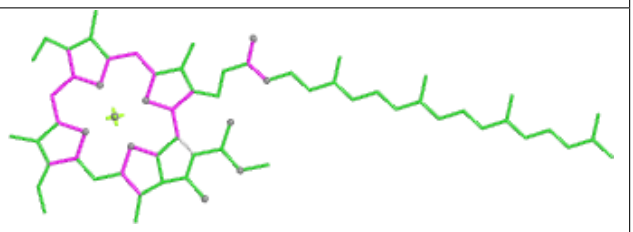

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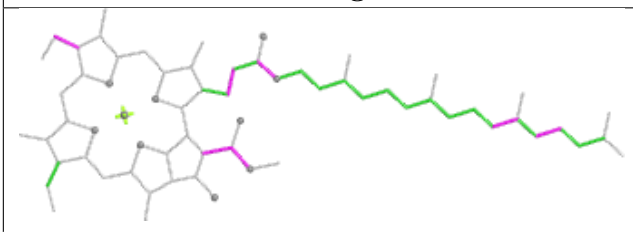

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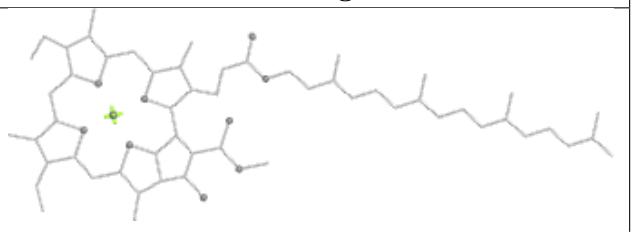
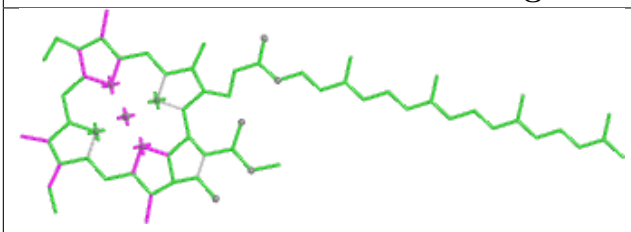


Rings

Ligand CLA B 610



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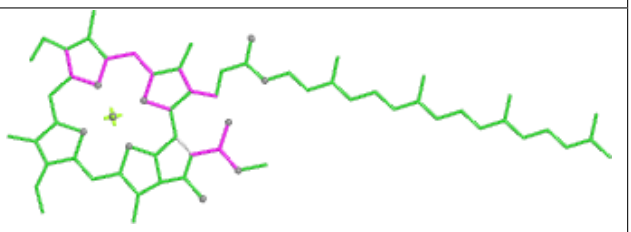

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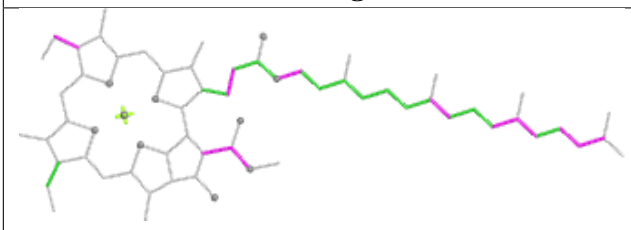

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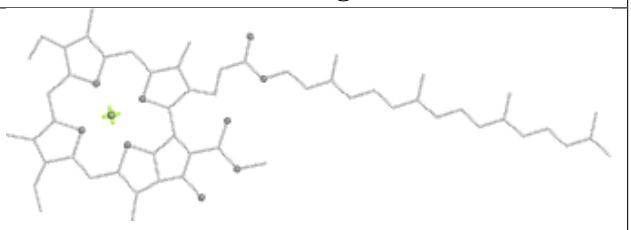
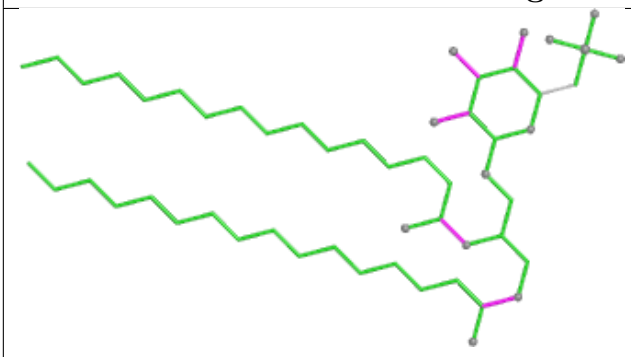


Rings

Ligand SQD L 103



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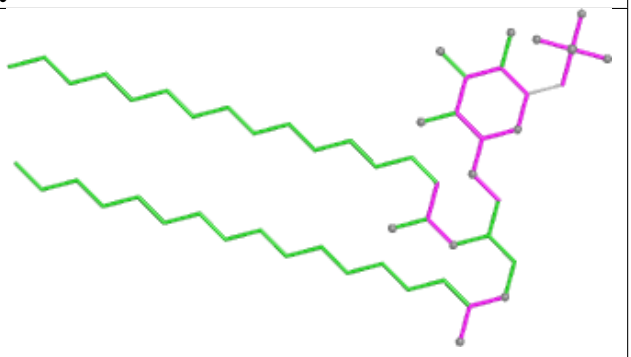

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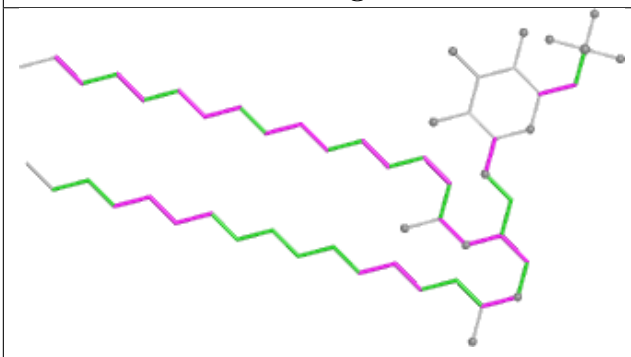

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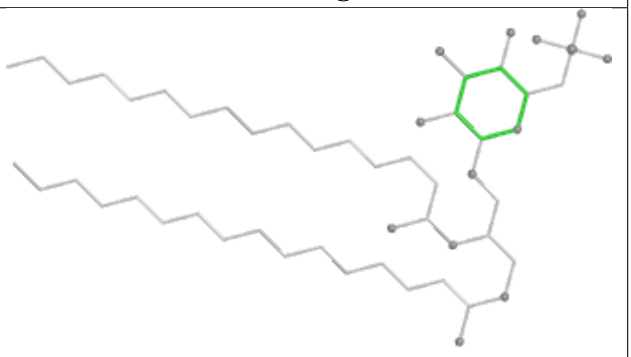
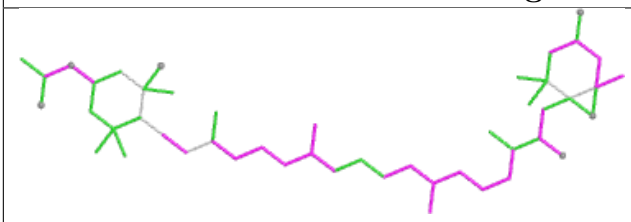


Rings

Ligand A86 20 201



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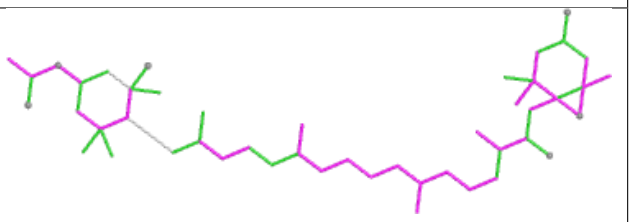

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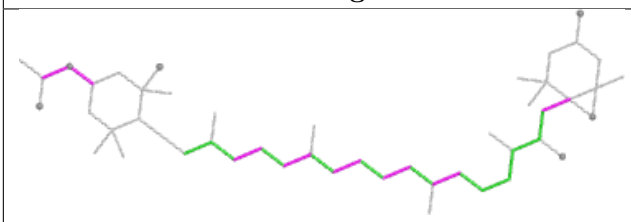

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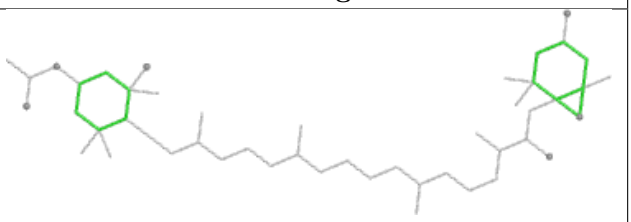
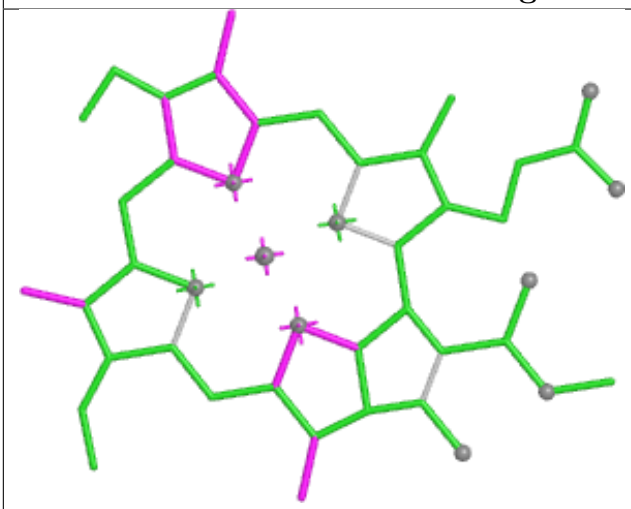


Rings

Ligand CLA 19 302



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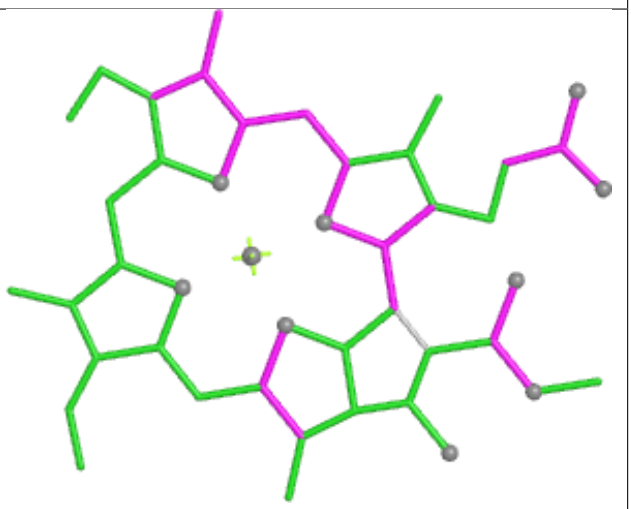

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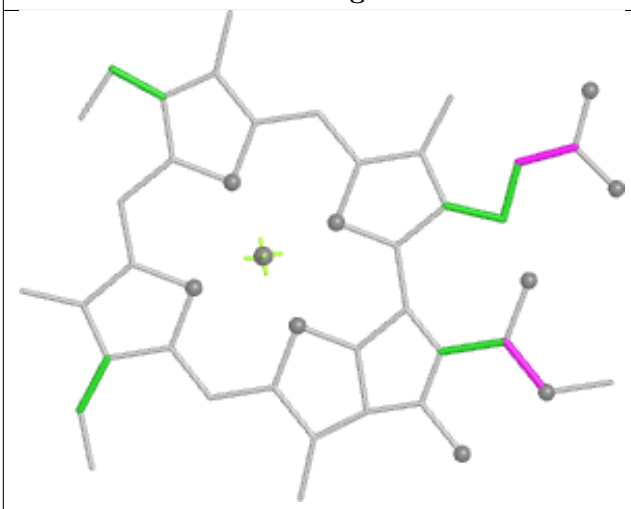

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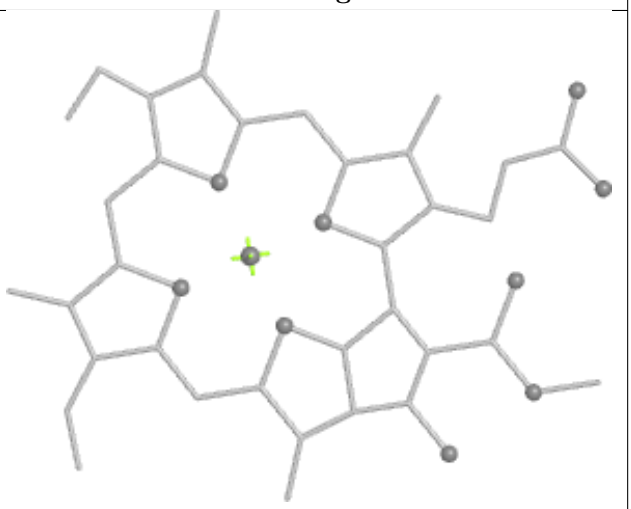
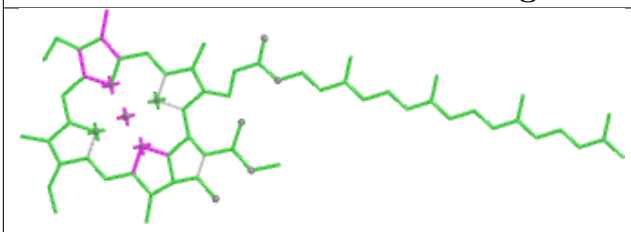


Rings

Ligand CLA 21 303



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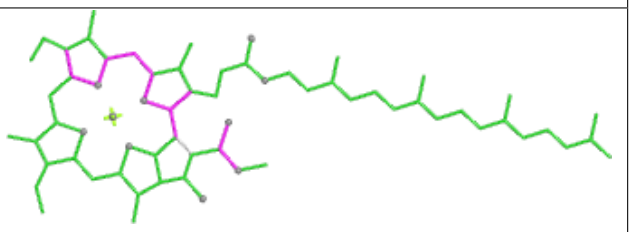

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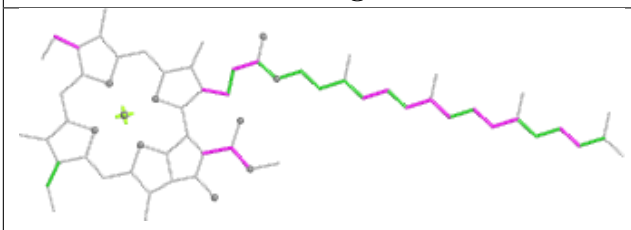

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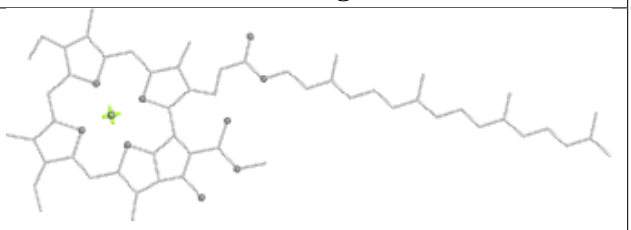
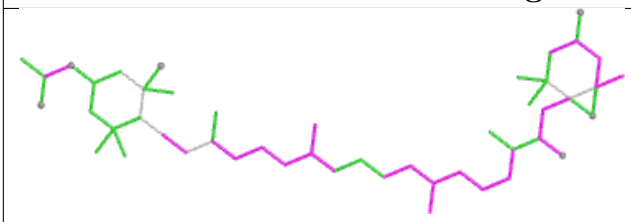


Rings

Ligand A86 12 317



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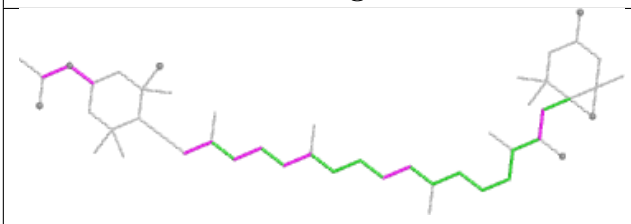
Bond angles



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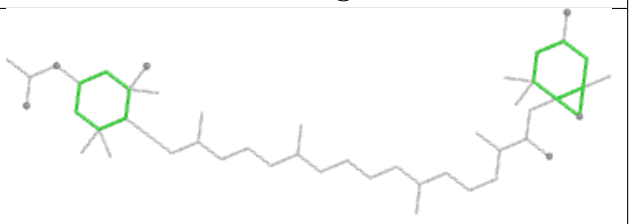
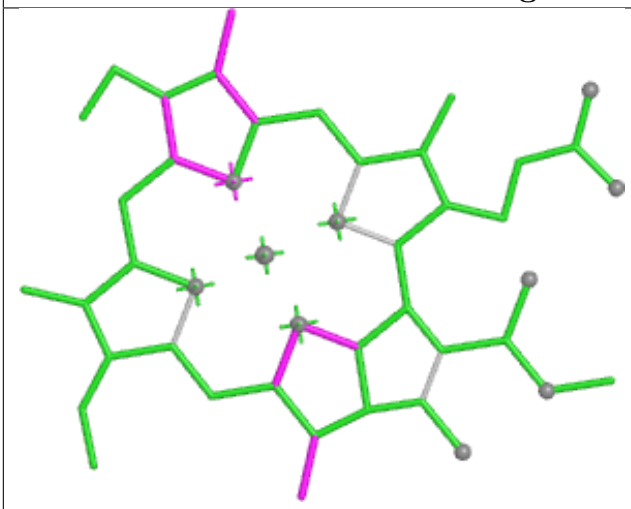


Rings

Ligand CLA 21 308



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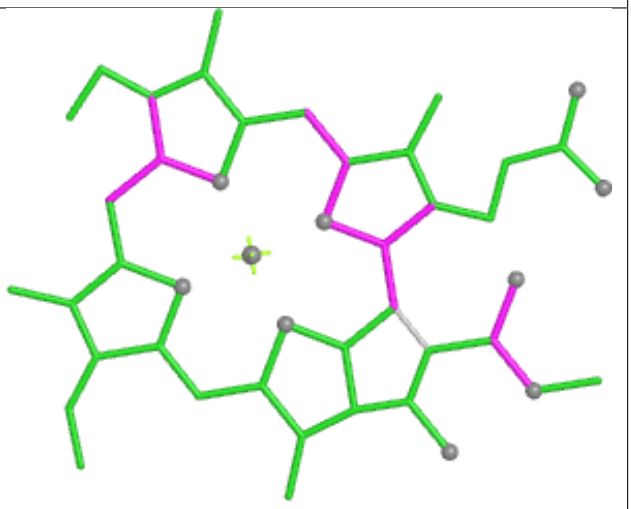

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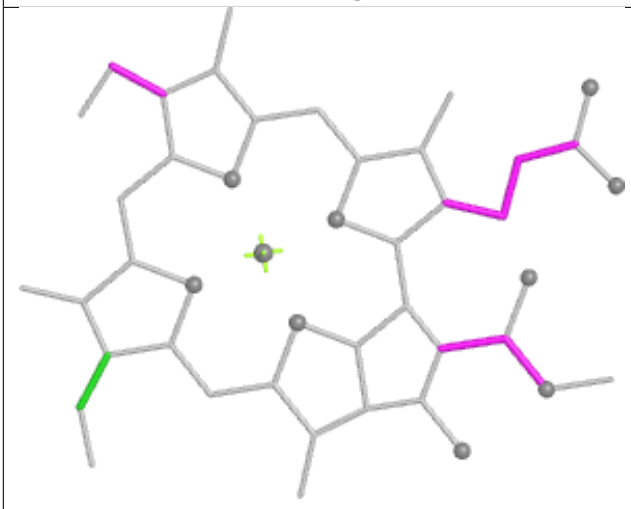

Torsions

Rings

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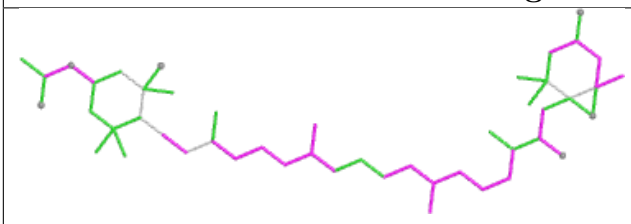

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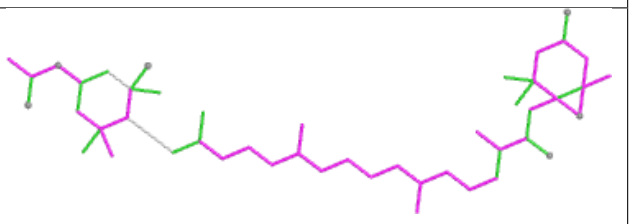

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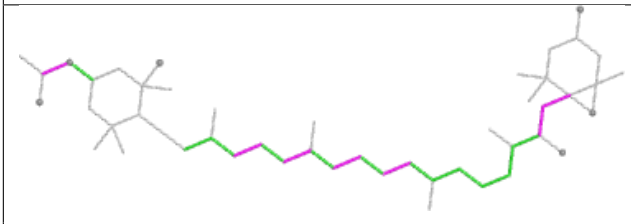

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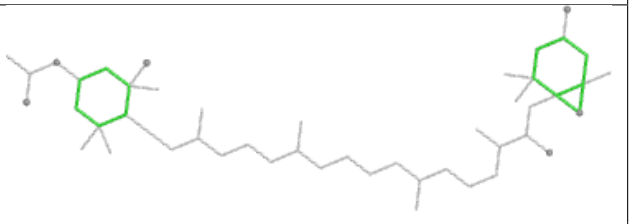

Rings

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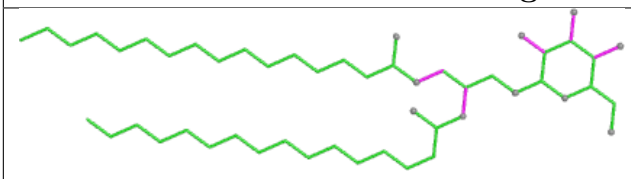
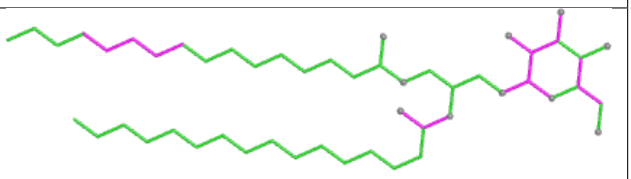
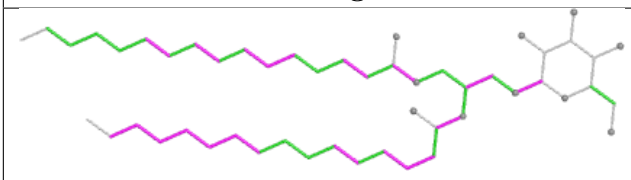
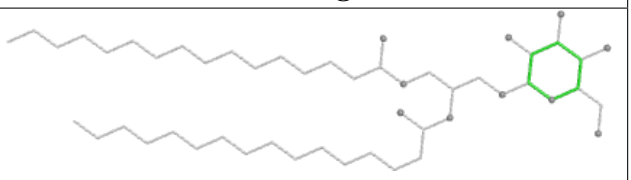
 Bond lengths	 Bond angles
 Torsions	 Rings

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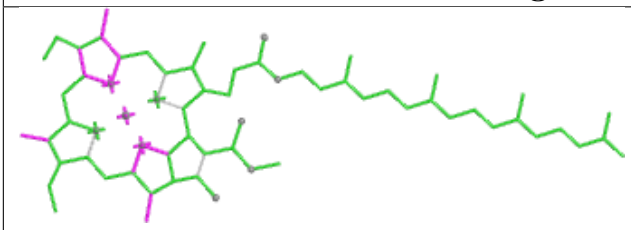
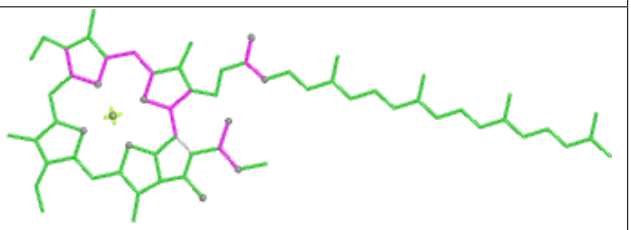
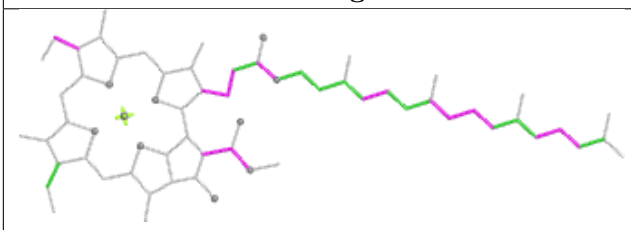
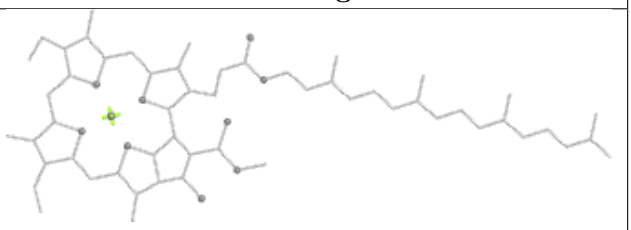
 Bond lengths	 Bond angles
 Torsions	 Rings

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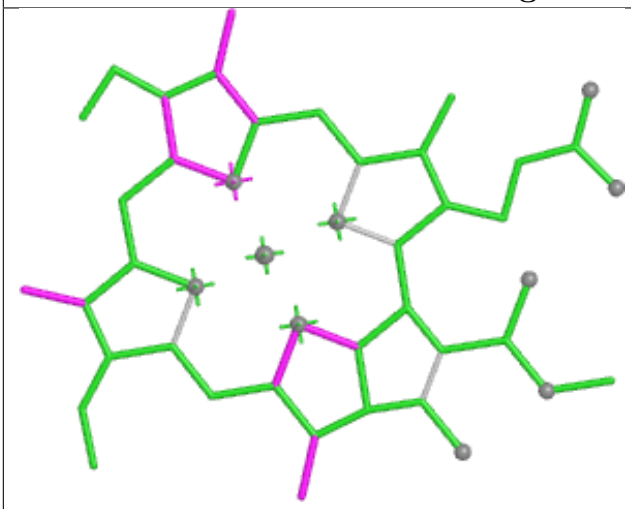

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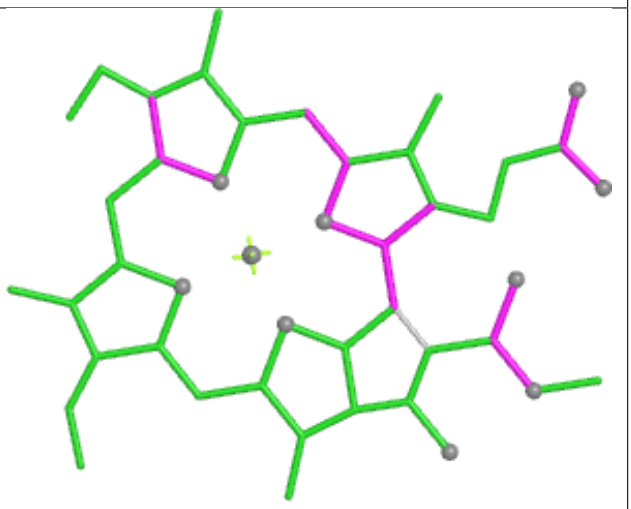

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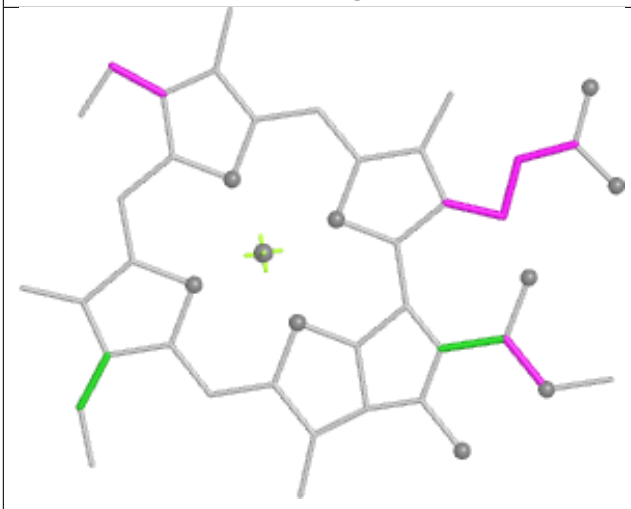
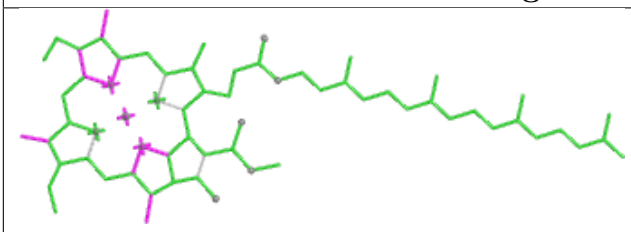


Torsions

Rings

Ligand CLA m 101



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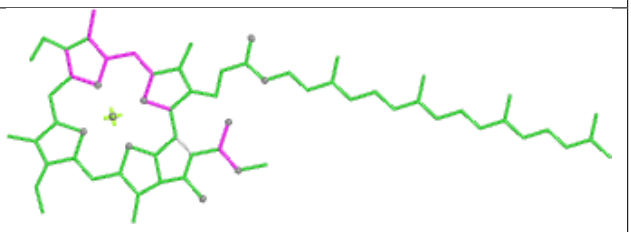

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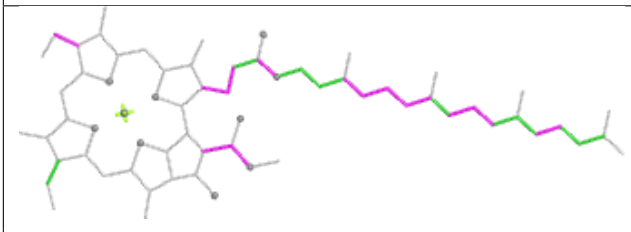

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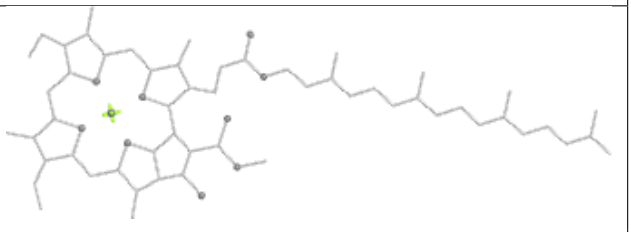

Rings

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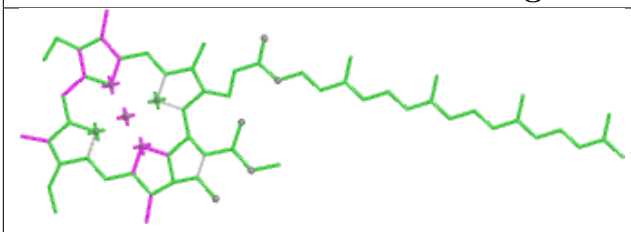

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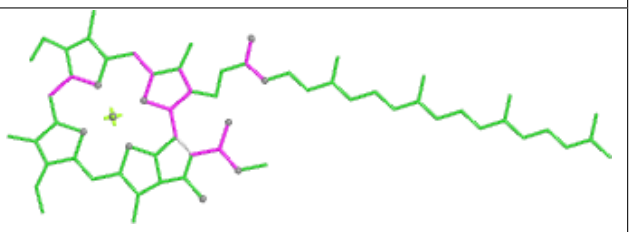

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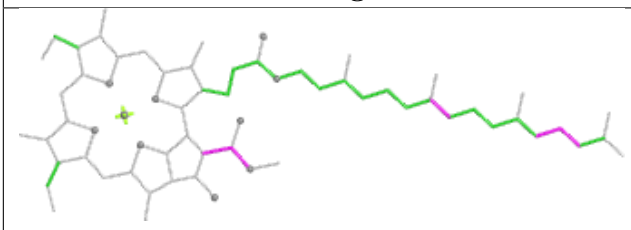

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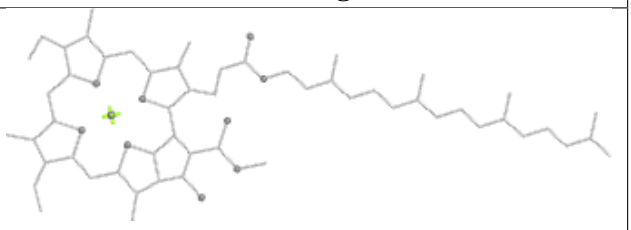
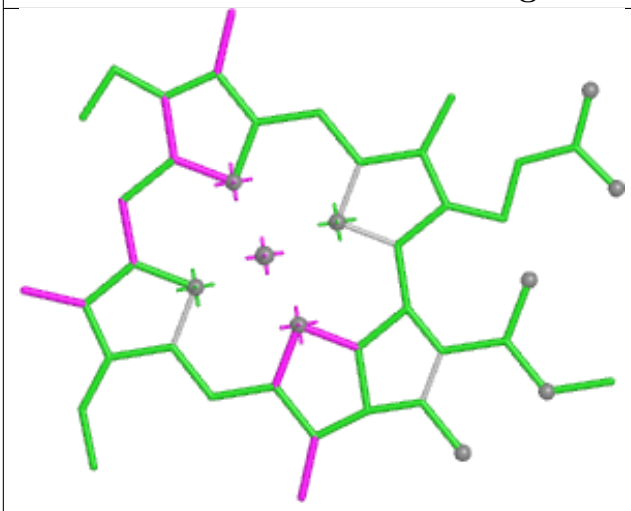


Rings

Ligand CLA 16 307



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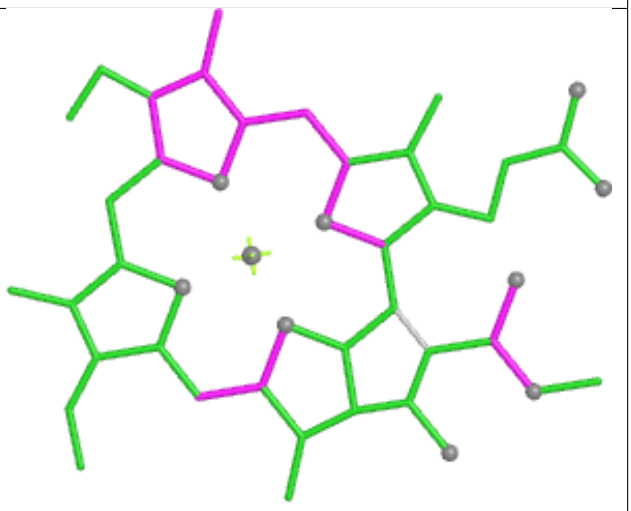

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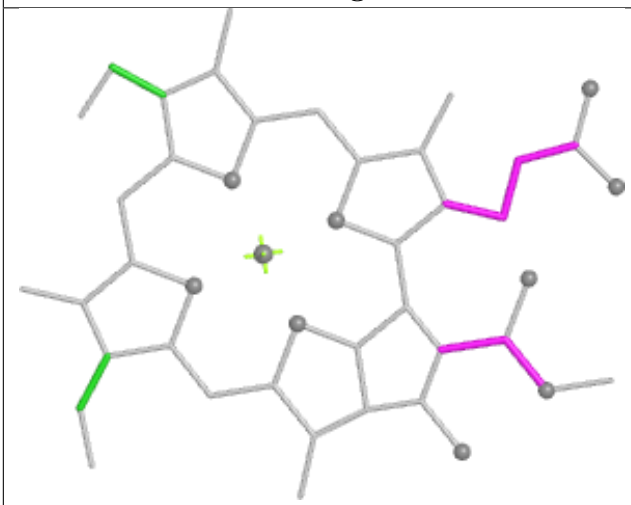

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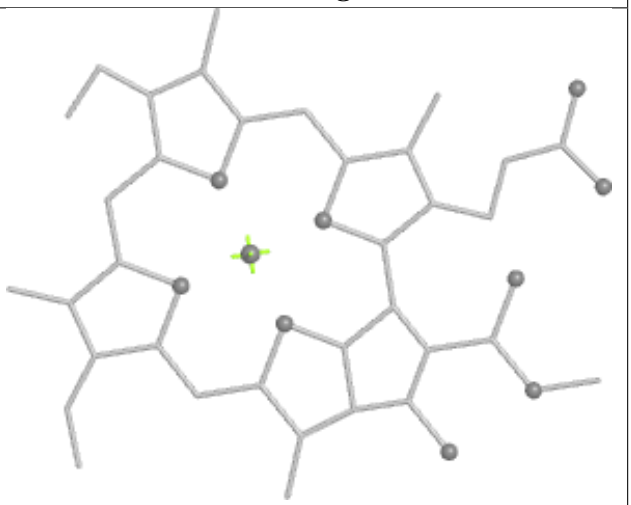
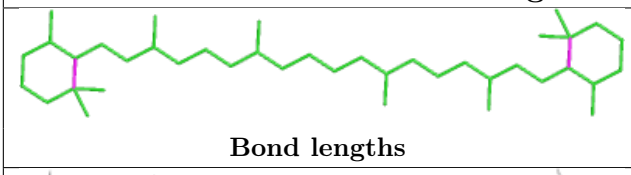


Rings

Ligand BCR a 404



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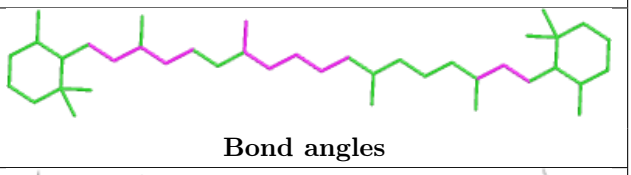

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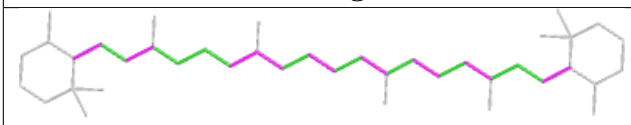

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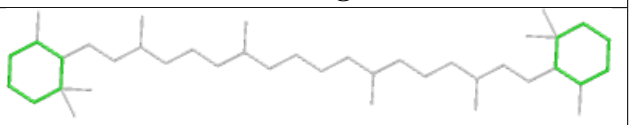
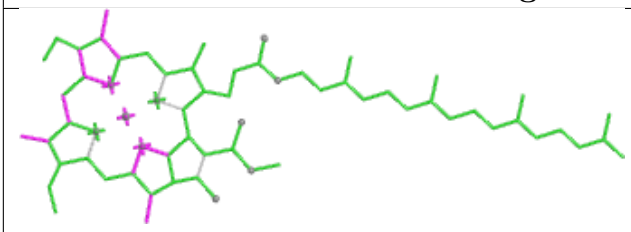


Rings

Ligand CLA 15 307



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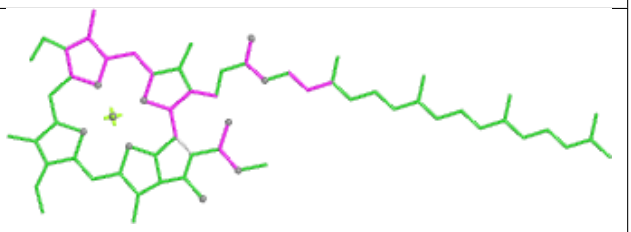

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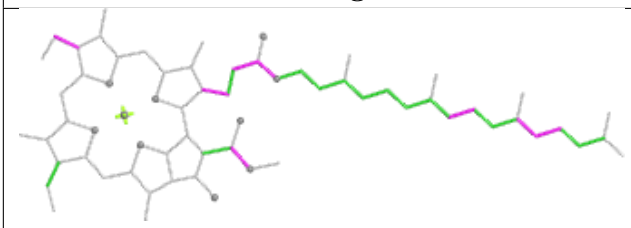

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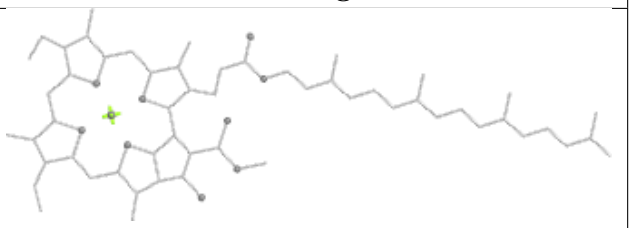
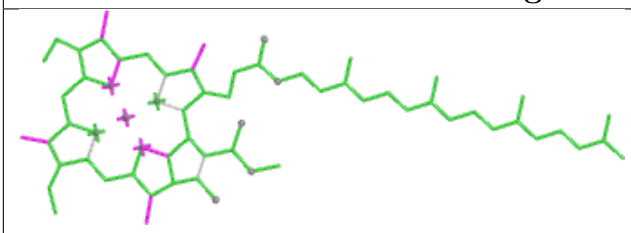


Rings

Ligand CLA B 612



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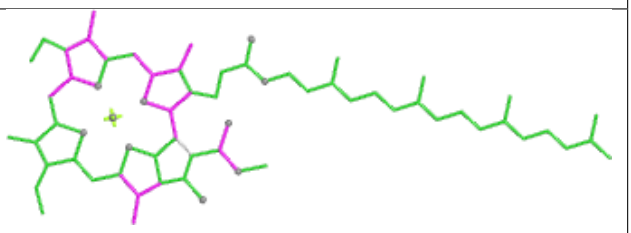

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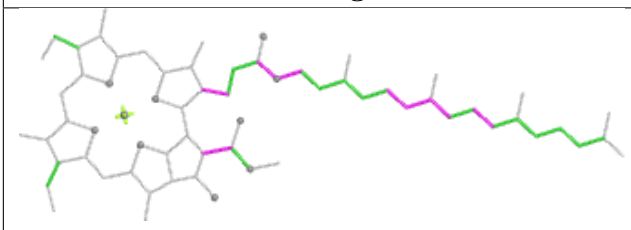

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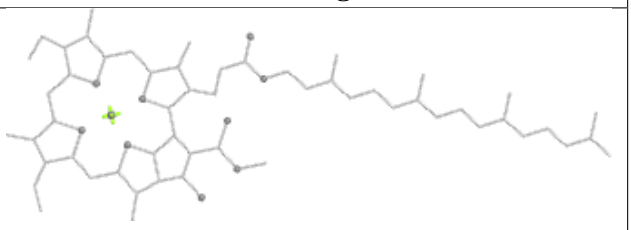
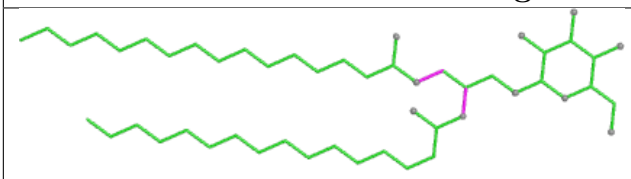


Rings

Ligand LMG W 101



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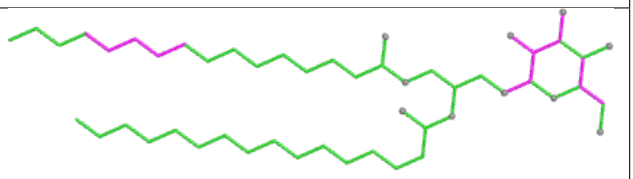
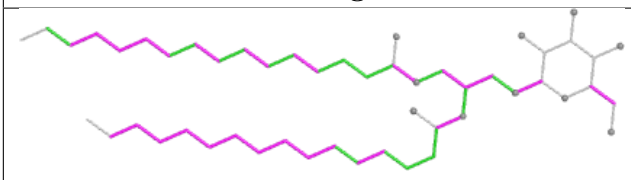


Bond angles



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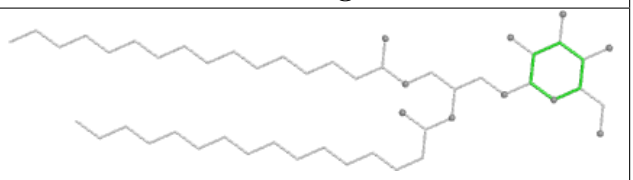
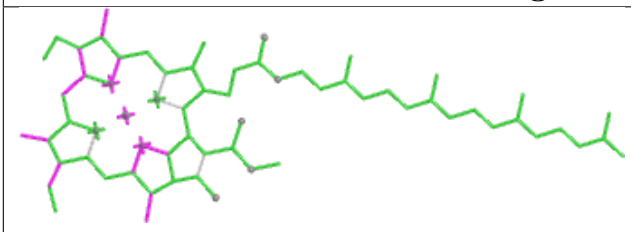


Rings

Ligand CLA c 505



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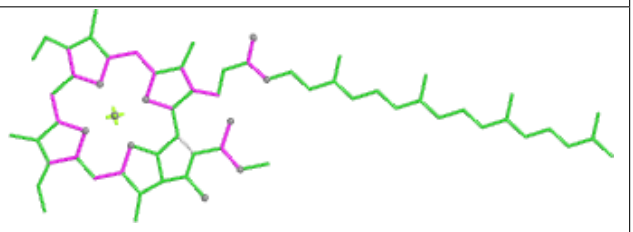

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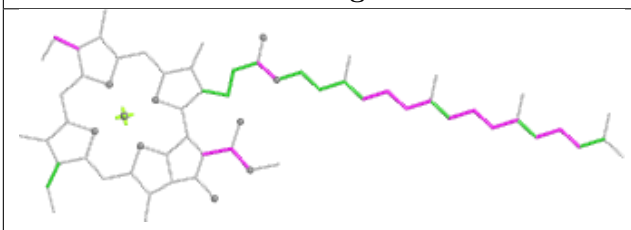

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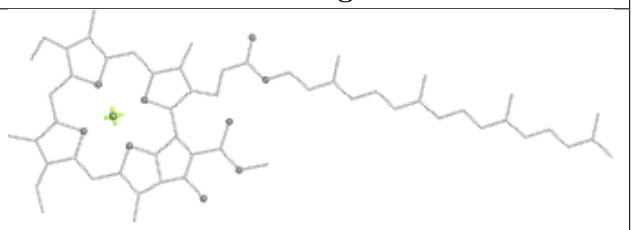
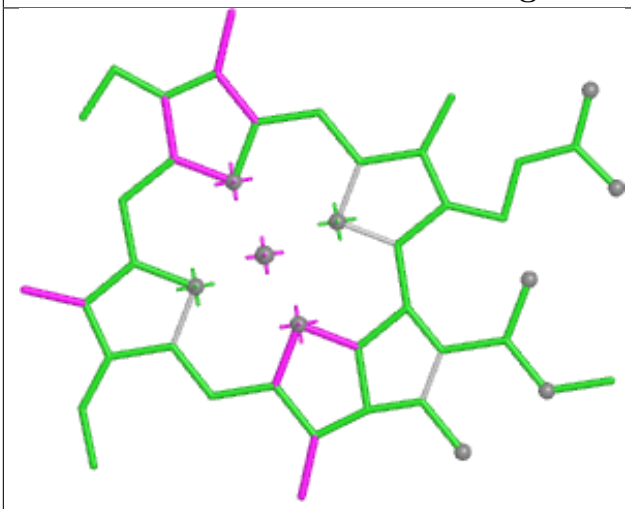


Rings

Ligand CLA 16 308



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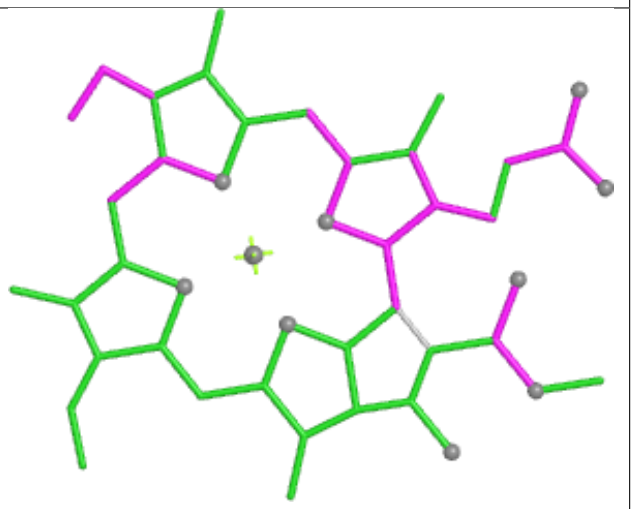
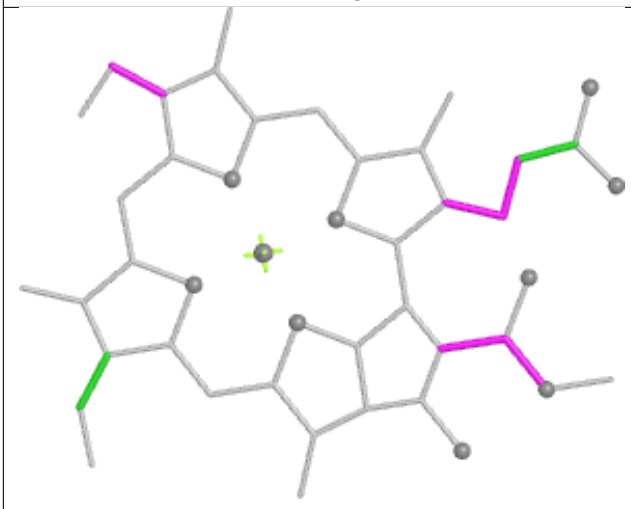


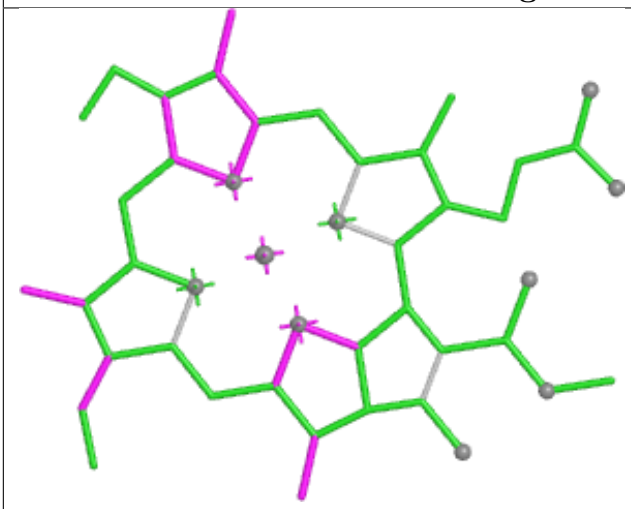
Bond angles



Torsions

Rings

Ligand CLA 17 304



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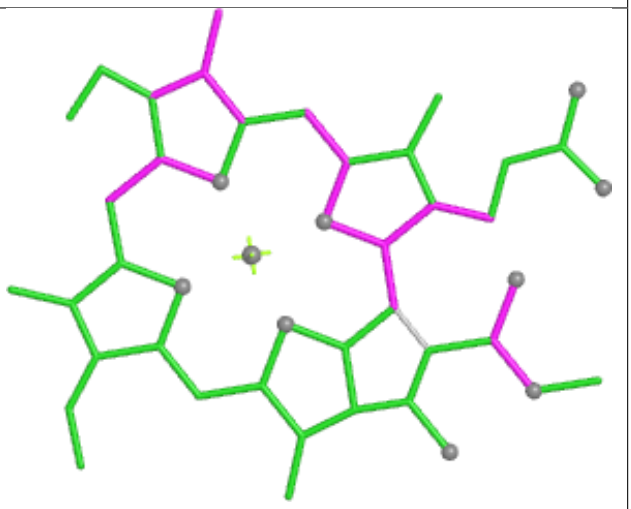

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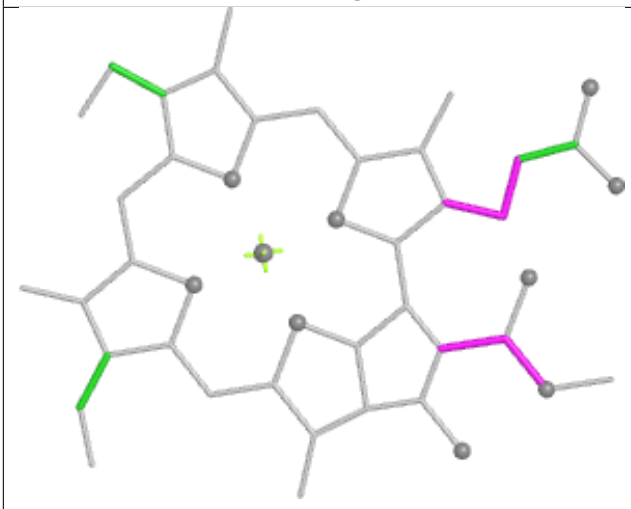
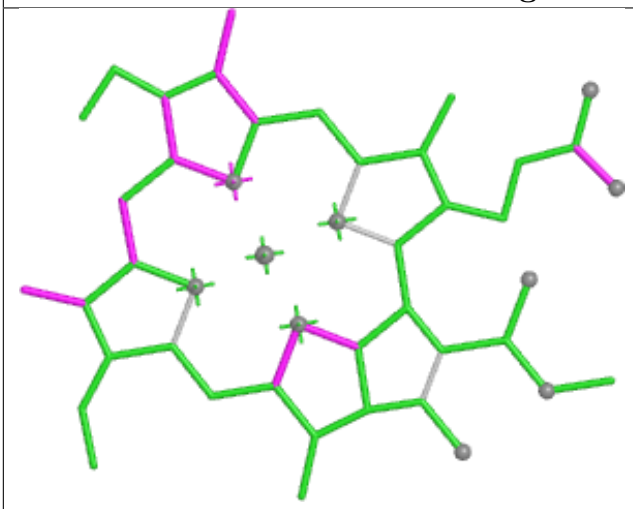


Torsions

Rings

Ligand CLA 21 309



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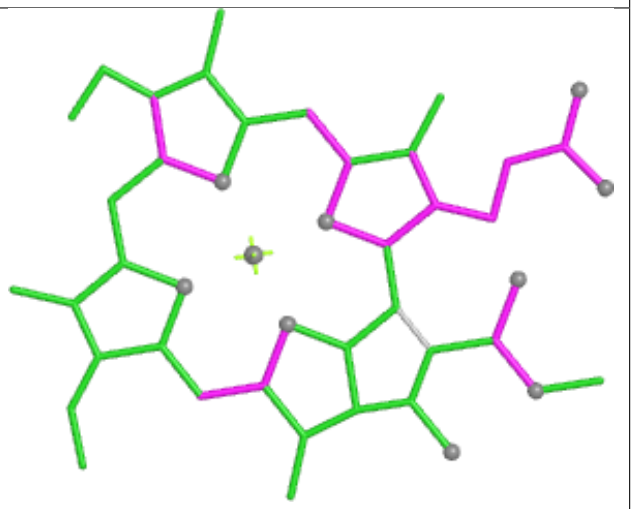

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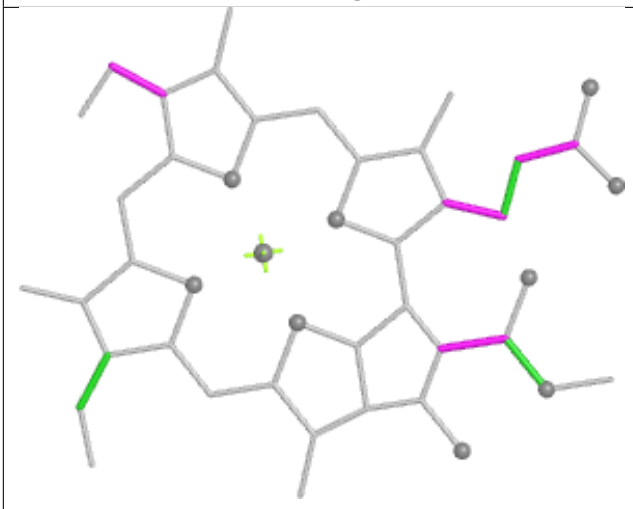
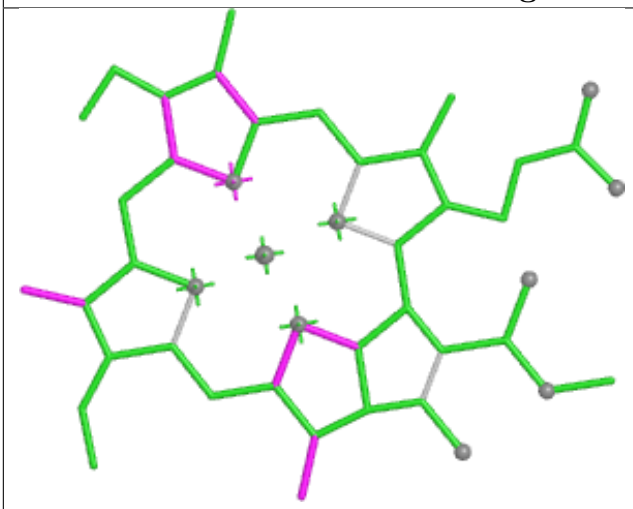


Torsions

Rings

Ligand CLA 20 208



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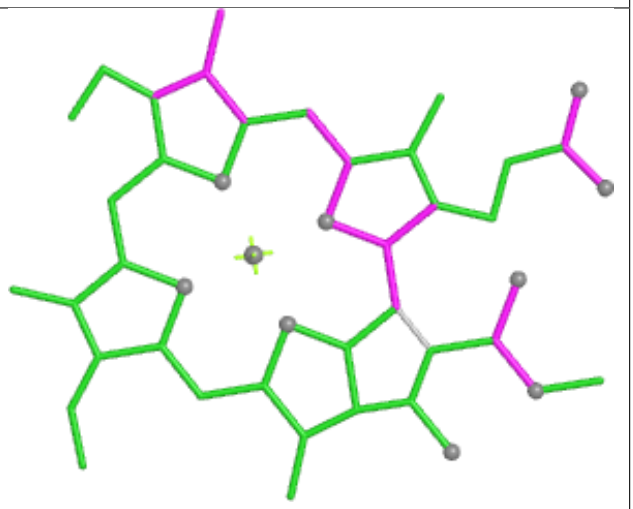

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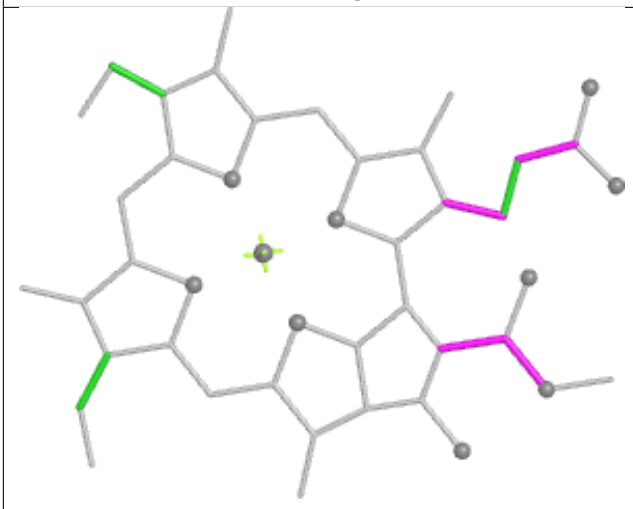
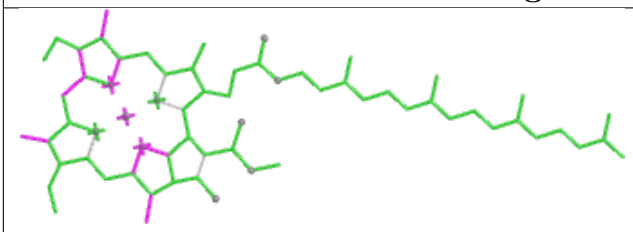


Torsions

Rings

Ligand CLA C 509



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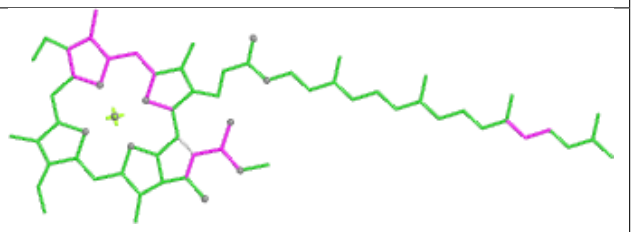

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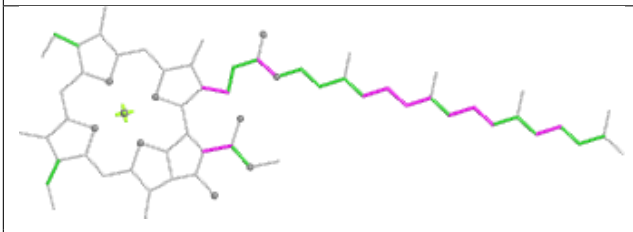

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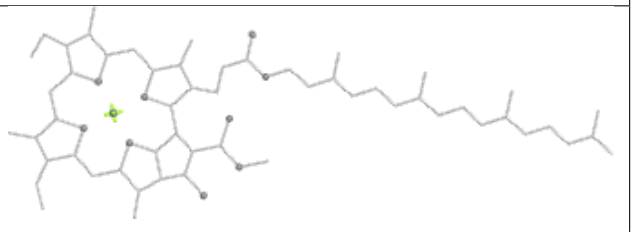
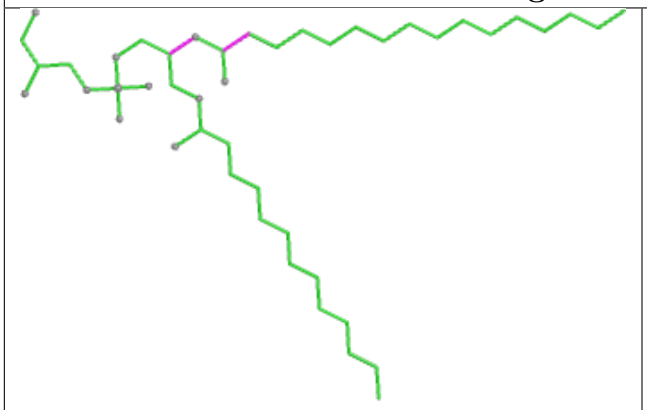


Rings

Ligand LHG a 407



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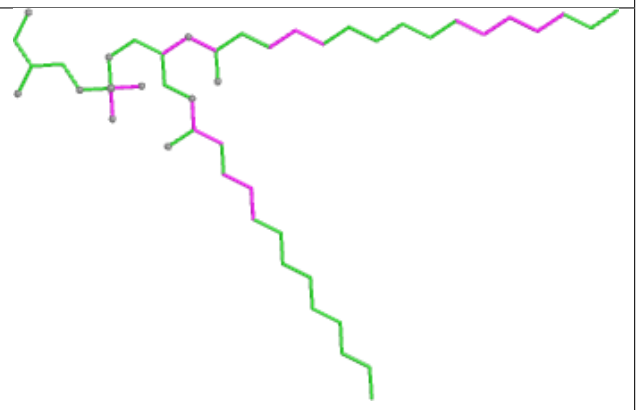

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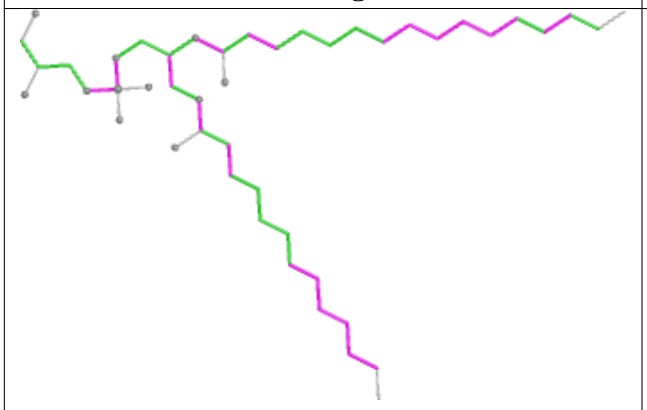

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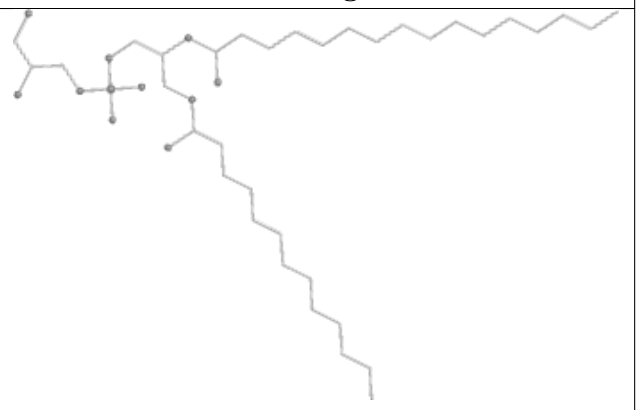
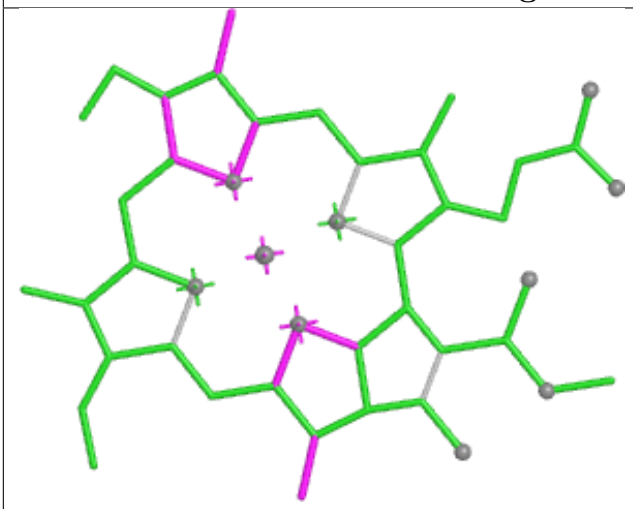


Rings

Ligand CLA 19 304



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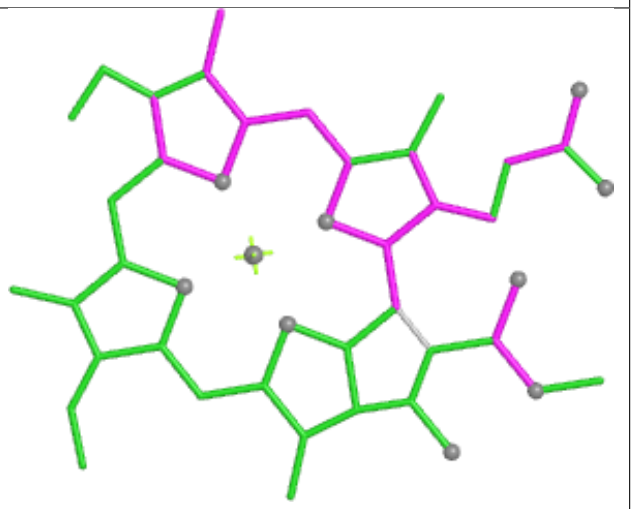

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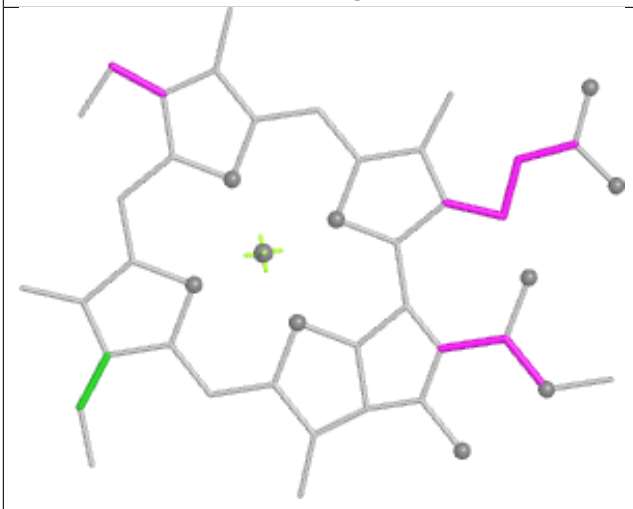

Torsions

Rings

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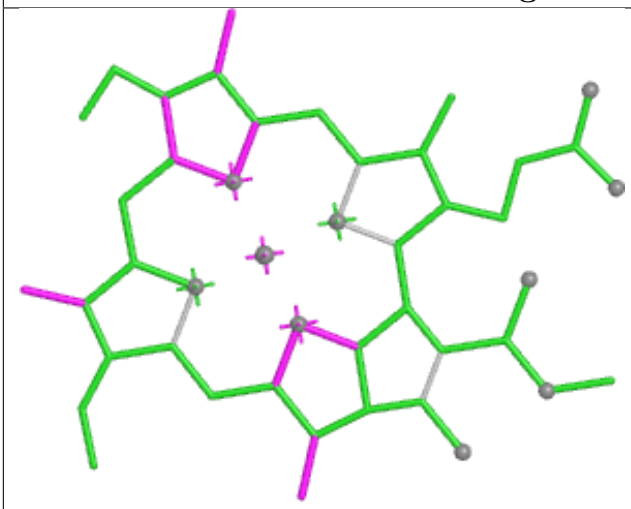

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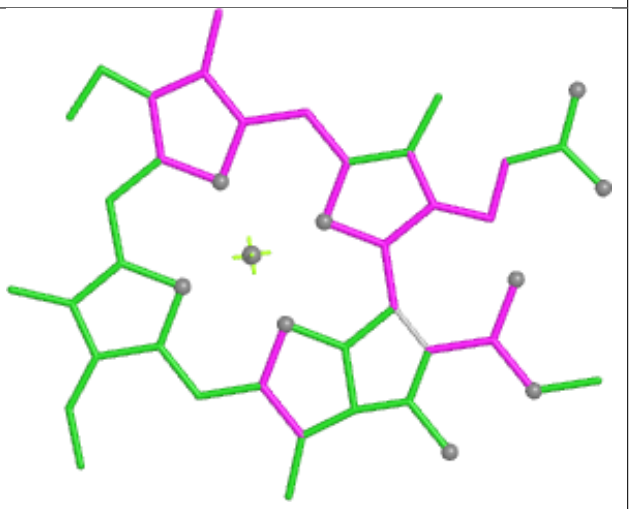

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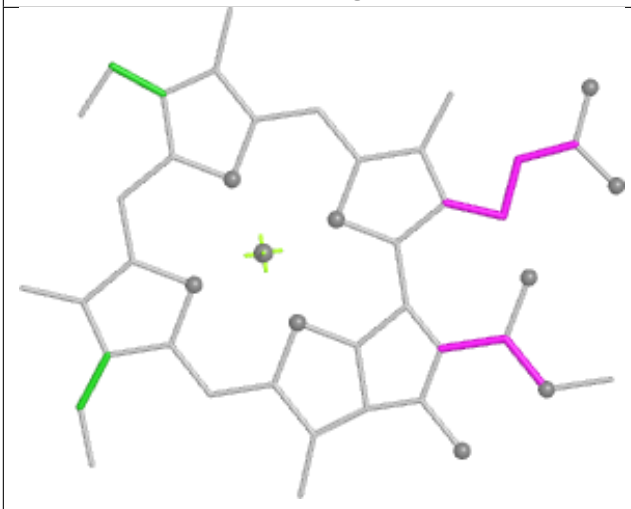
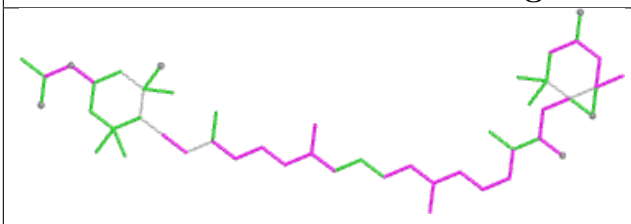


Torsions

Rings

Ligand A86 12 319



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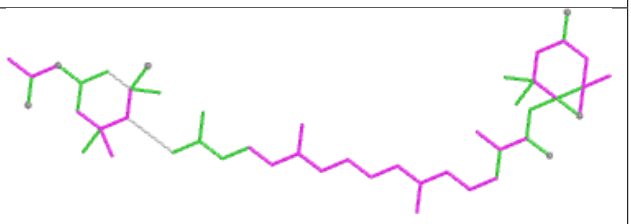

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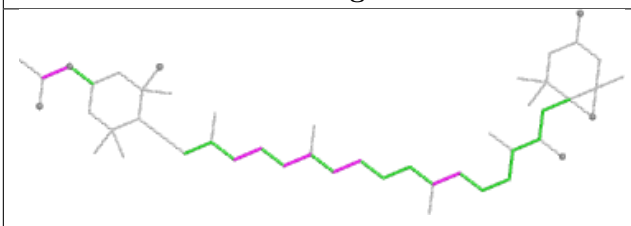

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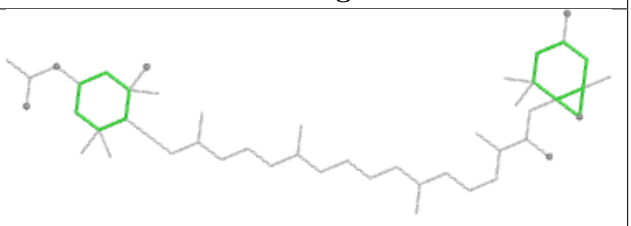
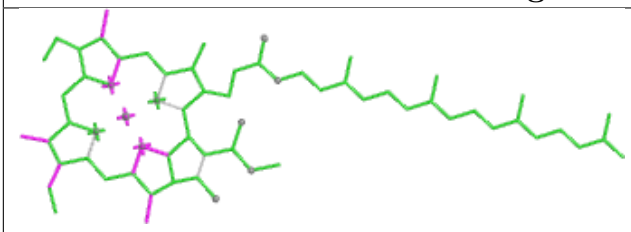


Rings

Ligand CLA d 401



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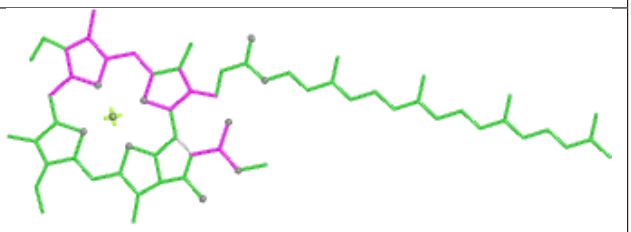

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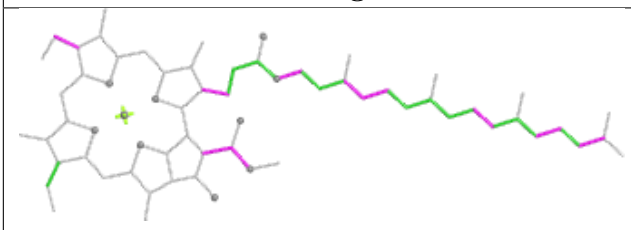

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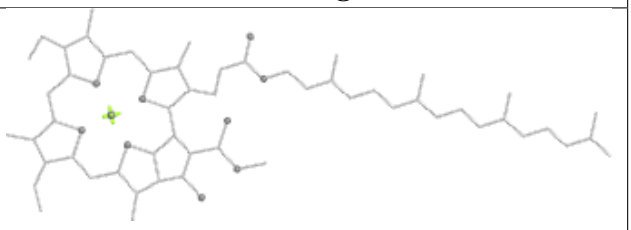
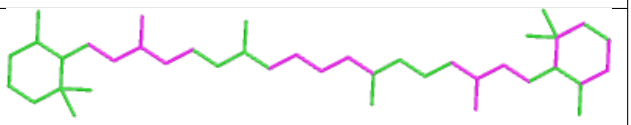


Rings

Ligand BCR c 520

Bond lengths



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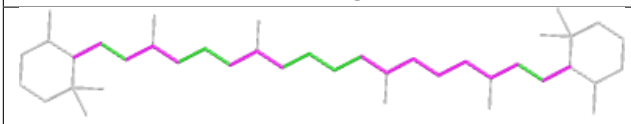

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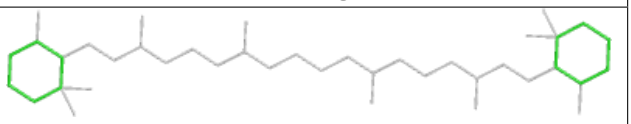
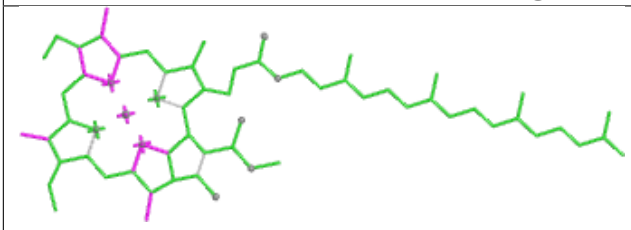


Rings

Ligand CLA z 101



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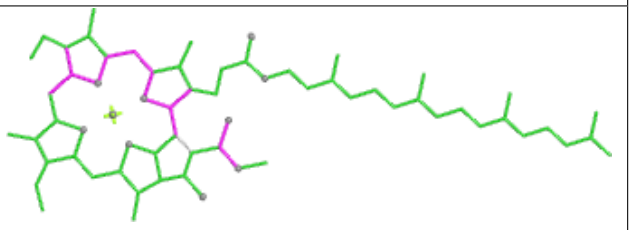

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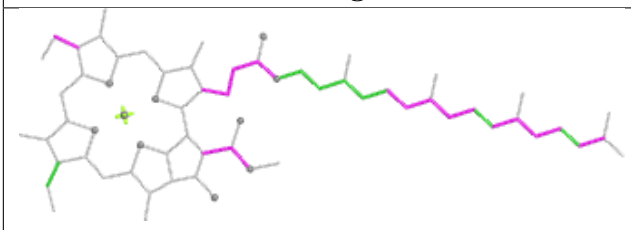

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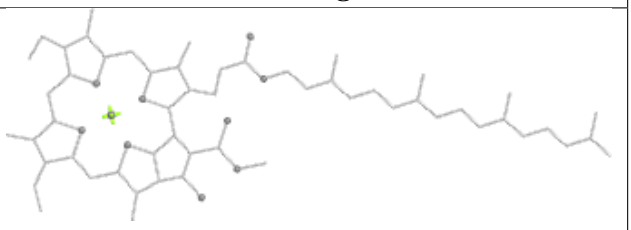
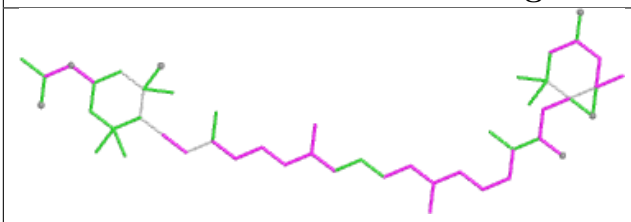


Rings

Ligand A86 14 316



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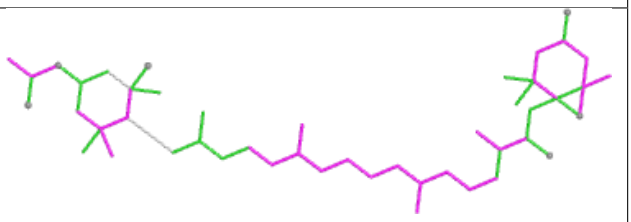

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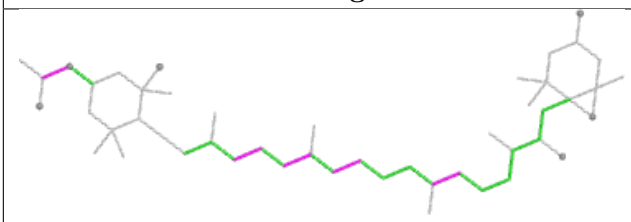

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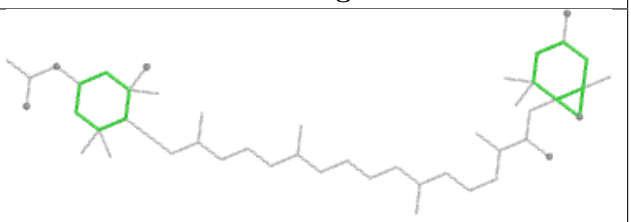
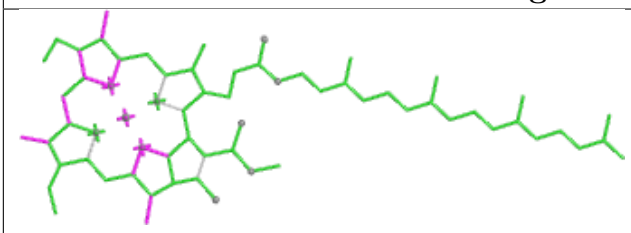


Rings

Ligand CLA c 512



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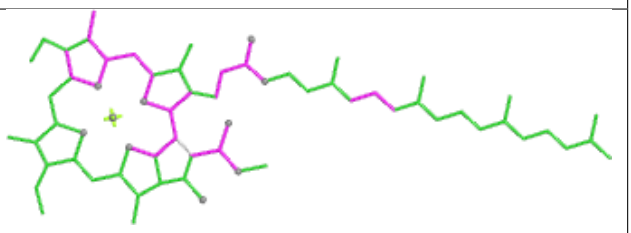
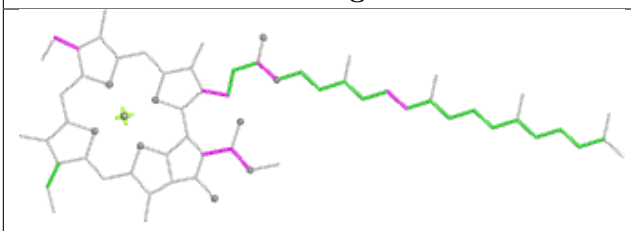


Bond angles



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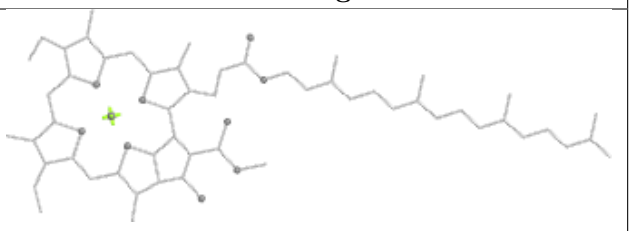
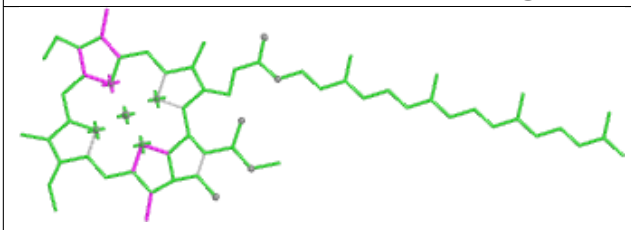


Rings

Ligand CLA 21 307



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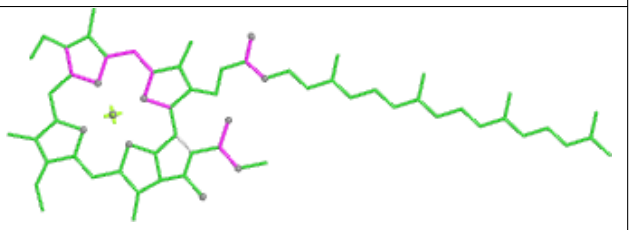
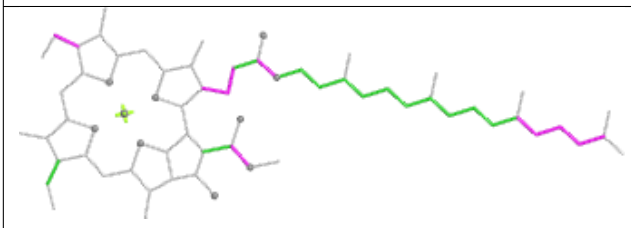


Bond angles



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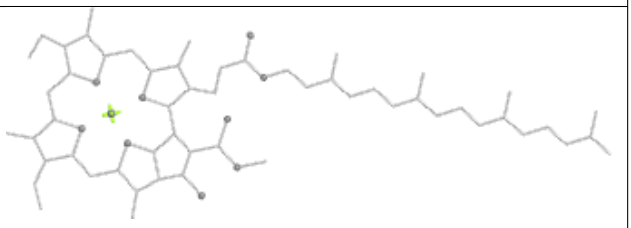
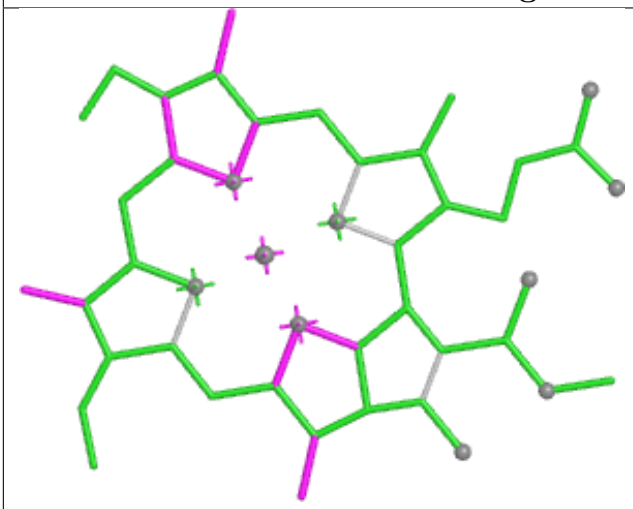


Rings

Ligand CLA 12 308



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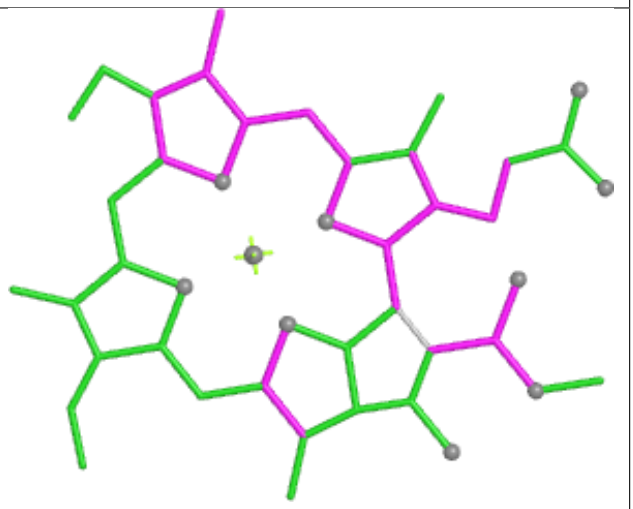
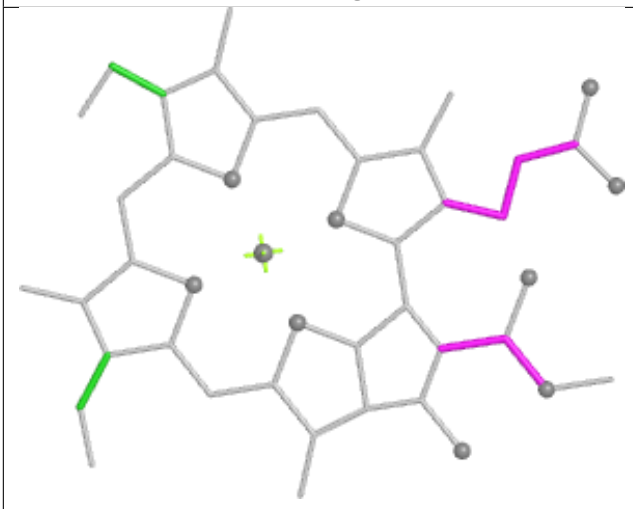


Bond angles



Torsions

Rings

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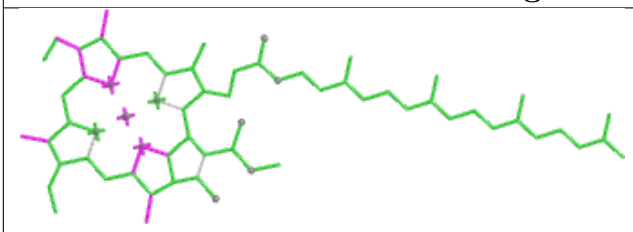

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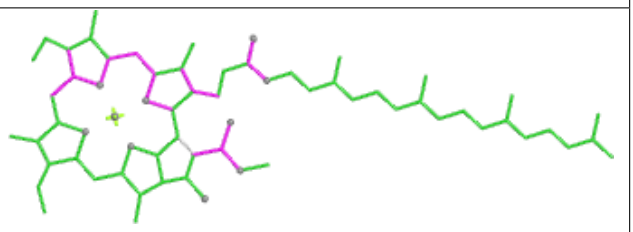
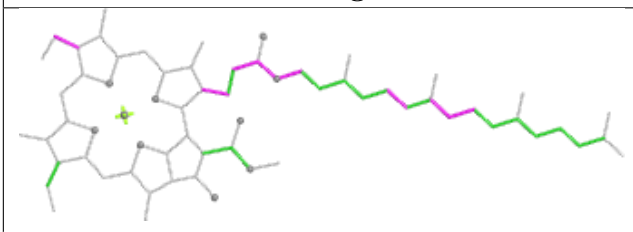
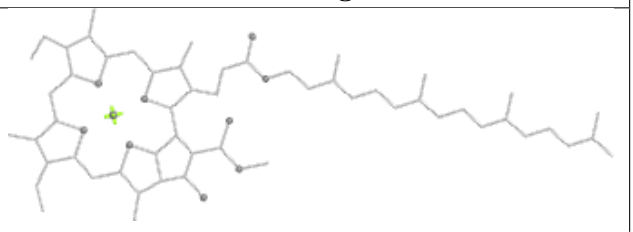


Bond angles

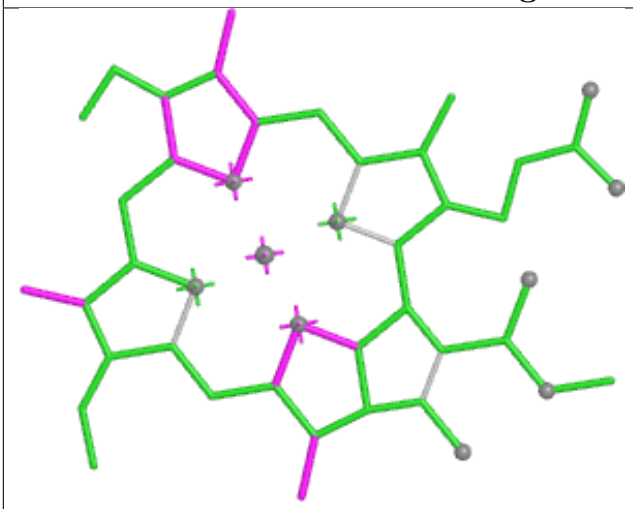


Torsions



Rings

Ligand CLA 16 309



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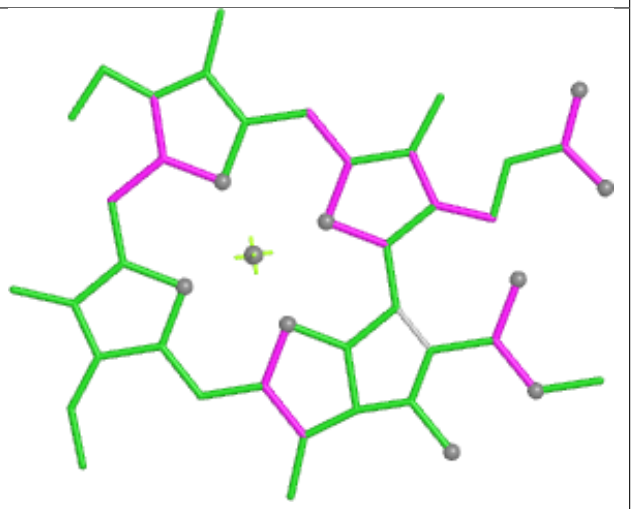
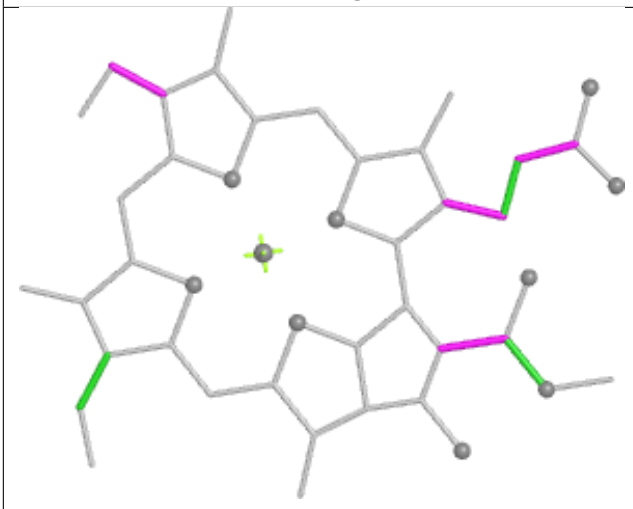


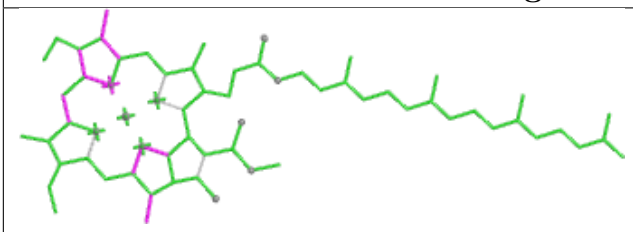
Bond angles



Torsions

Rings

Ligand CLA w 103



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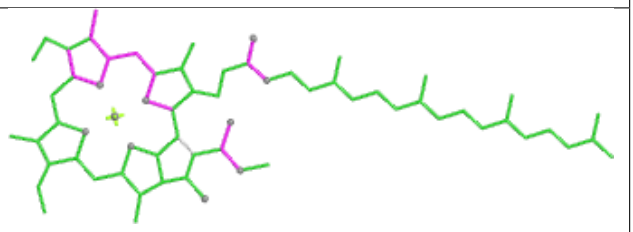

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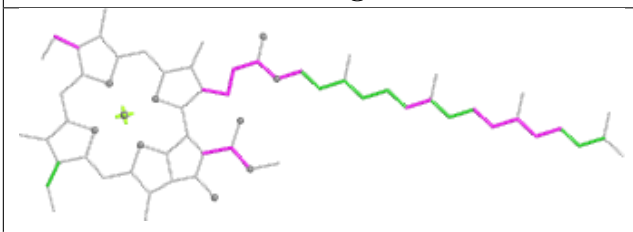

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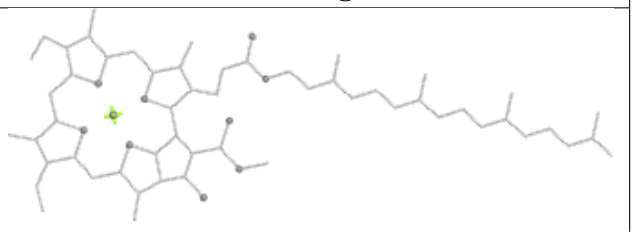
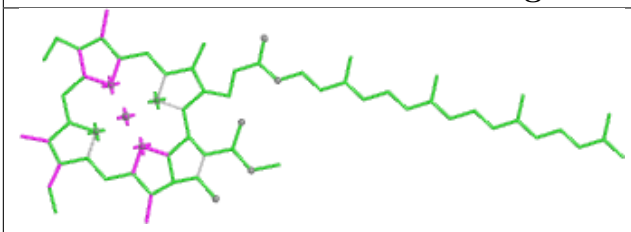


Rings

Ligand CLA B 611



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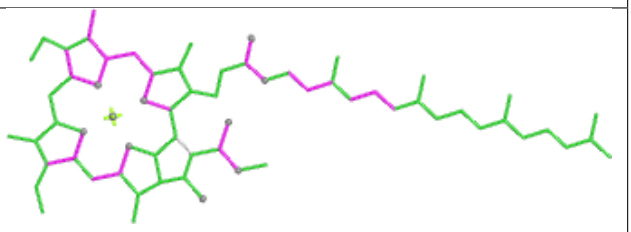

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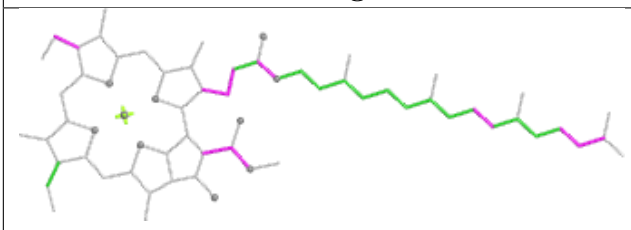

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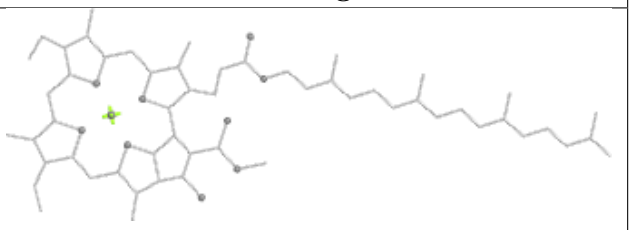
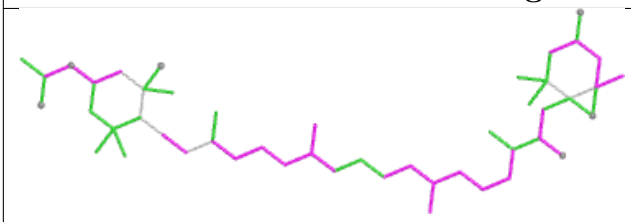


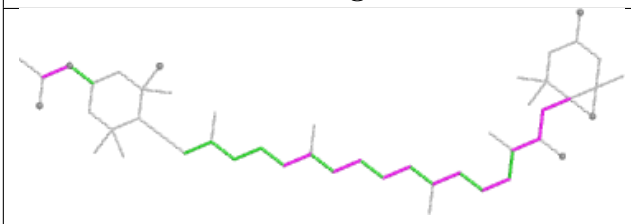
Rings

Ligand A86 17 302



Bond lengths

Bond angles



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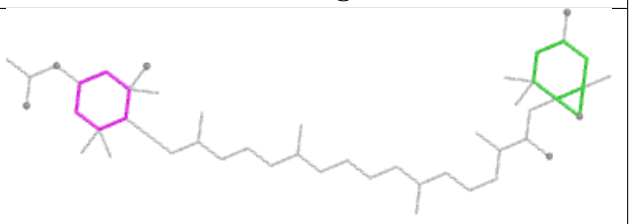
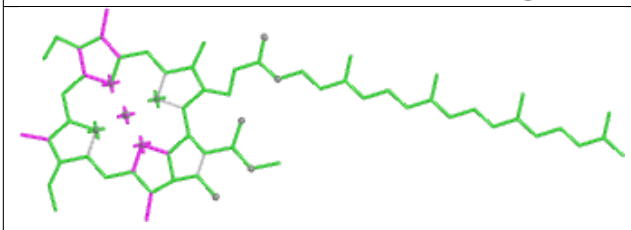


Rings

Ligand CLA 13 302



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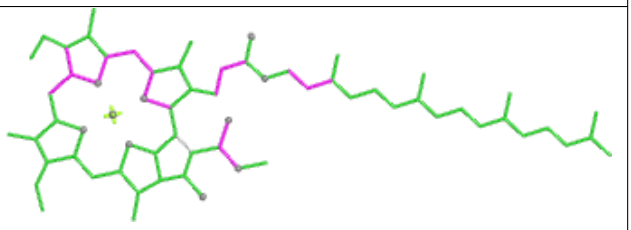

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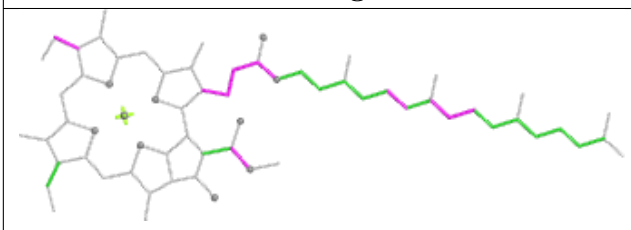

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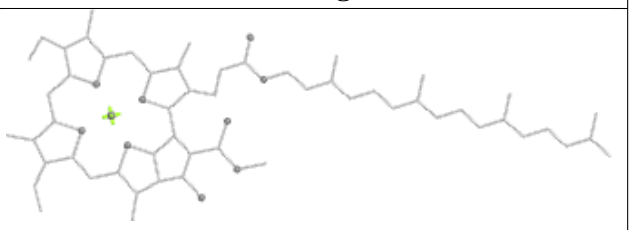
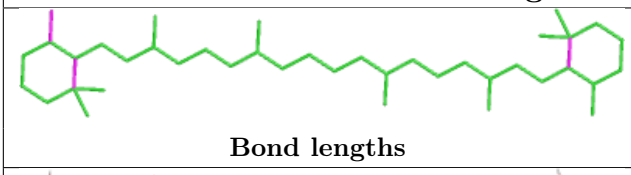


Rings

Ligand BCR b 623



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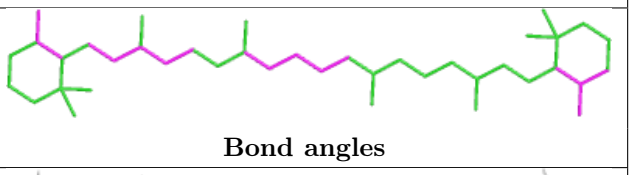

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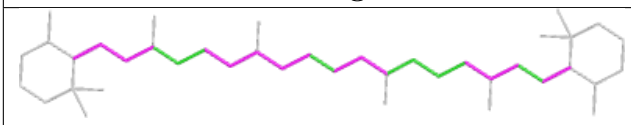

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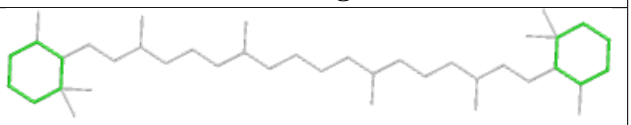
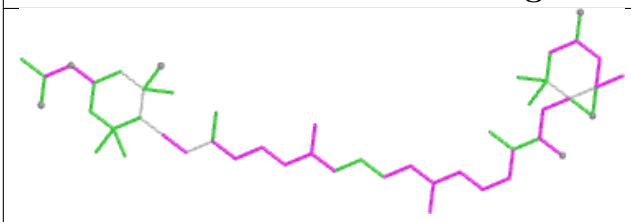


Rings

Ligand A86 18 314



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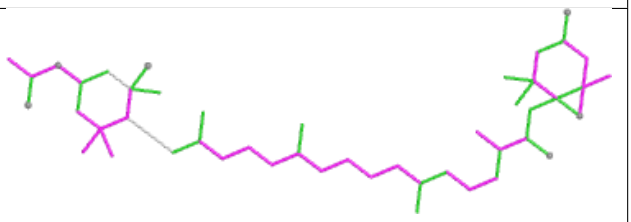

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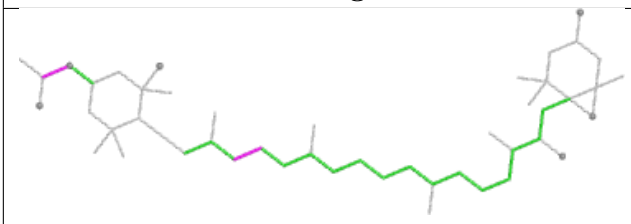

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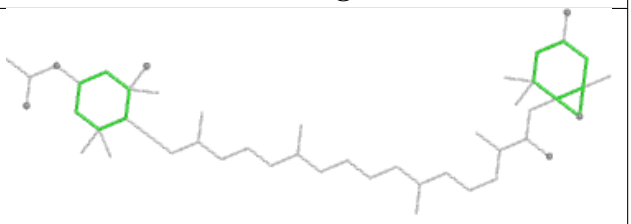
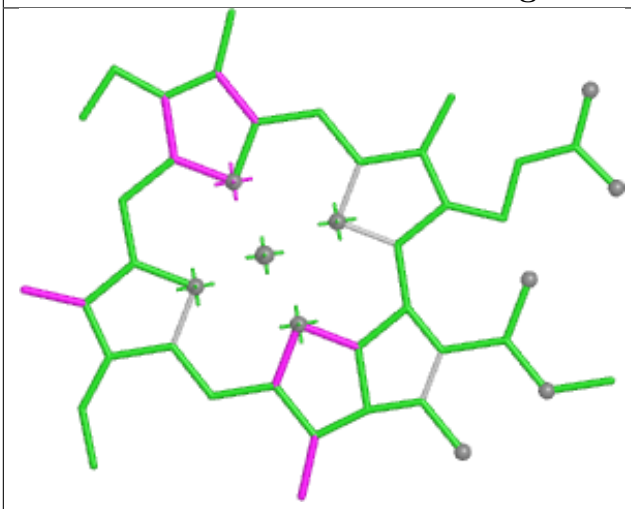


Rings

Ligand CLA 15 302



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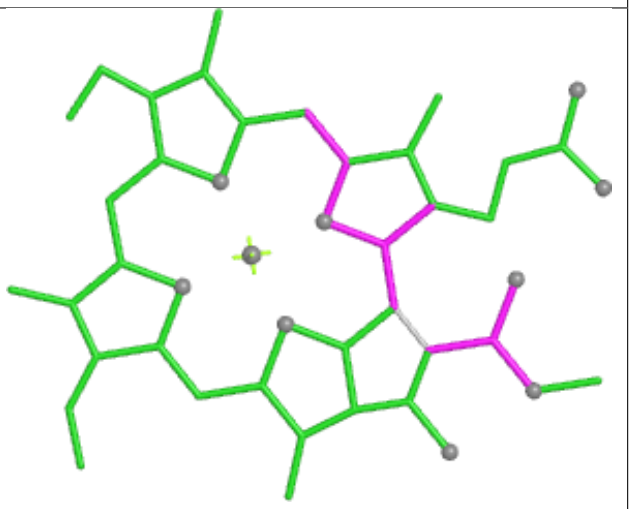

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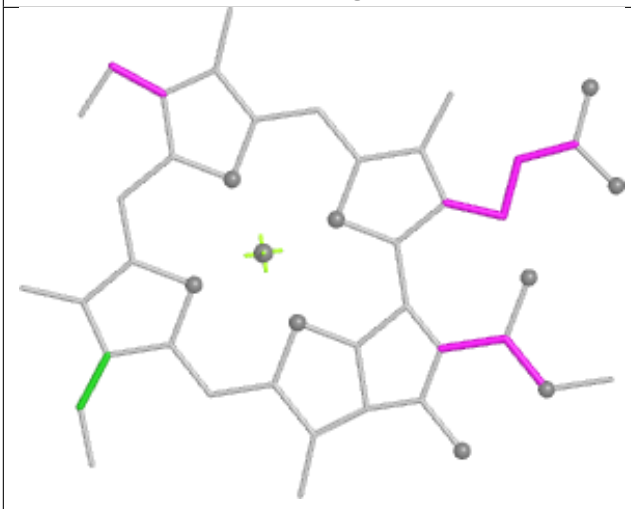
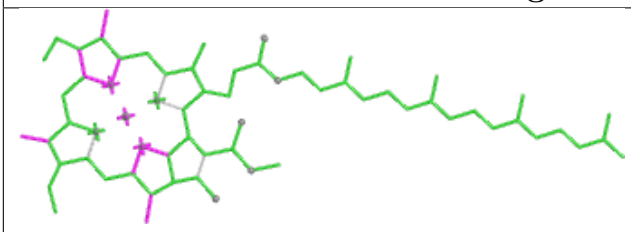


Torsions

Rings

Ligand CLA b 607



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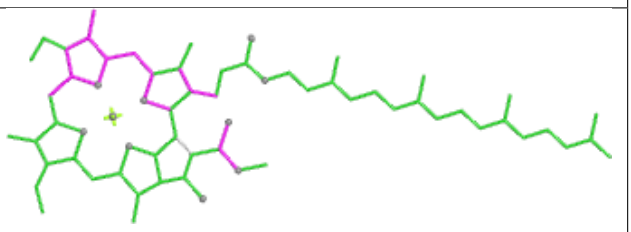

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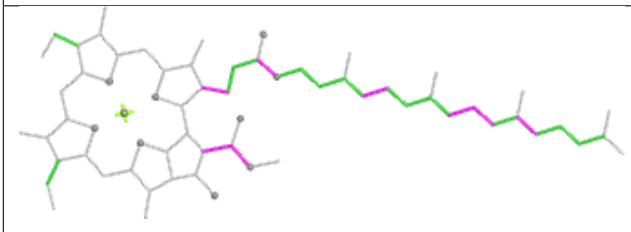

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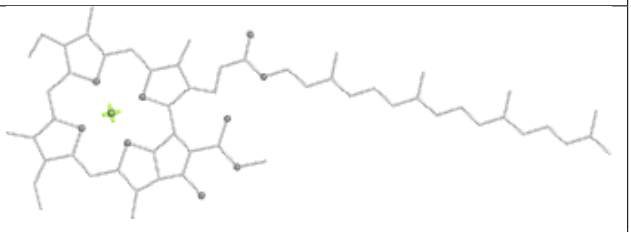
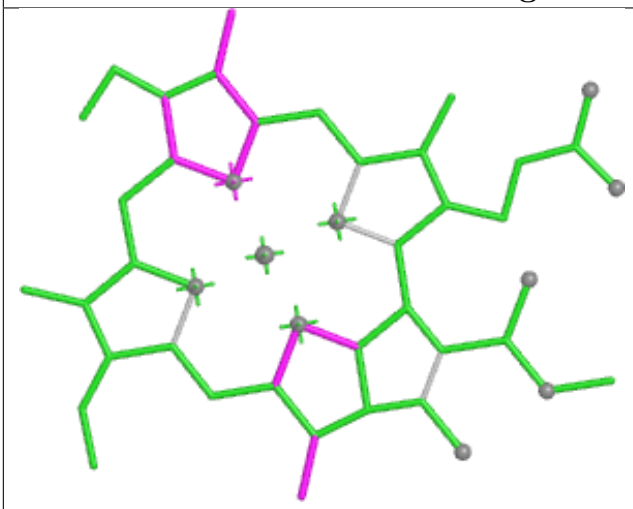


Rings

Ligand CLA 18 304



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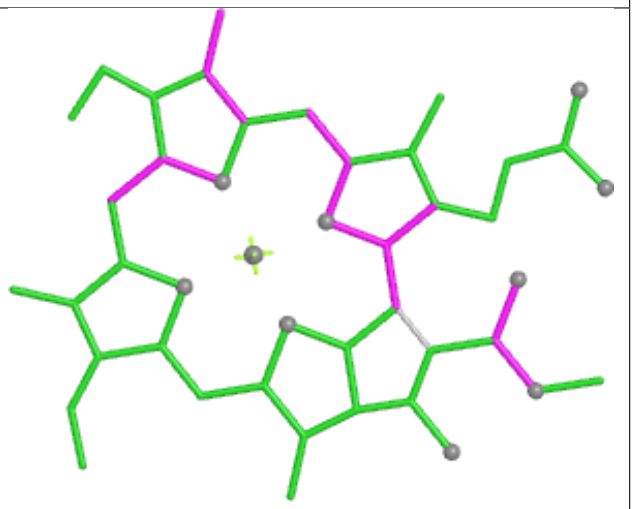

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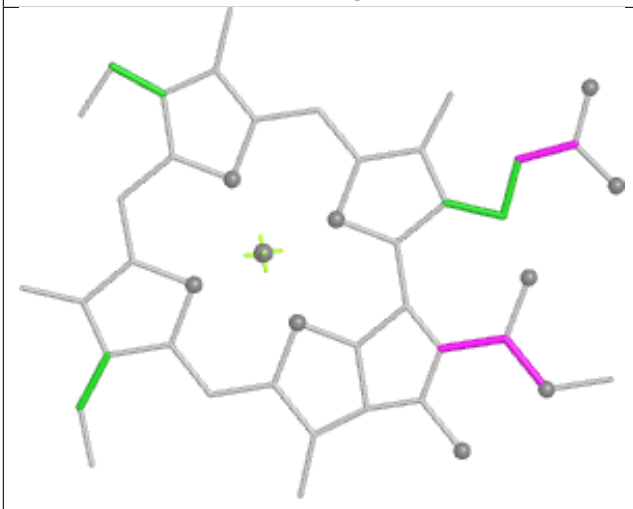

Torsions

Rings

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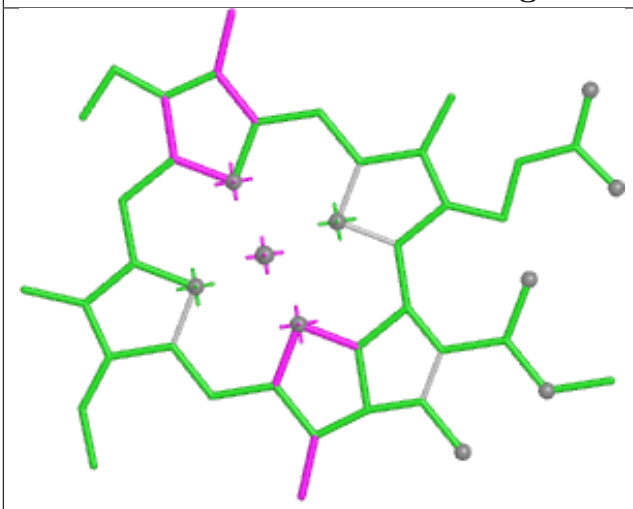

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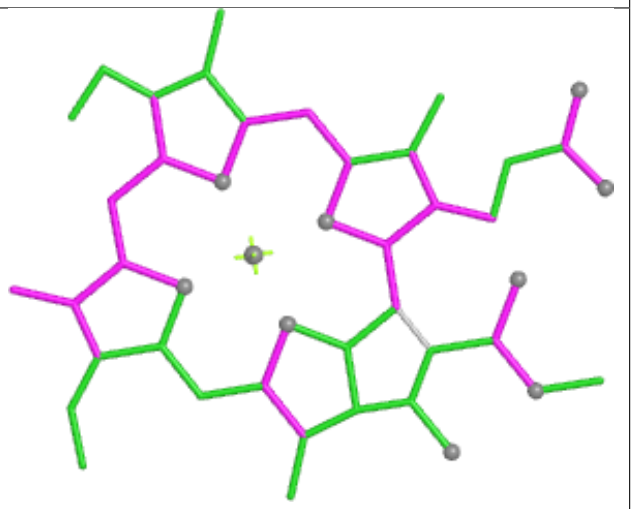

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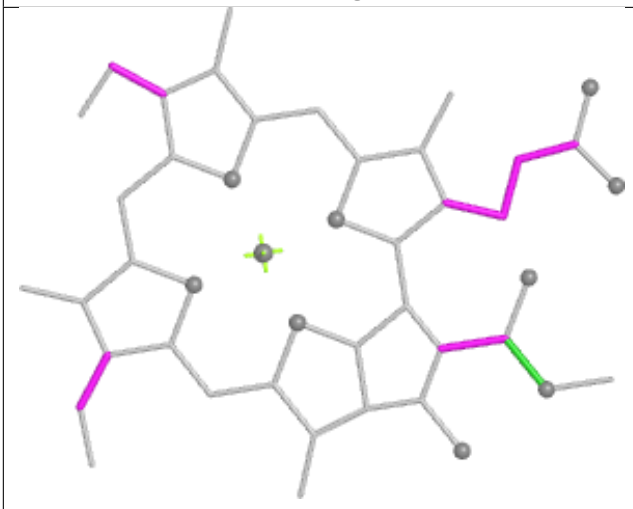
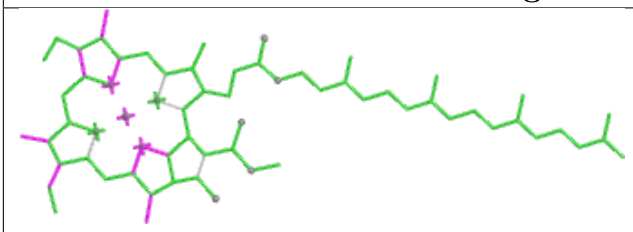


Torsions

Rings

Ligand CLA D 401



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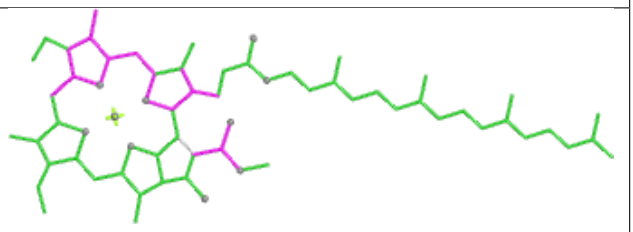

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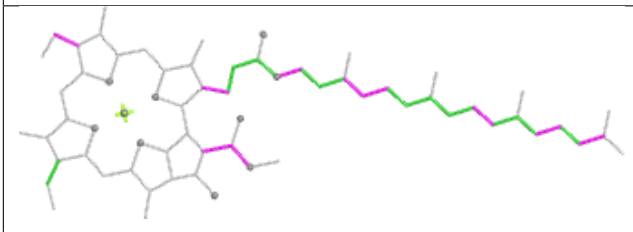

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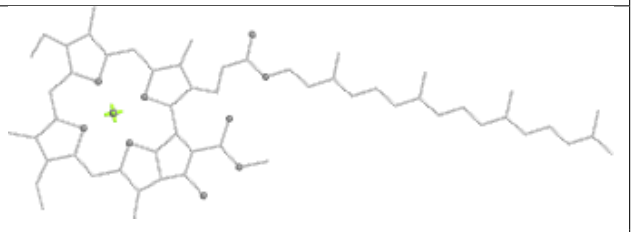
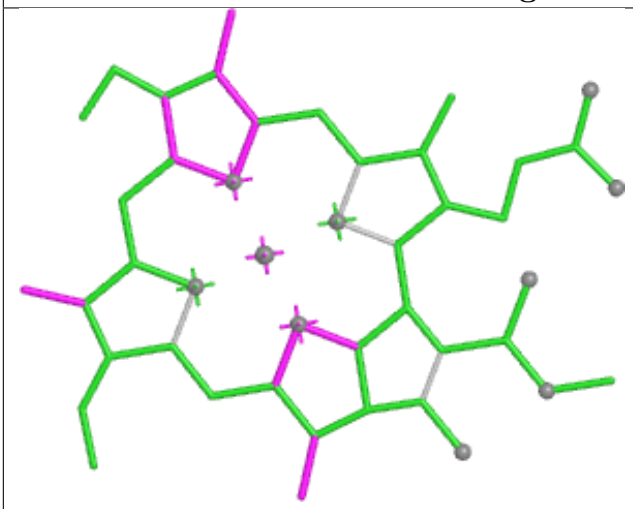


Rings

Ligand CLA 16 303



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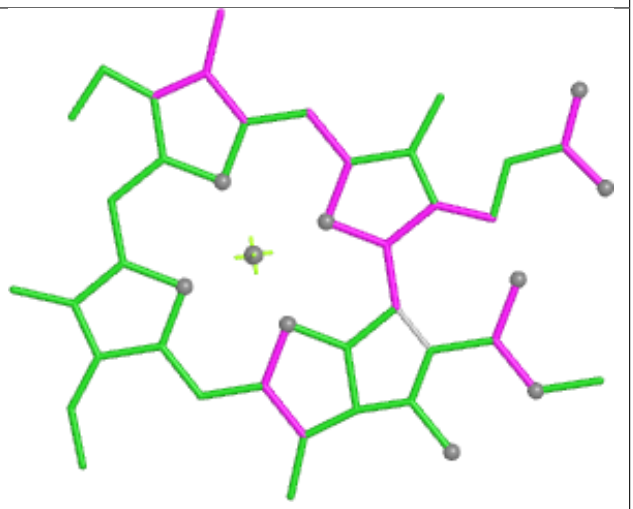
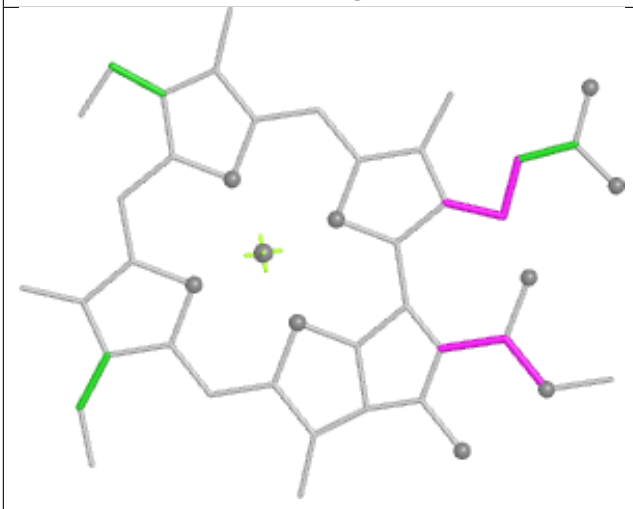


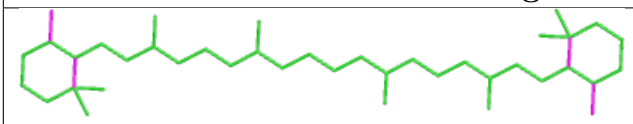
Bond angles



Torsions

Rings

Ligand BCR C 515



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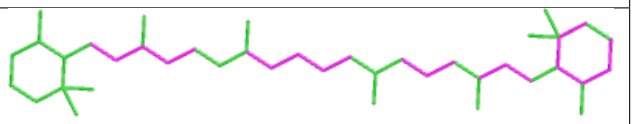
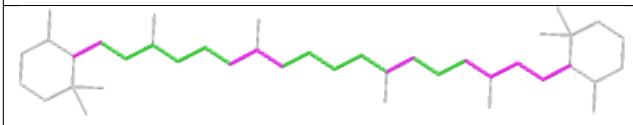


Bond angles



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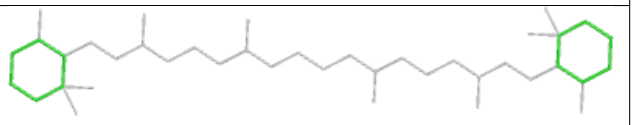
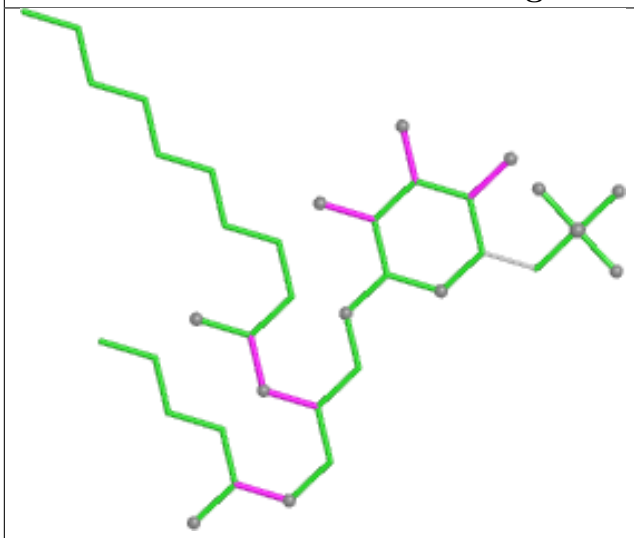


Rings

Ligand SQD B 621



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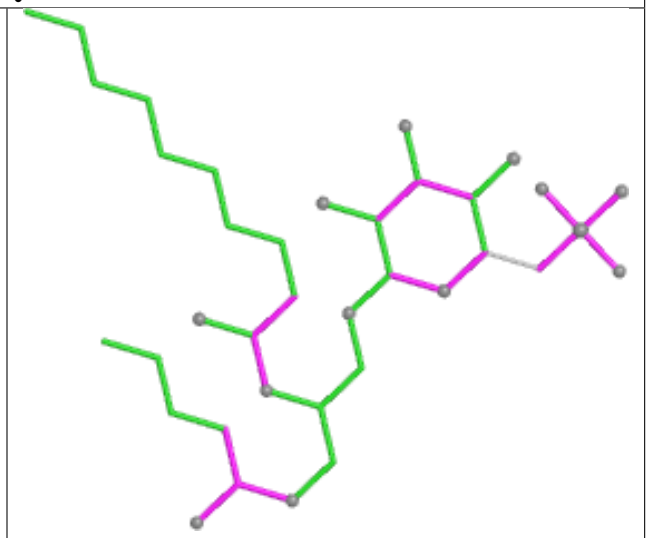
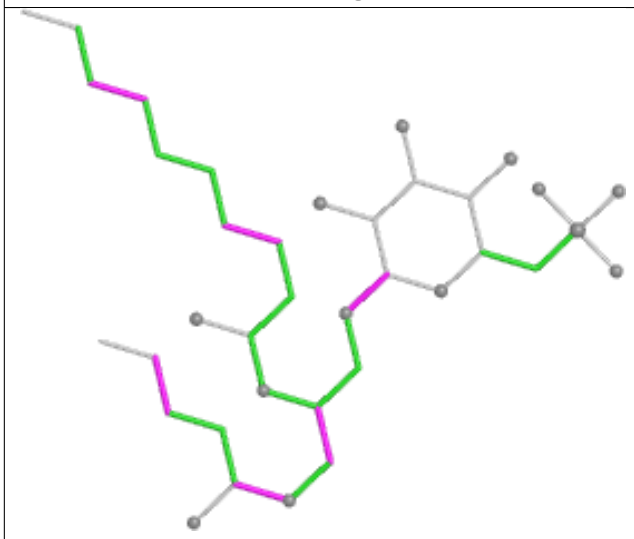


Bond angles



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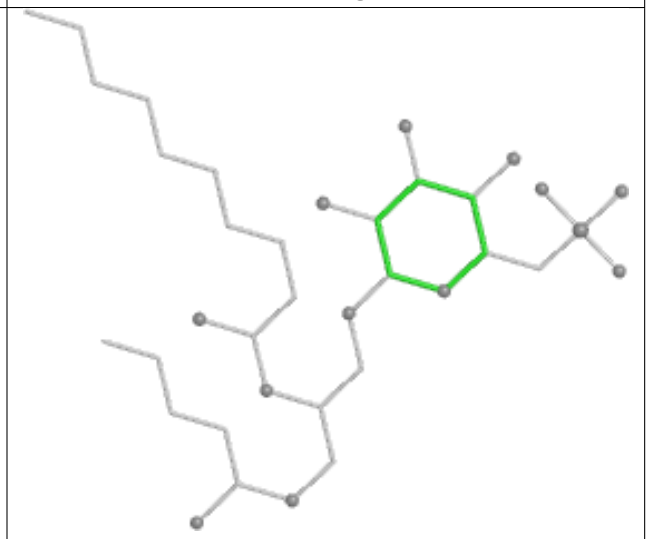
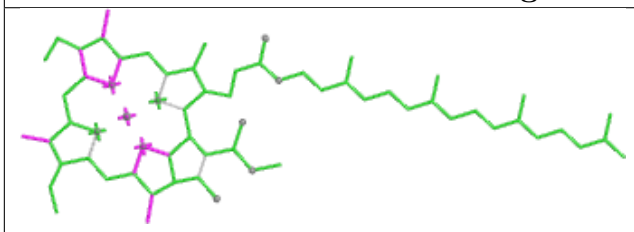


Rings

Ligand CLA 13 308



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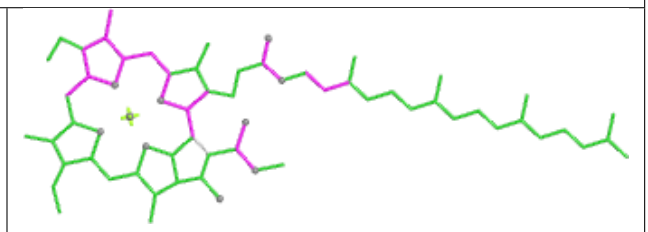

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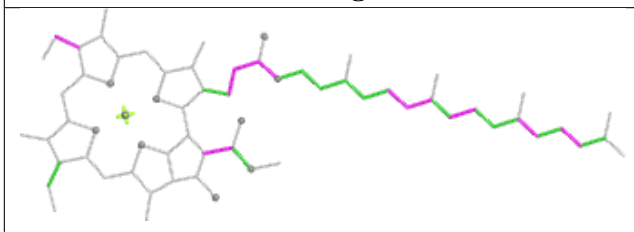
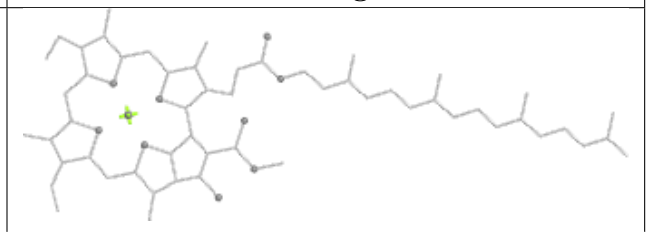
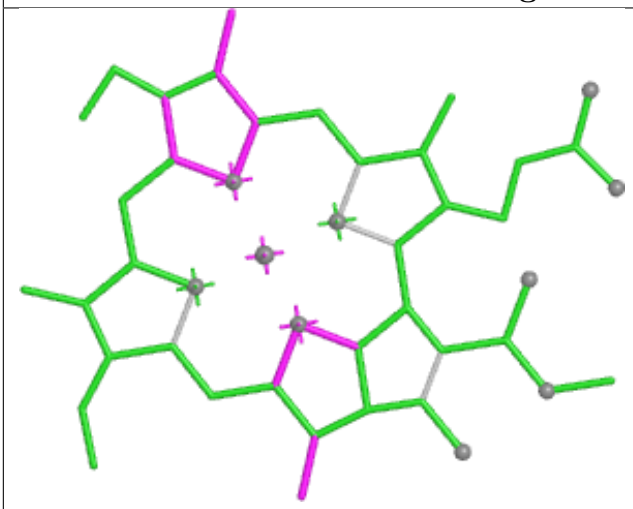


Torsions



Rings

Ligand CLA 20 206



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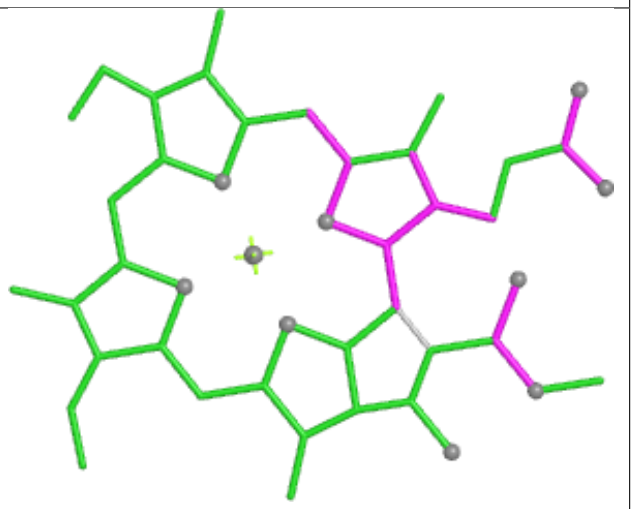

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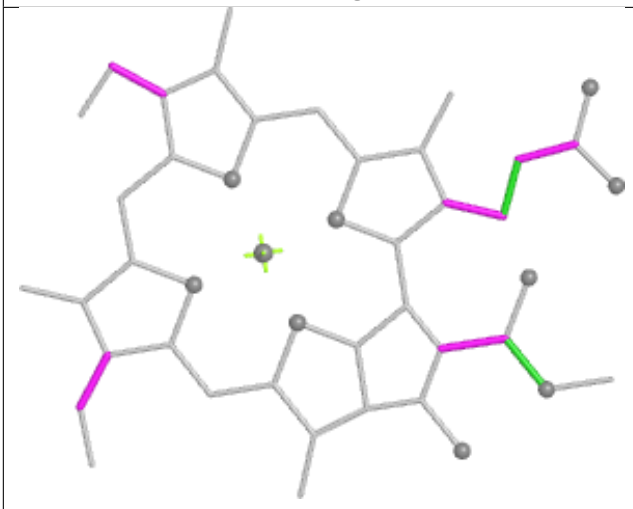
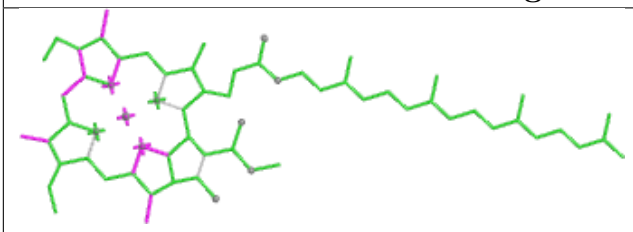


Torsions

Rings

Ligand CLA B 603



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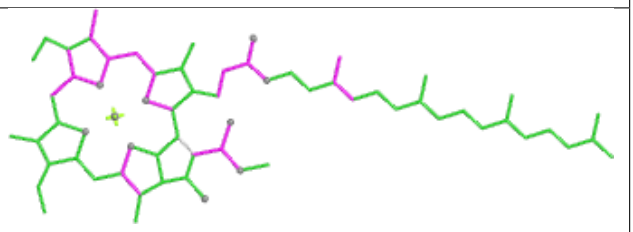

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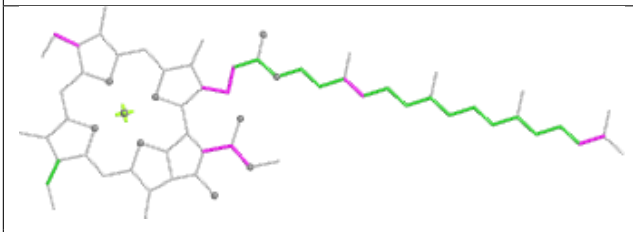

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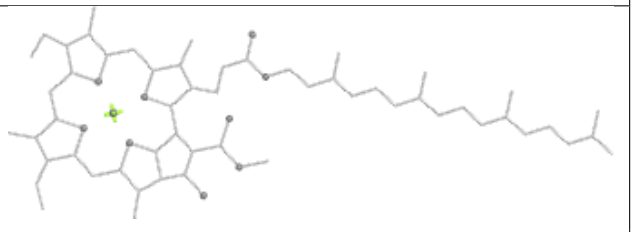
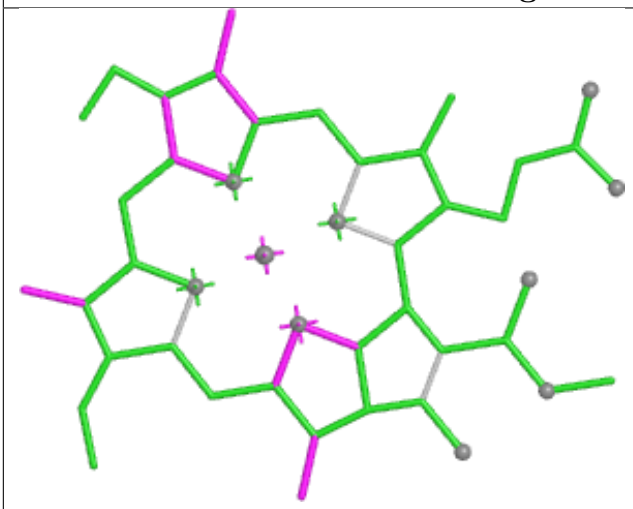


Rings

Ligand CLA 18 311



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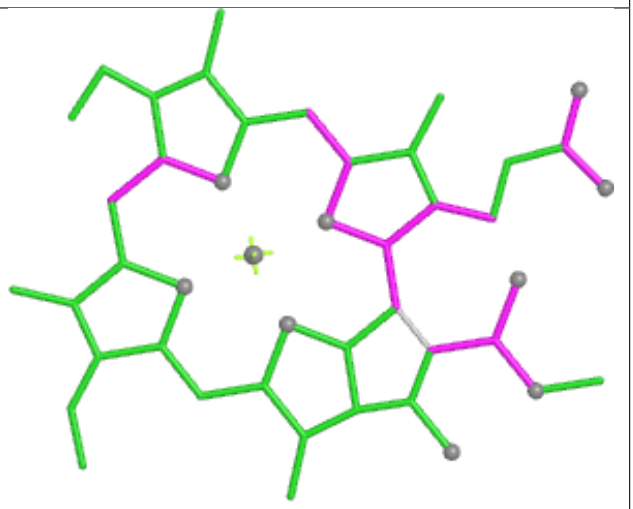

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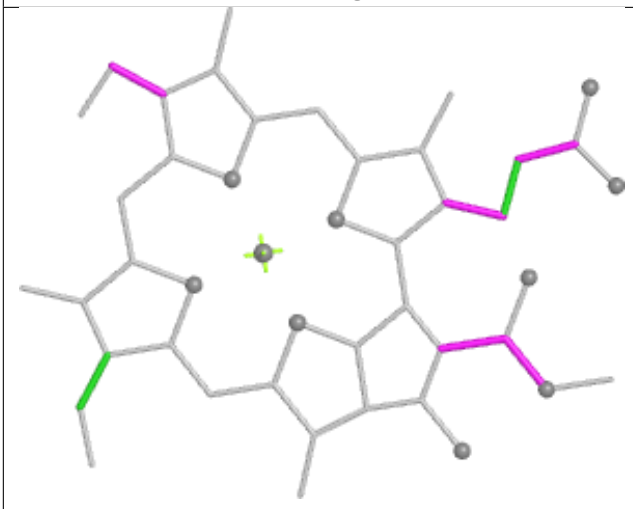
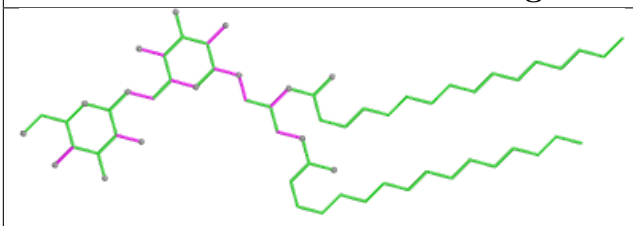


Torsions

Rings

Ligand DGD c 518



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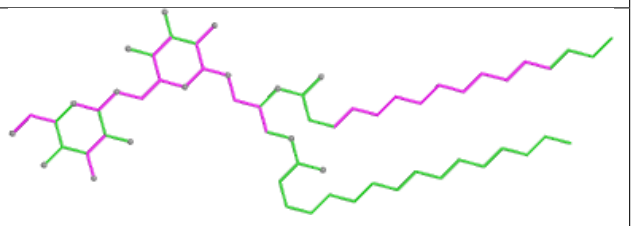

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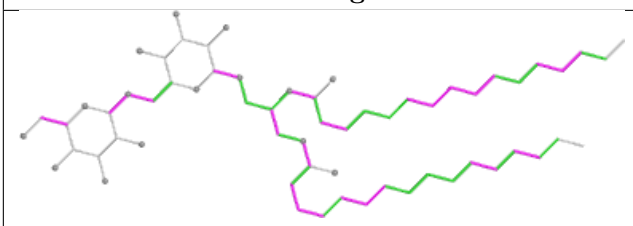

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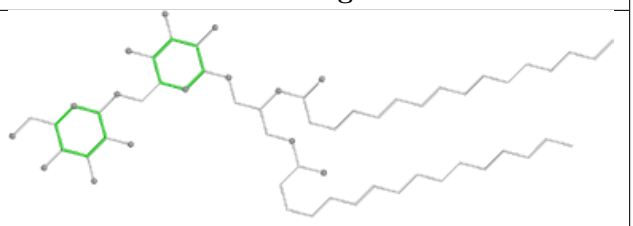
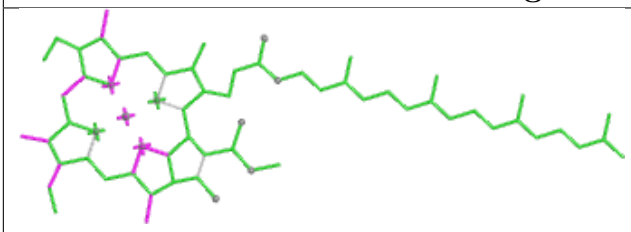


Rings

Ligand CLA C 508



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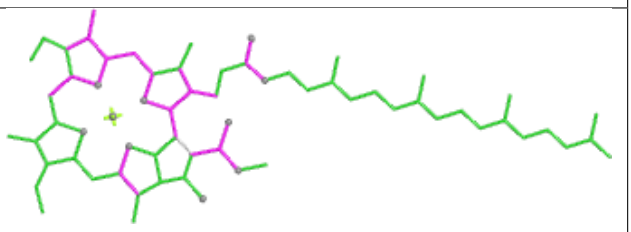

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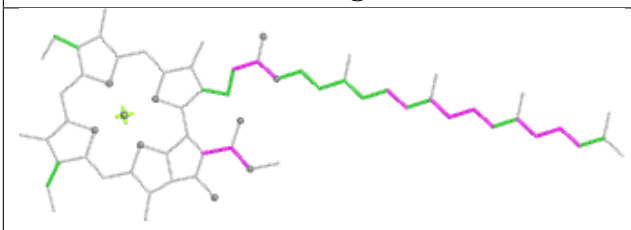

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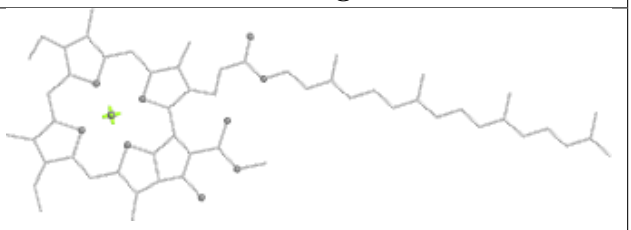
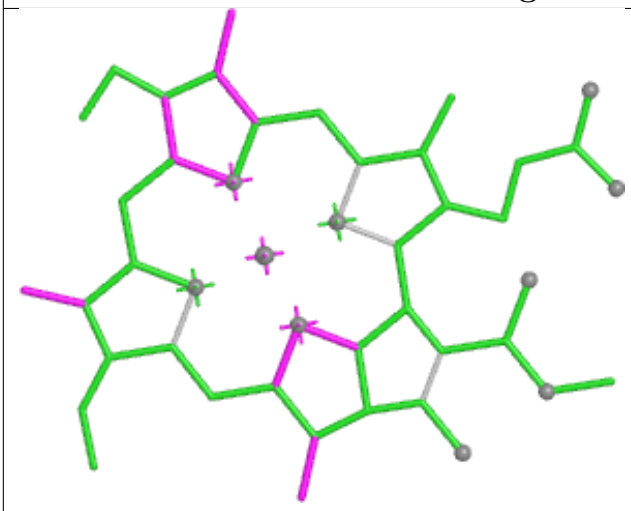


Rings

Ligand CLA 13 310



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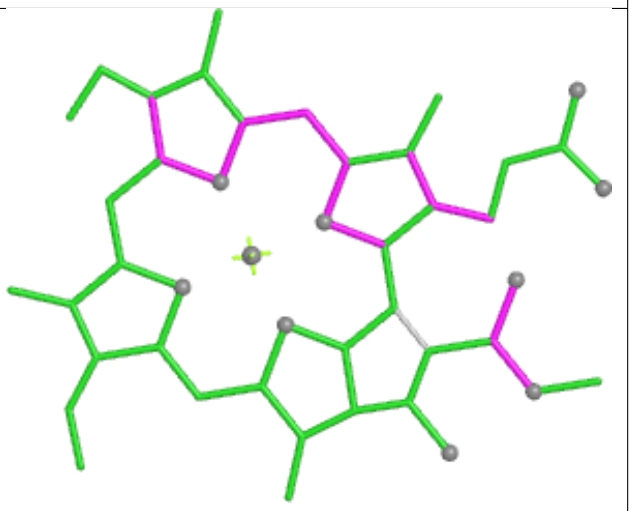

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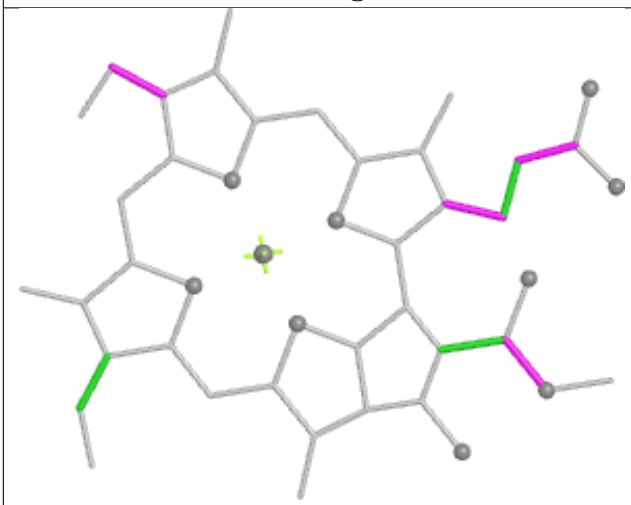

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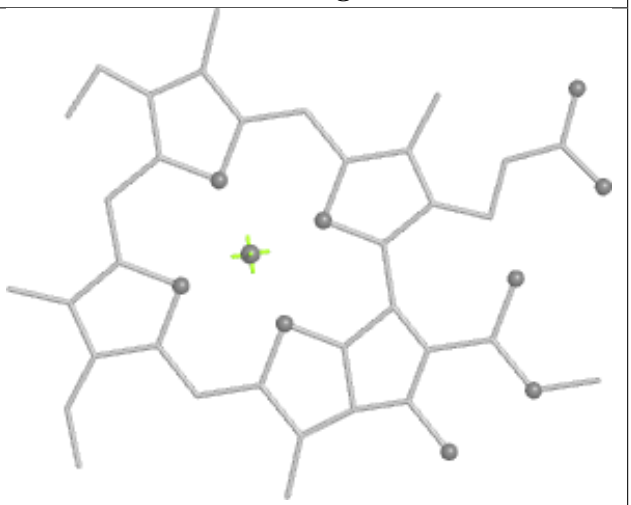
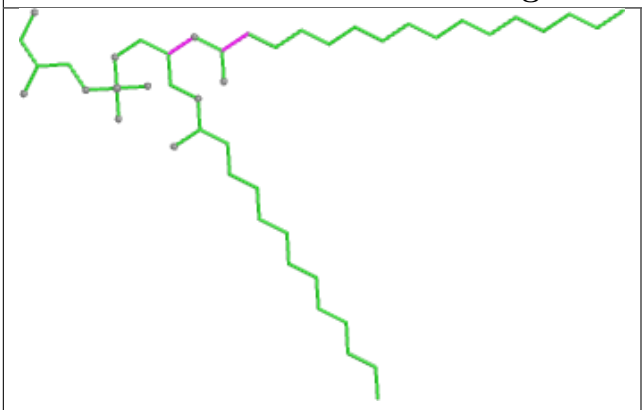


Rings

Ligand LHG A 408



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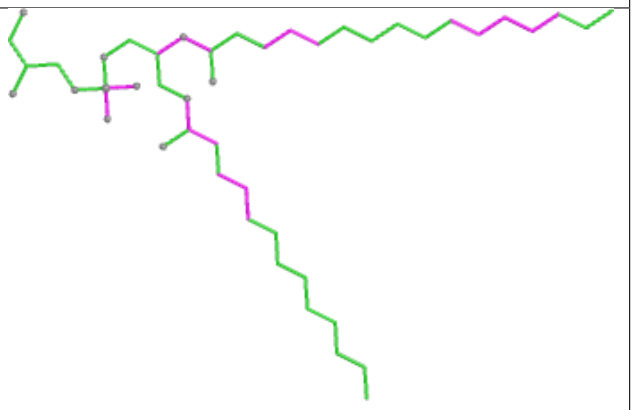

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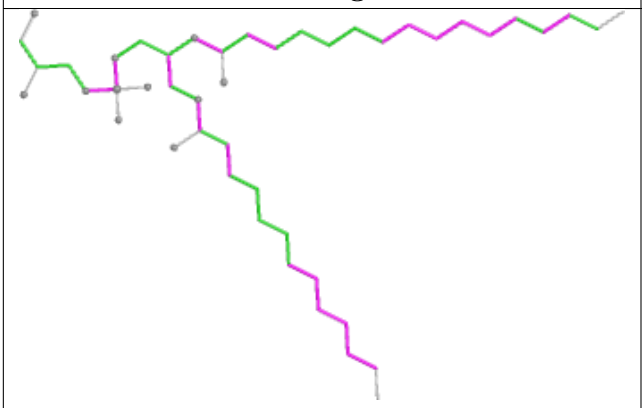

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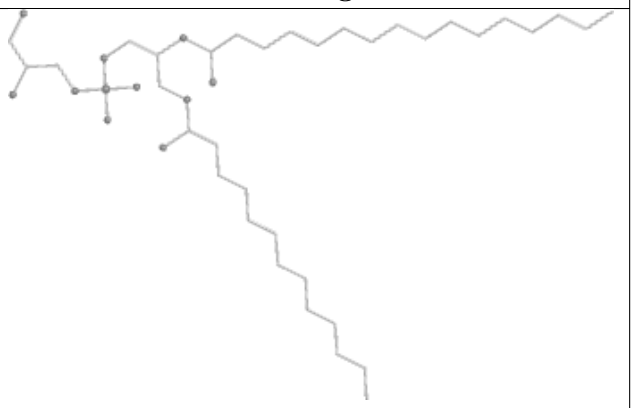
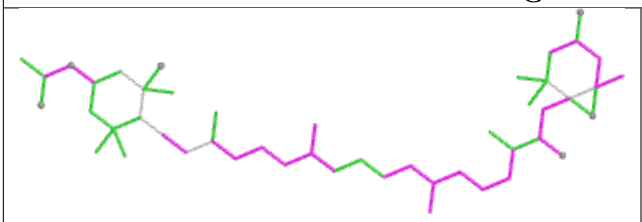


Rings

Ligand A86 15 315



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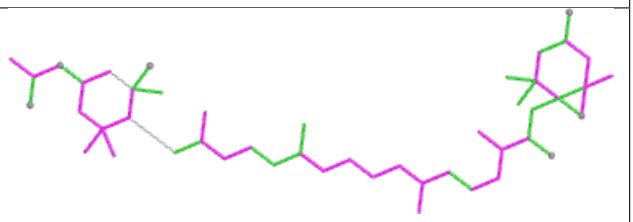

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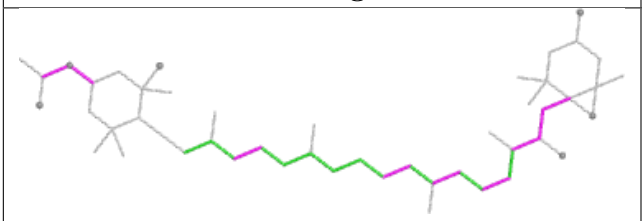

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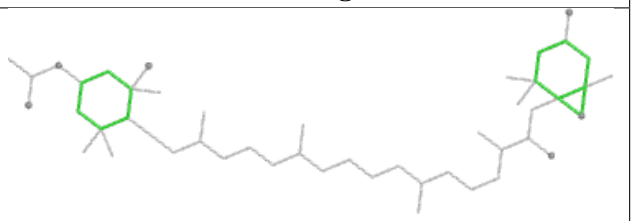
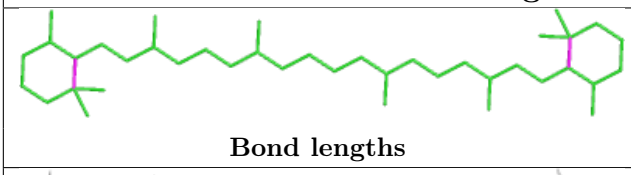


Rings

Ligand BCR B 617



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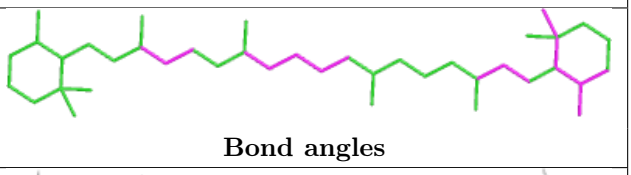

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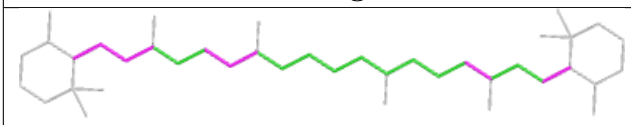

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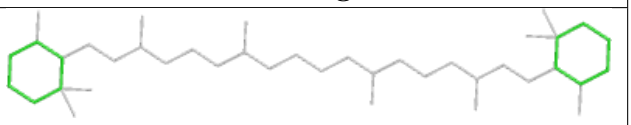
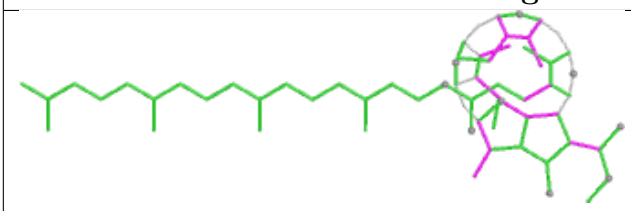


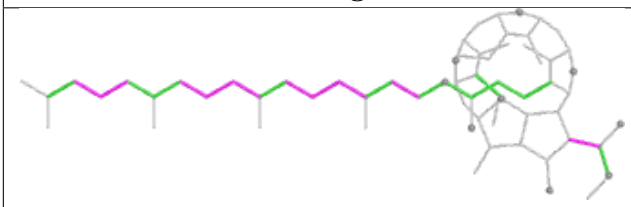
Rings

Ligand PHO A 403



Bond lengths

Bond angles



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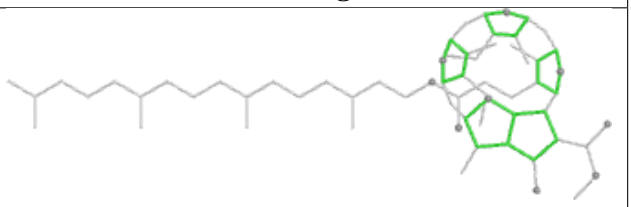
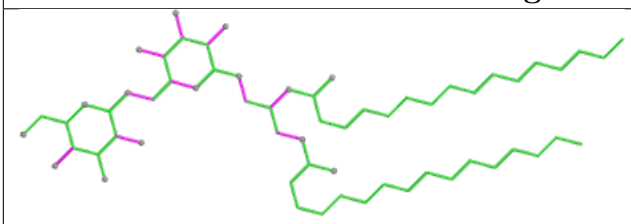


Rings

Ligand DGD J 101



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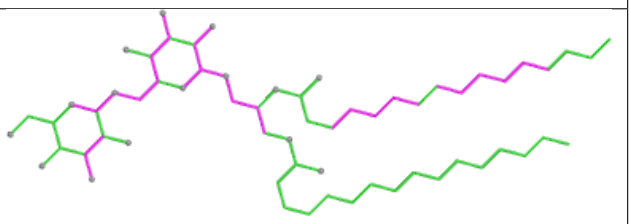

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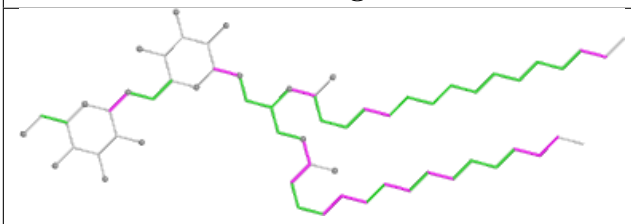

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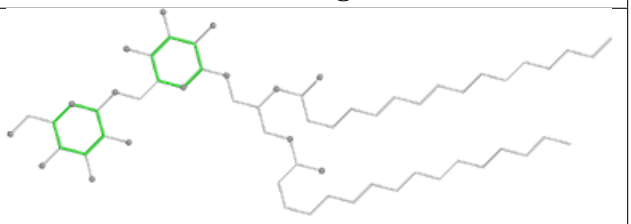
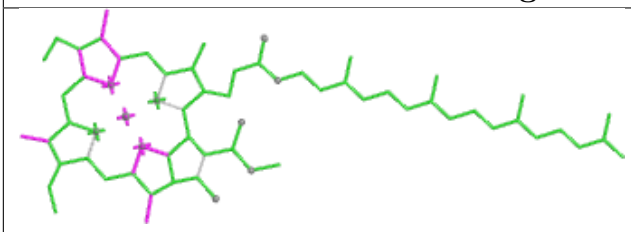


Rings

Ligand CLA 19 307



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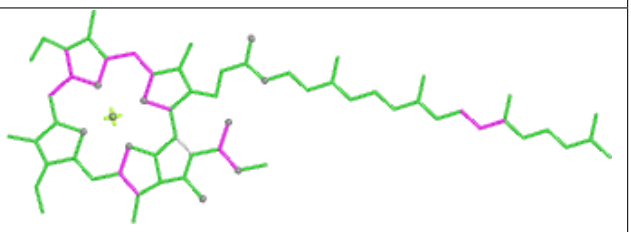
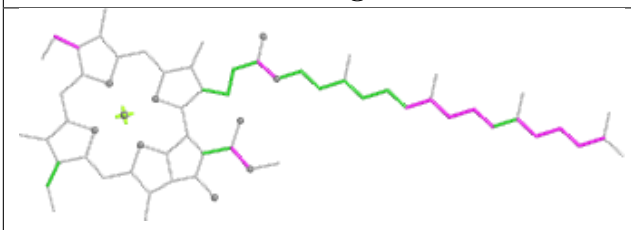


Bond angles



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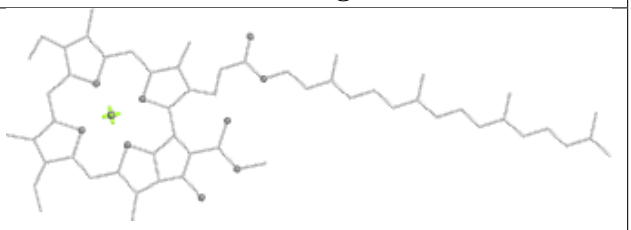
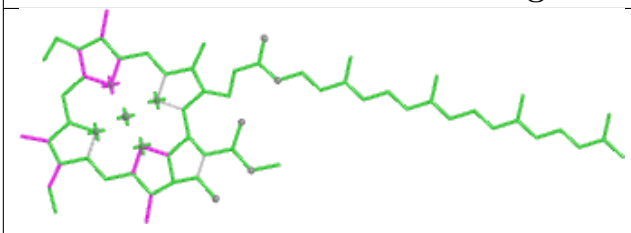


Rings

Ligand CLA b 605



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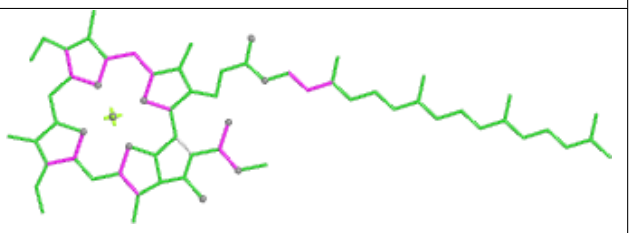
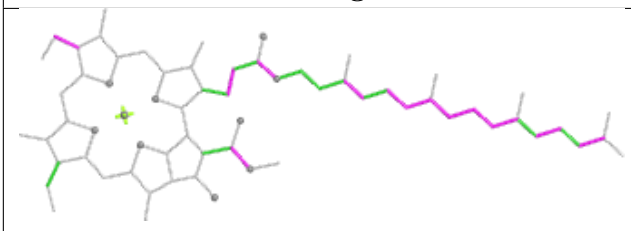


Bond angles



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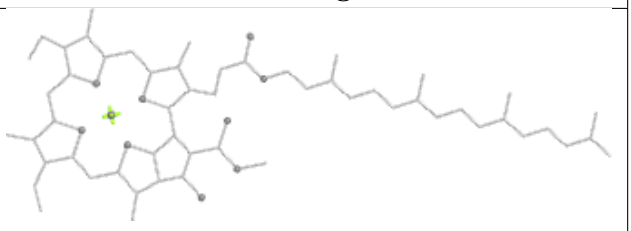

Rings

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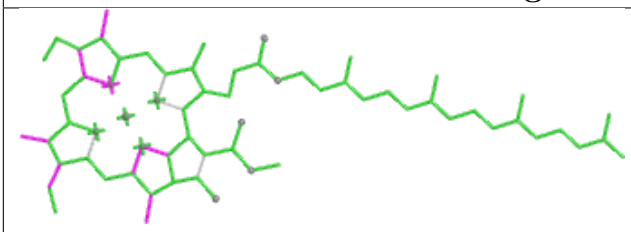

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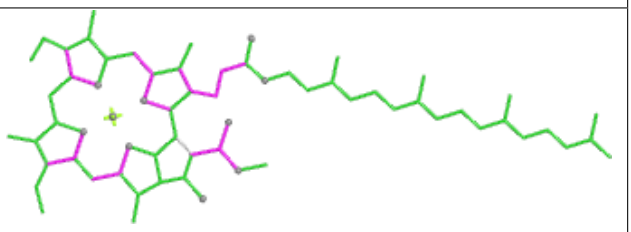
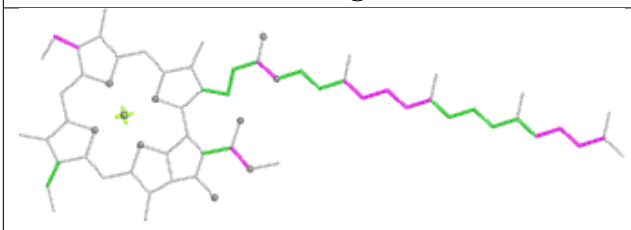
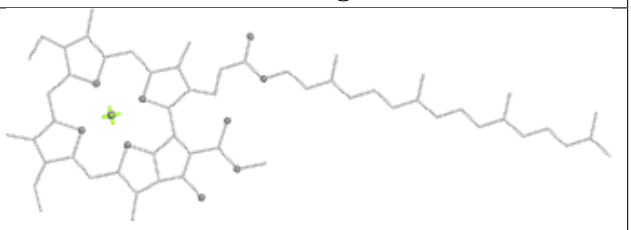


Bond angles

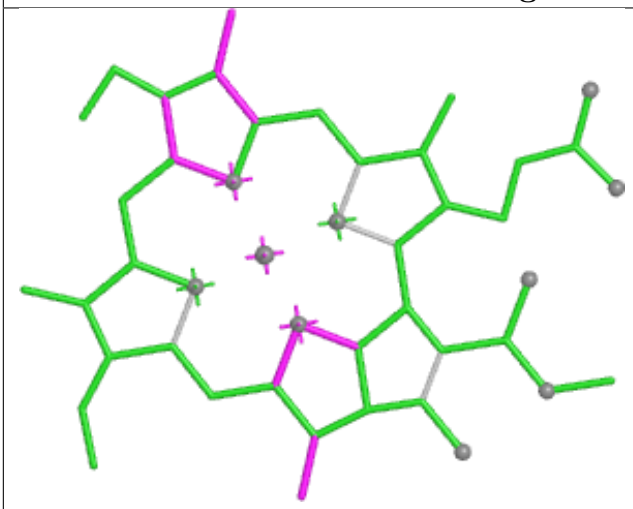


Torsions



Rings

Ligand CLA 20 203



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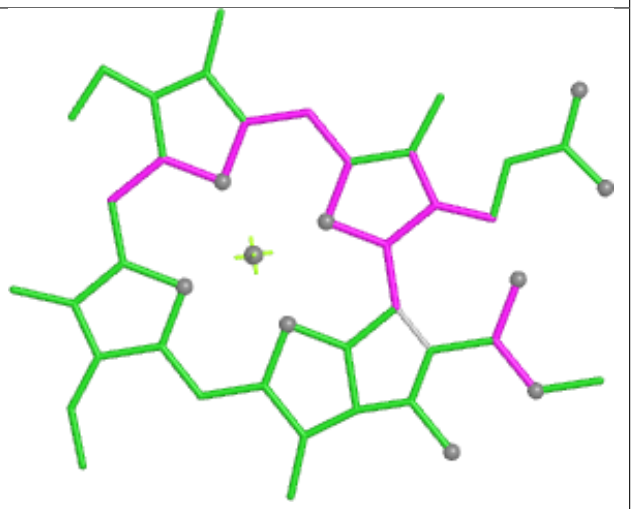
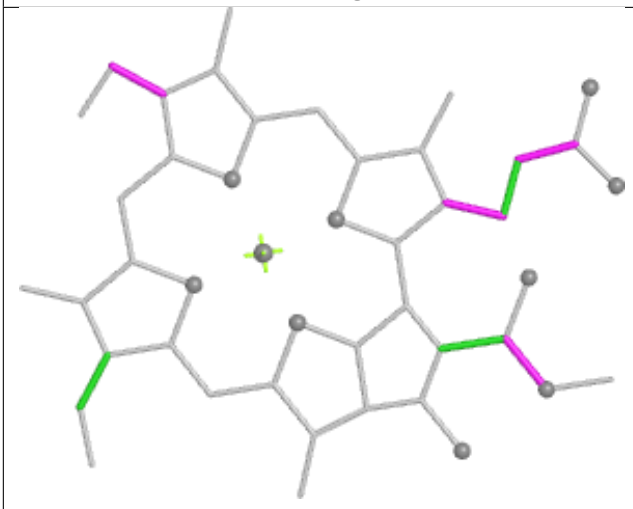


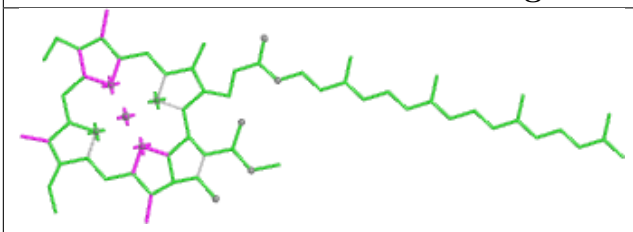
Bond angles



Torsions

Rings

Ligand CLA B 601



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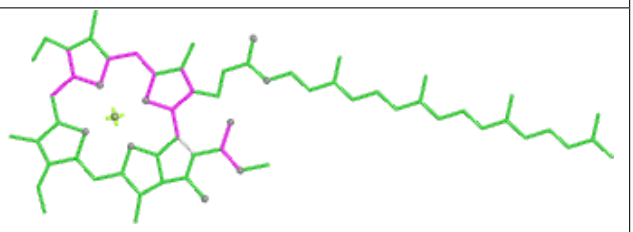

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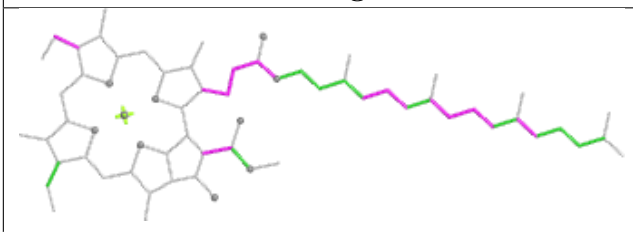

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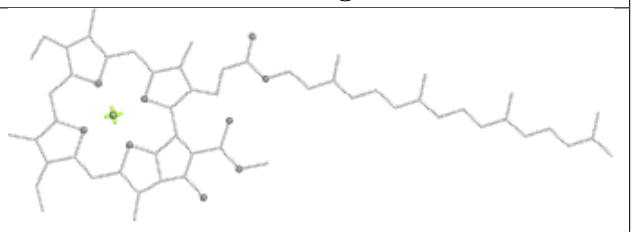
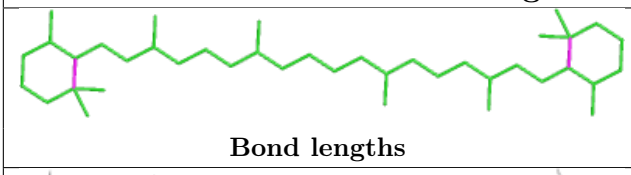


Rings

Ligand BCR B 616



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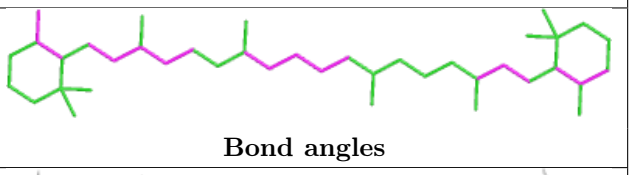

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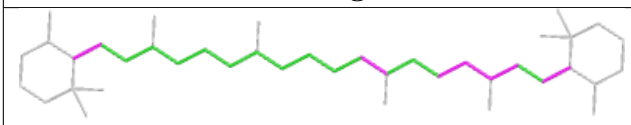

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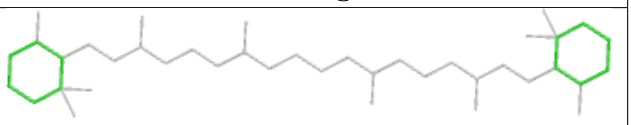
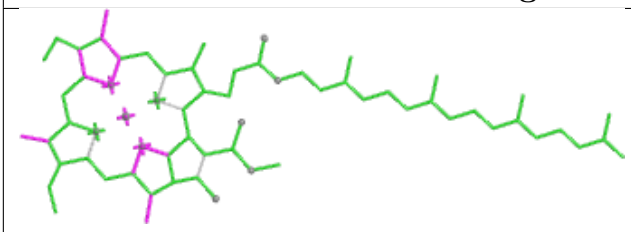


Rings

Ligand CLA 14 305



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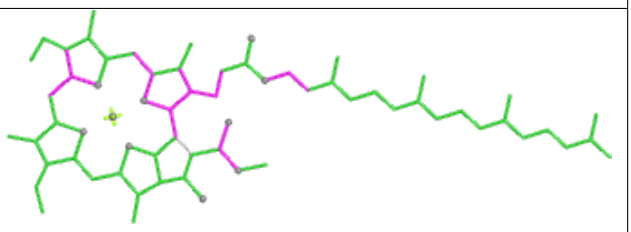

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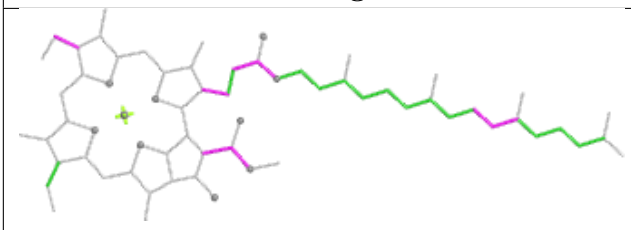

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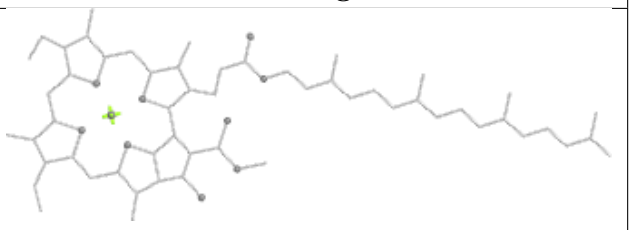
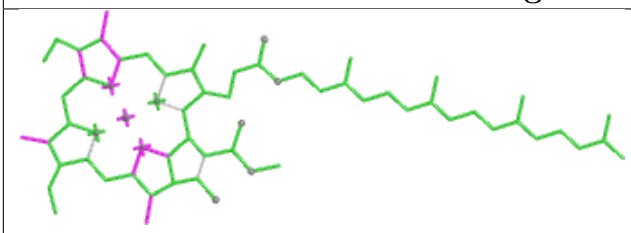


Rings

Ligand CLA C 514



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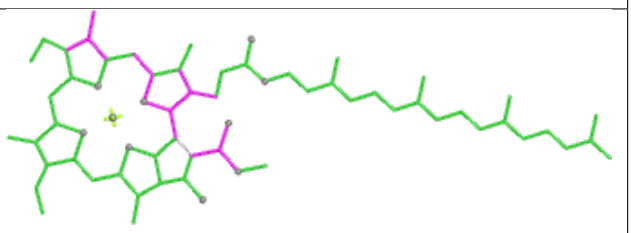

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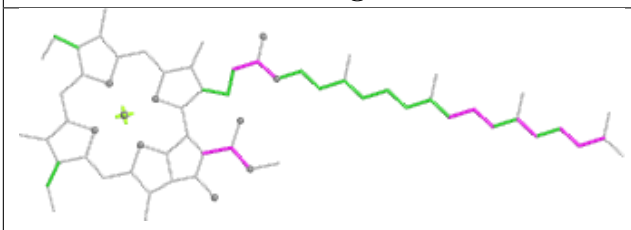

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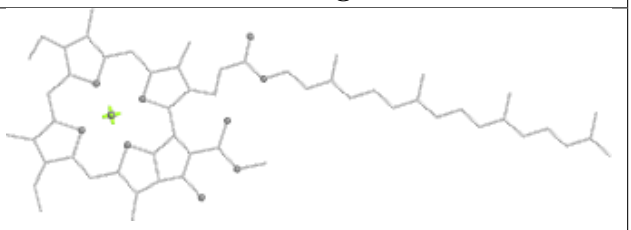
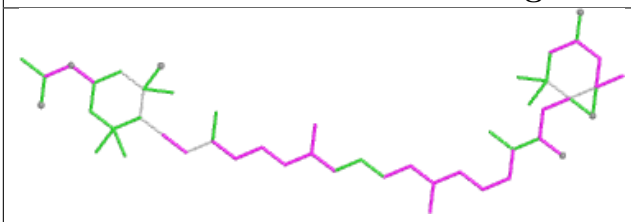


Rings

Ligand A86 20 211



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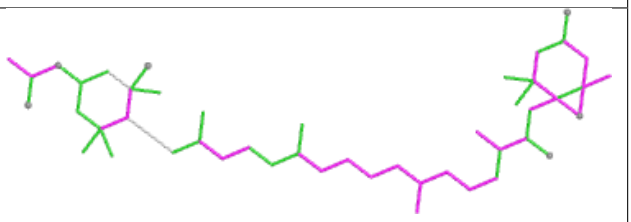

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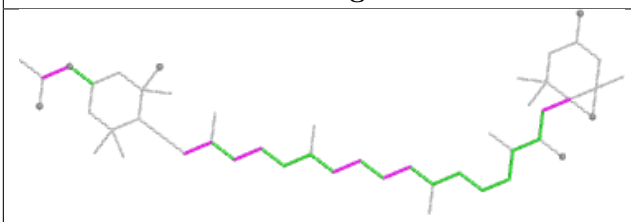

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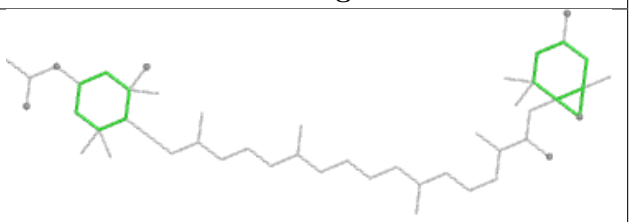
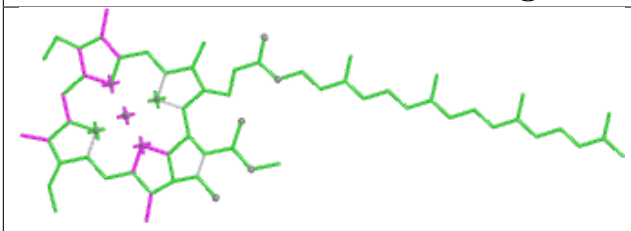


Rings

Ligand CLA 12 305



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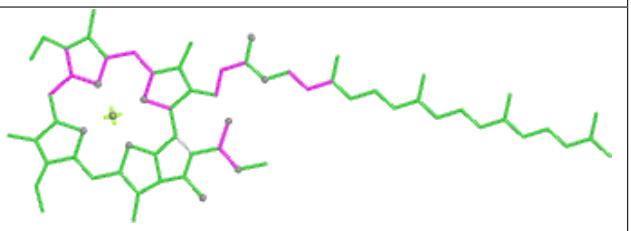

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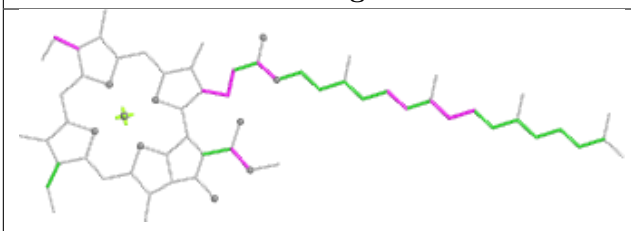

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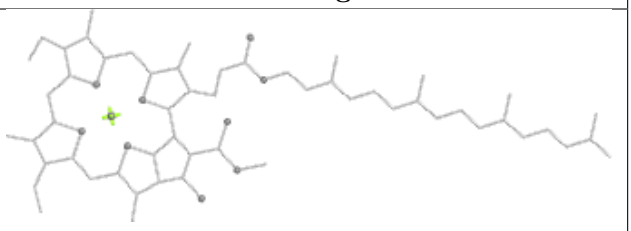

Rings

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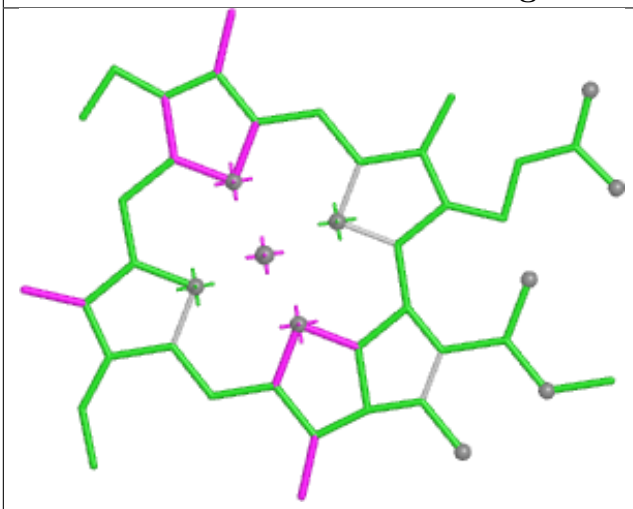

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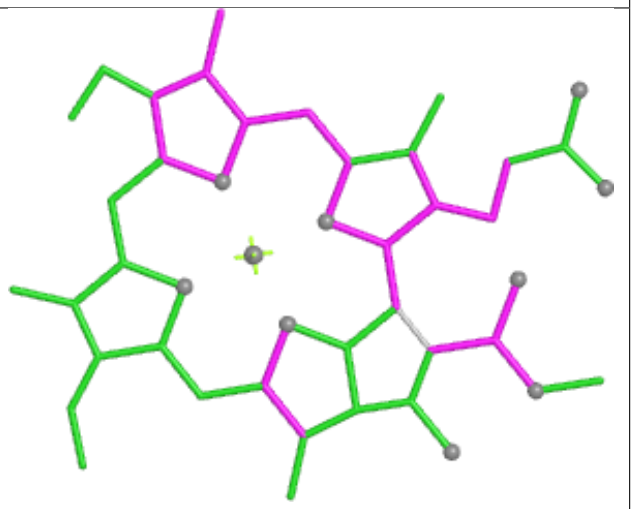

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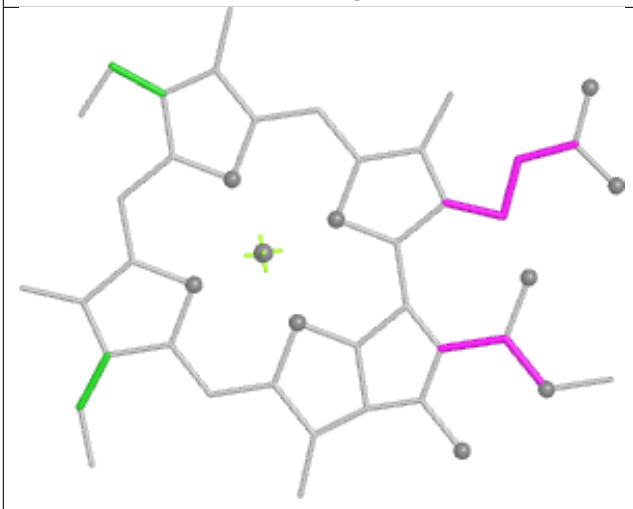

Torsions

Rings

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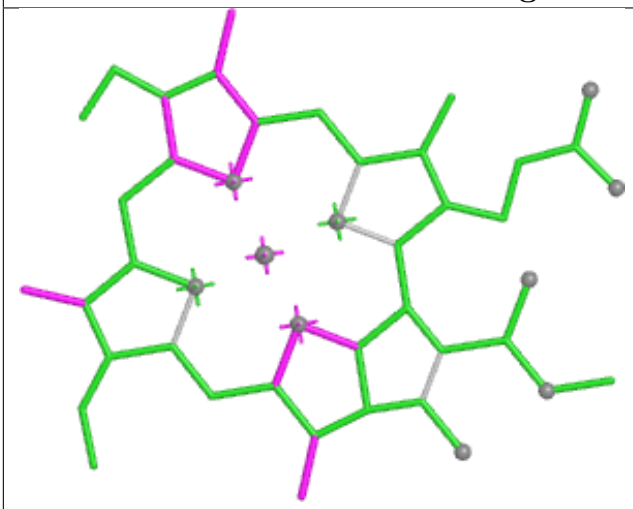

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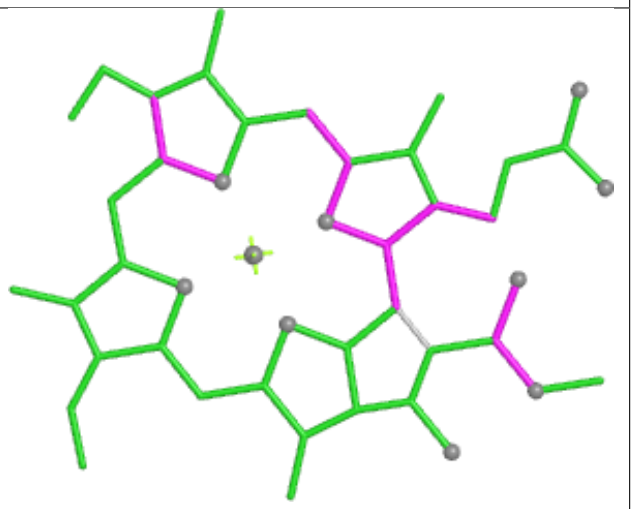

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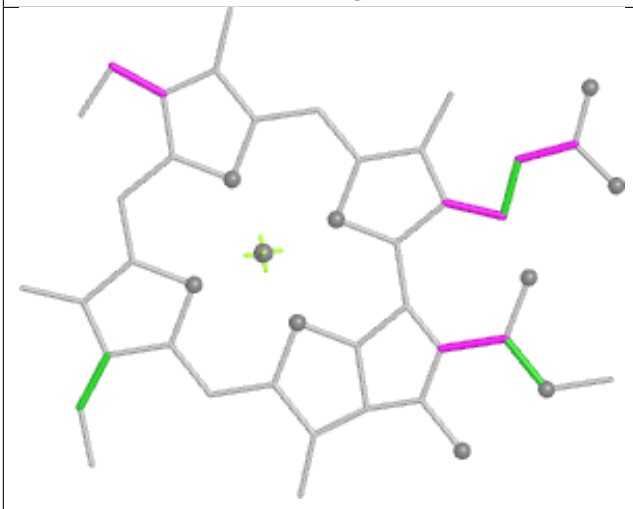

Torsions

Rings

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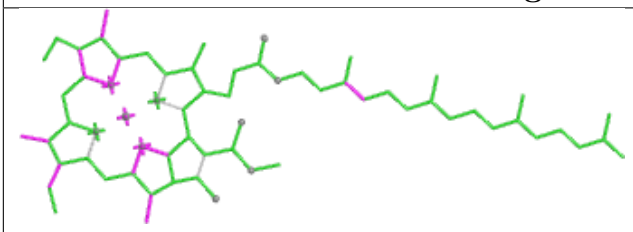

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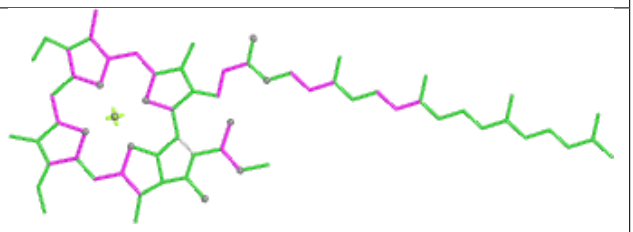

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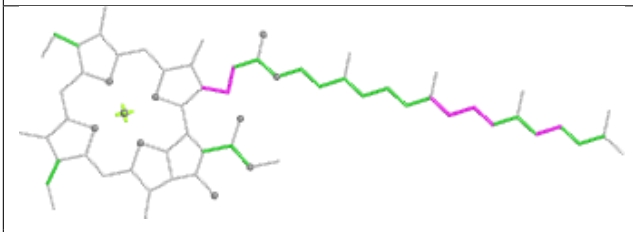

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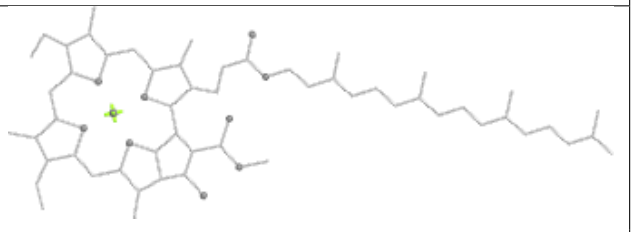
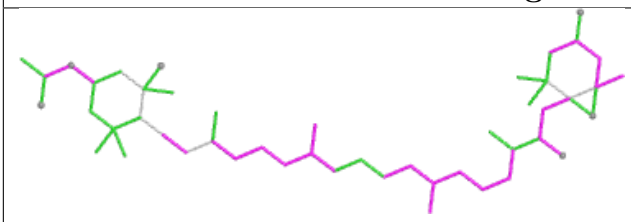


Rings

Ligand A86 11 314



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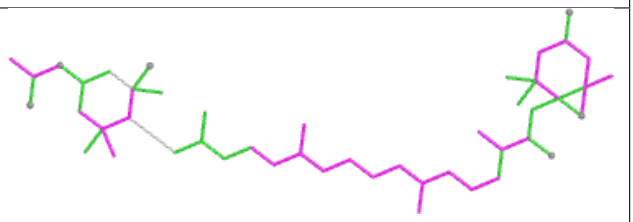

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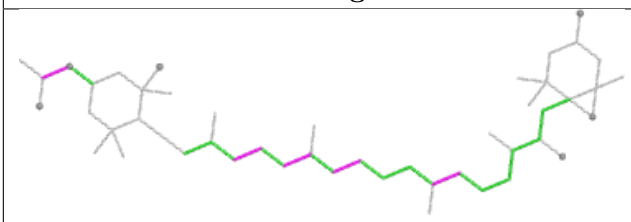

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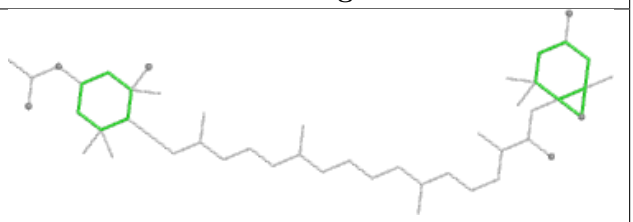
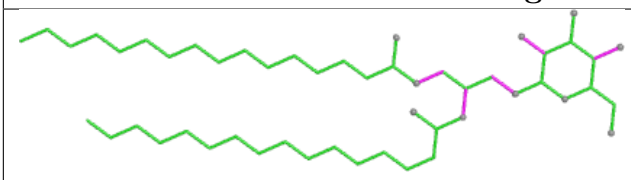


Rings

Ligand LMG c 519



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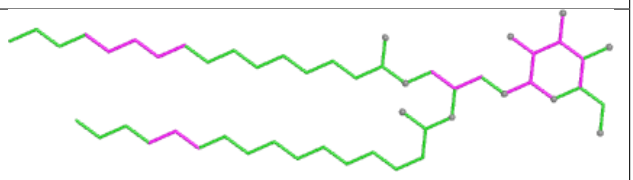
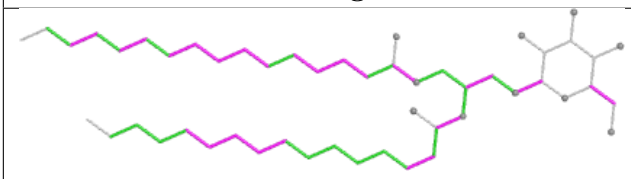


Bond angles



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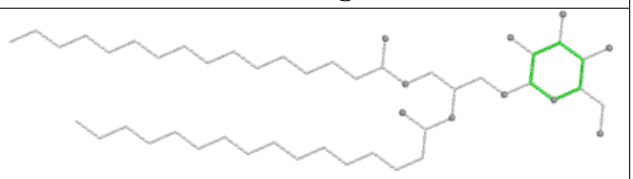
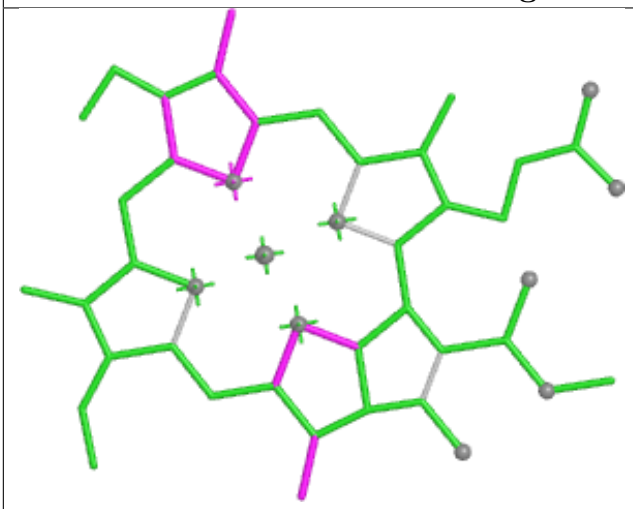


Rings

Ligand CLA 13 307



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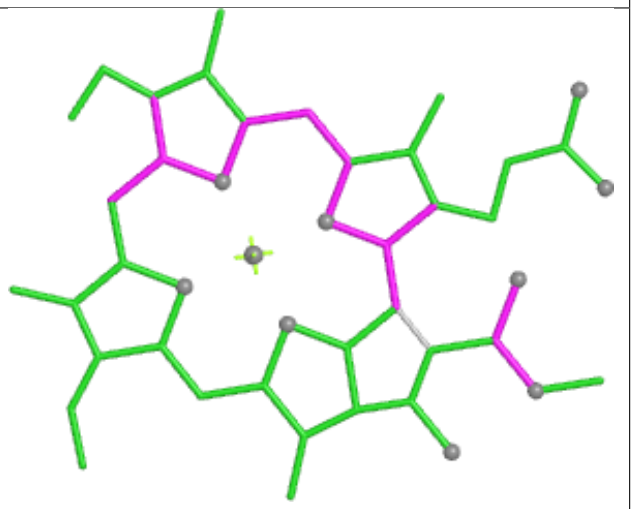
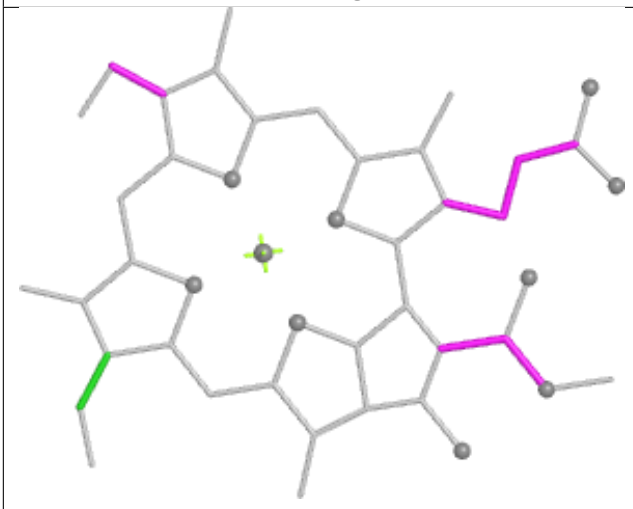


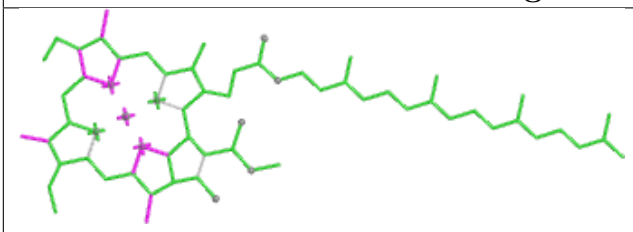
Bond angles



Torsions

Rings

Ligand CLA C 512



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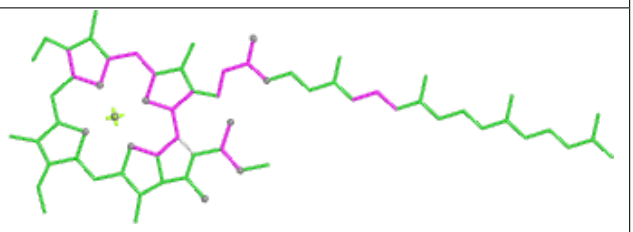
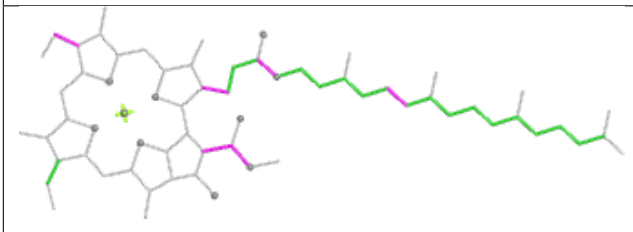


Bond angles



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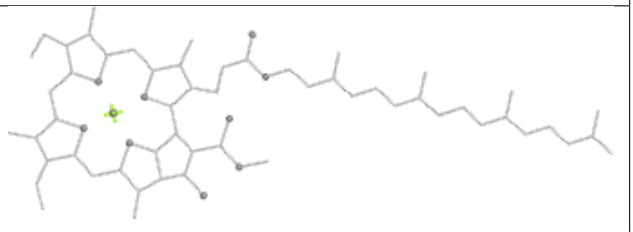
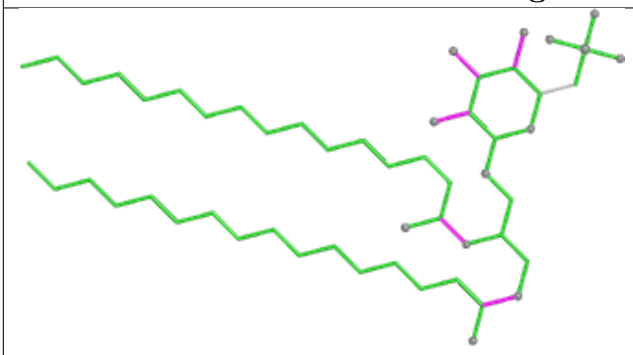


Rings

Ligand SQD a 405



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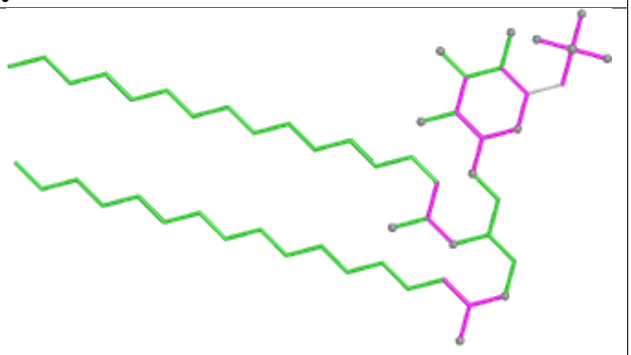
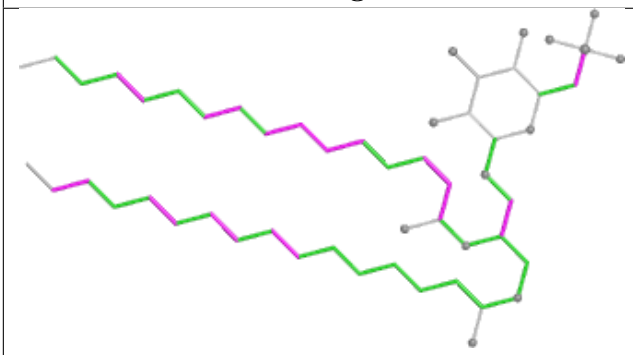
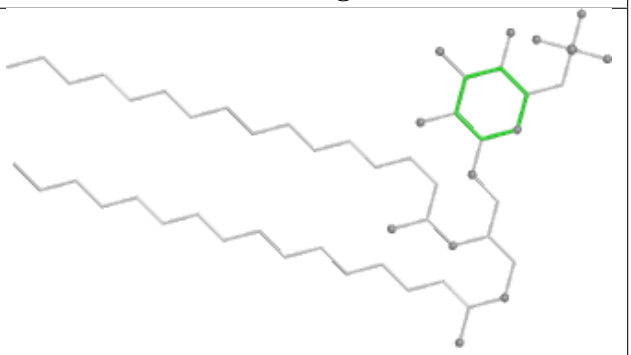


Bond angles

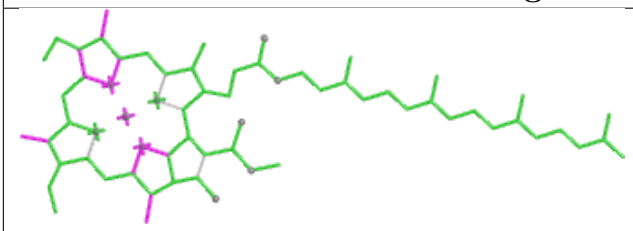


Torsions

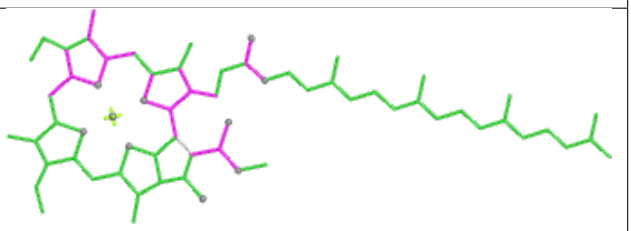


Rings

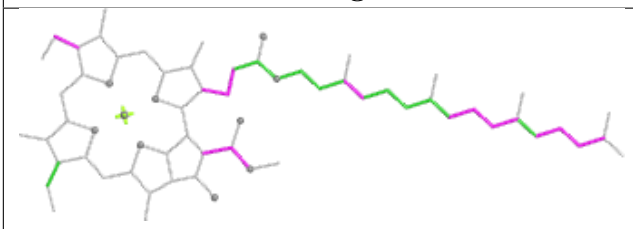
Ligand CLA C 507



Bond lengths



Bond angles



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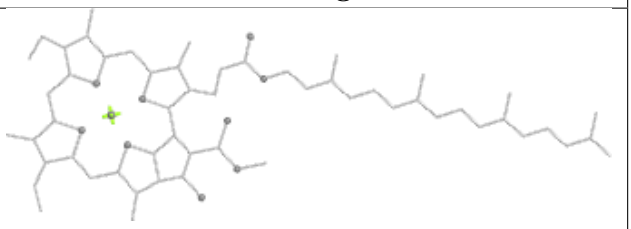
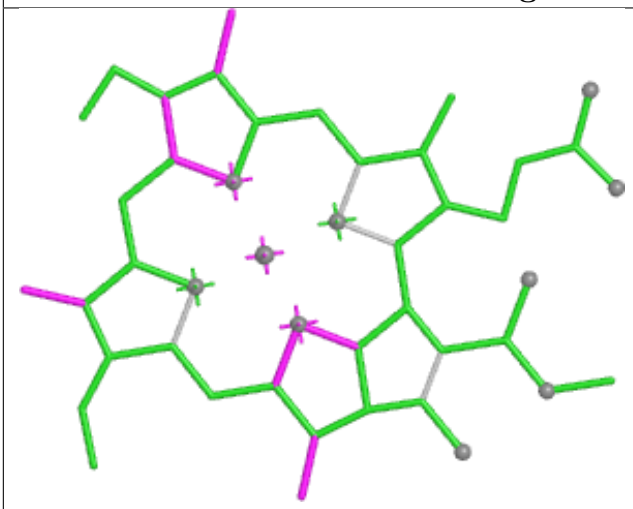


Rings

Ligand CLA 20 205



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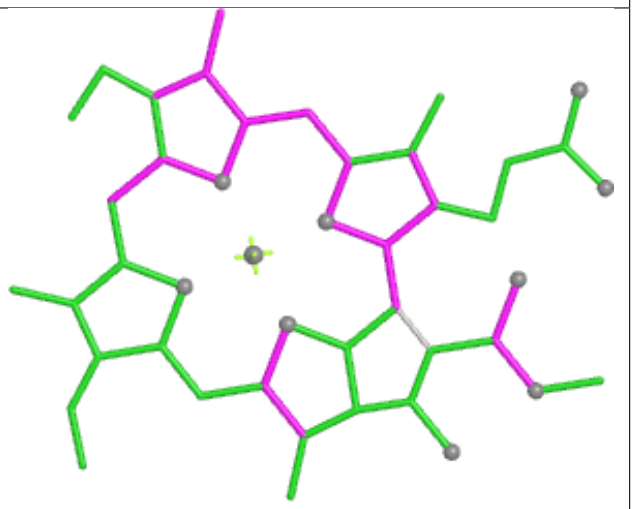
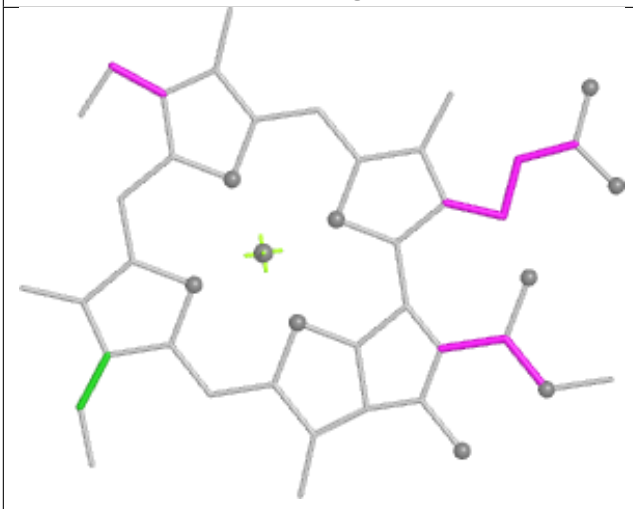


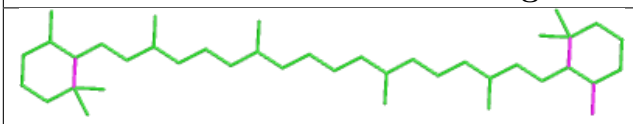
Bond angles



Torsions

Rings

Ligand BCR H 101



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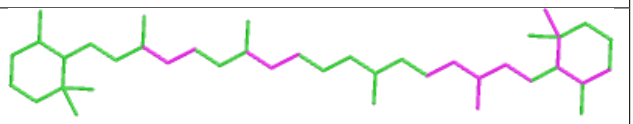
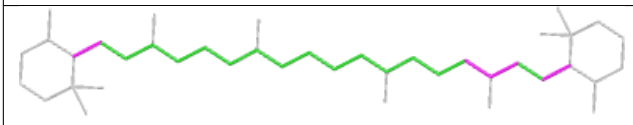


Bond angles



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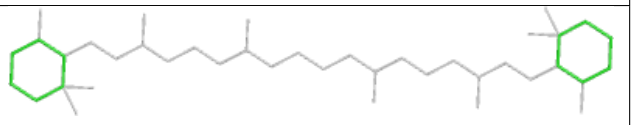
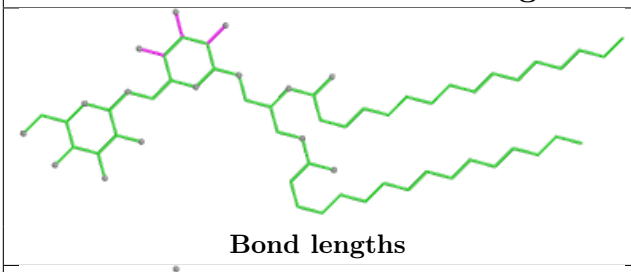


Rings

Ligand DGD H 102



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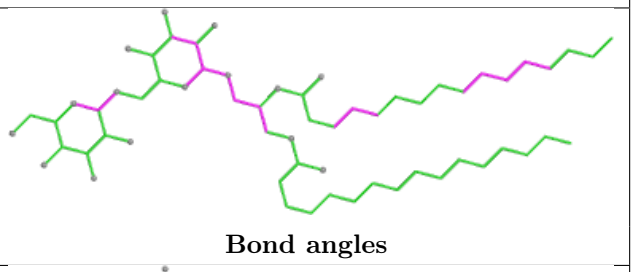
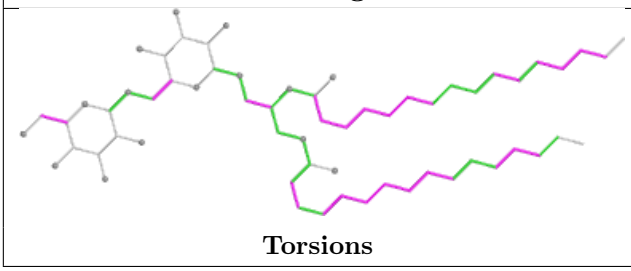


Bond angles



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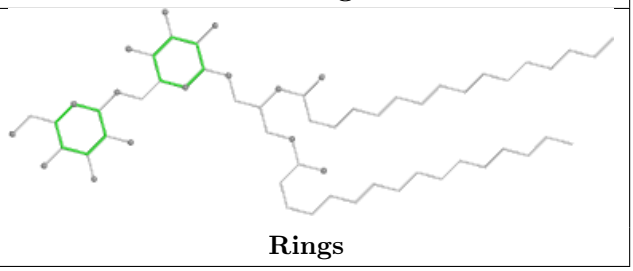
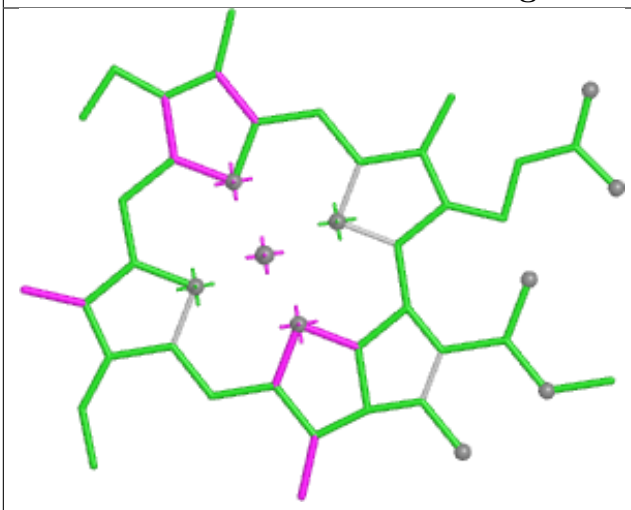


Rings

Ligand CLA 21 304



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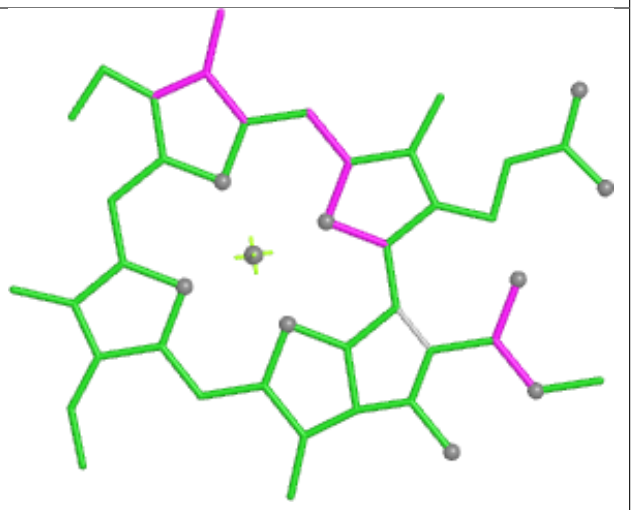

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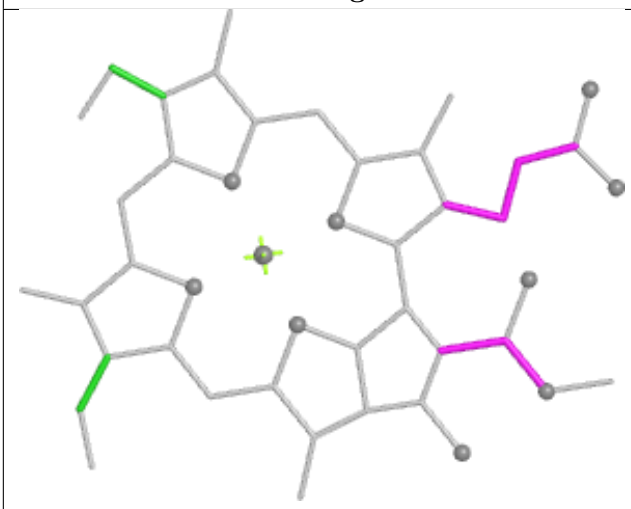
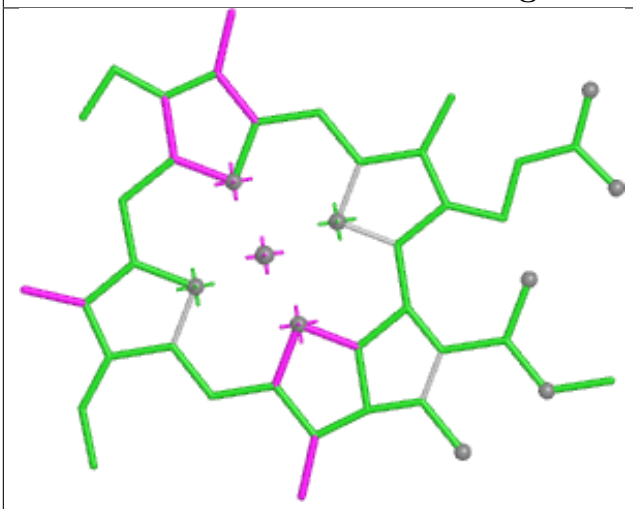


Torsions

Rings

Ligand CLA 13 306



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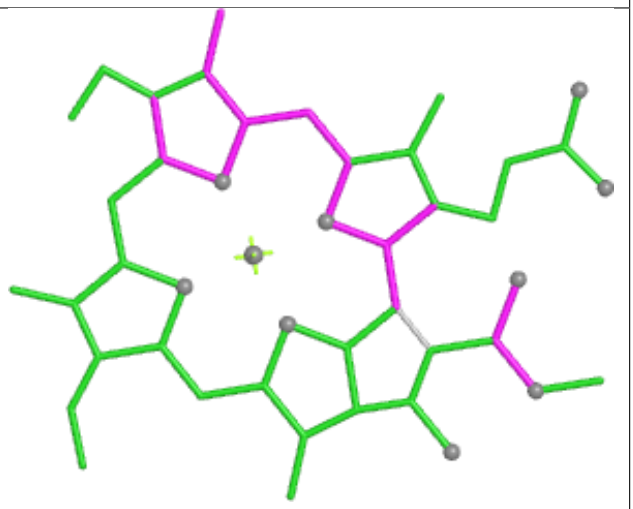
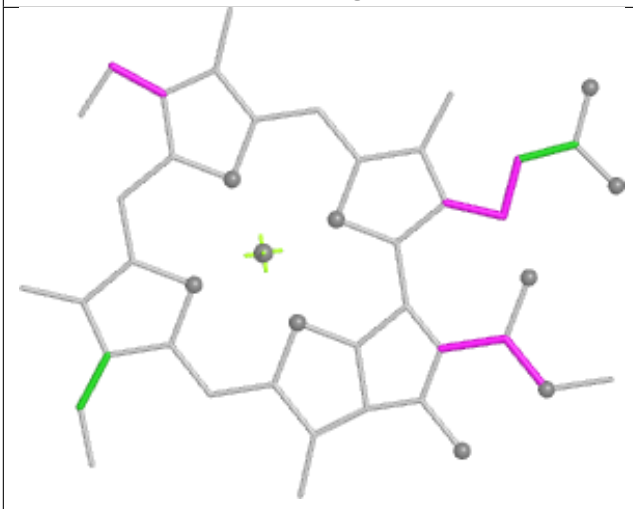


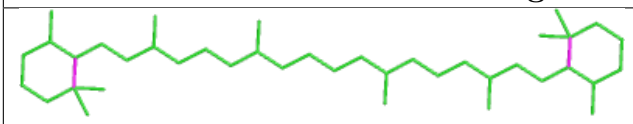
Bond angles



Torsions

Rings

Ligand BCR c 521



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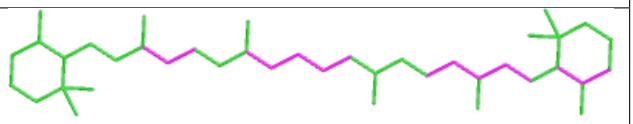

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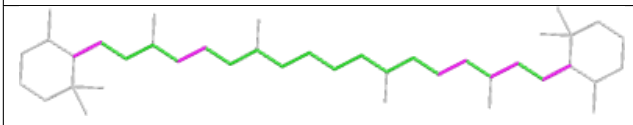

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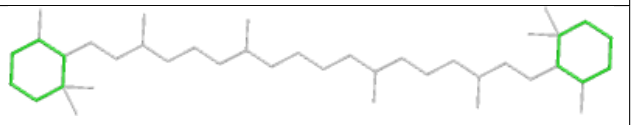
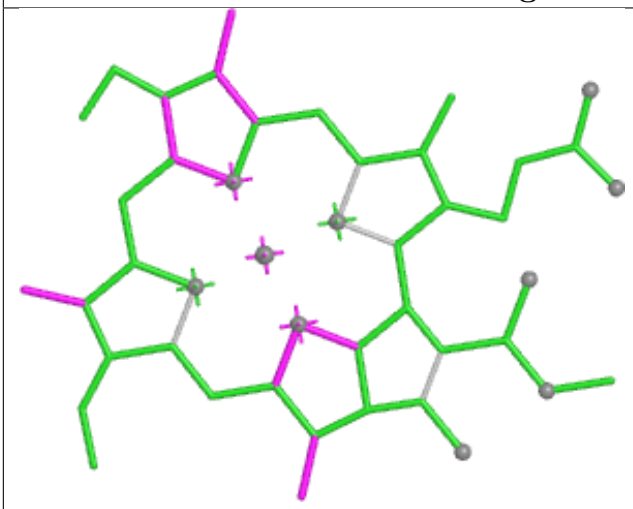


Rings

Ligand CLA 15 308



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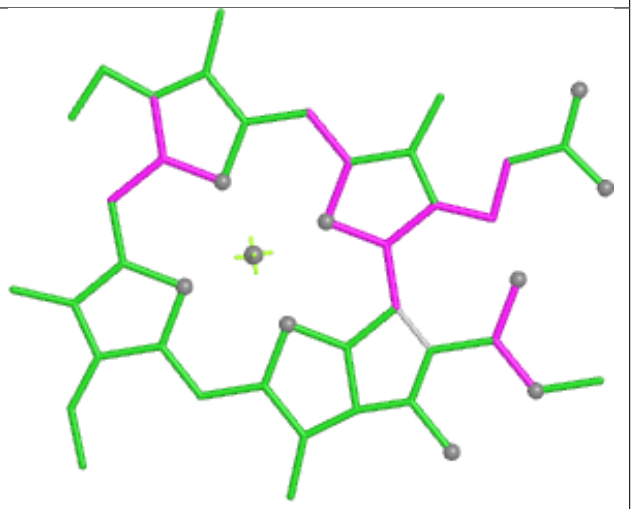

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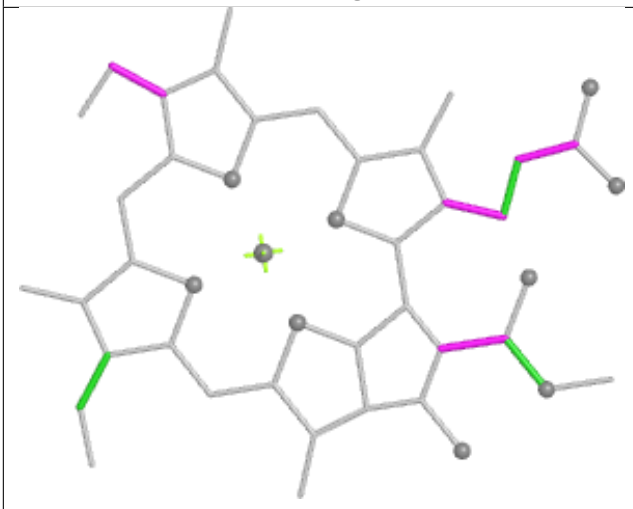
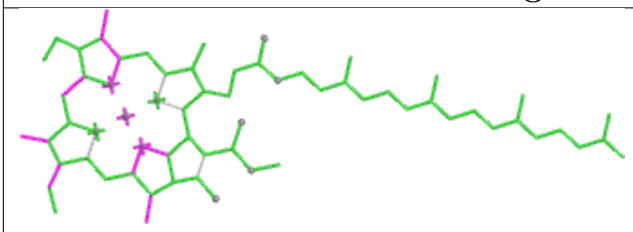


Torsions

Rings

Ligand CLA C 502



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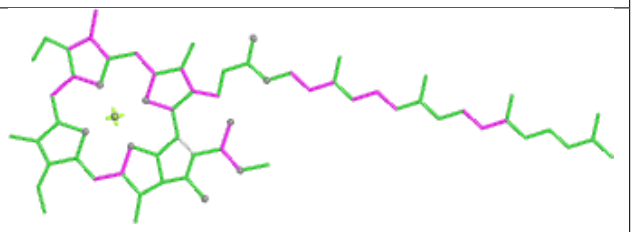

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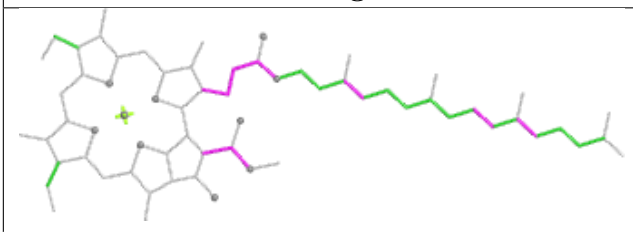

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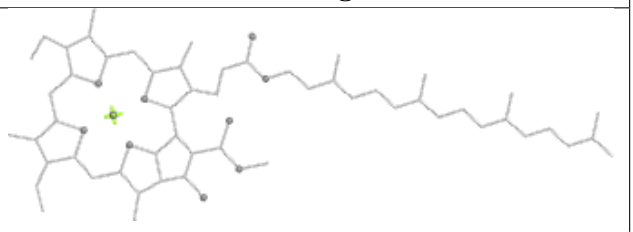
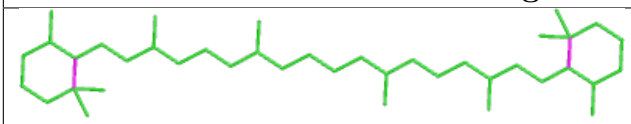


Rings

Ligand BCR A 405



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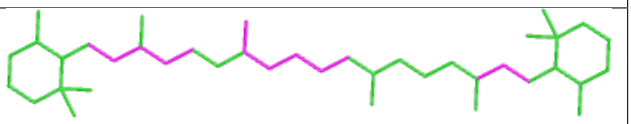
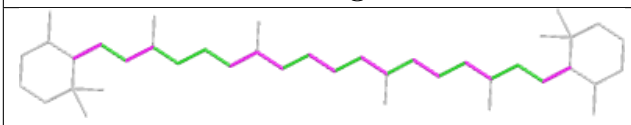


Bond angles



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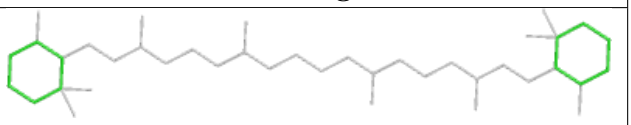
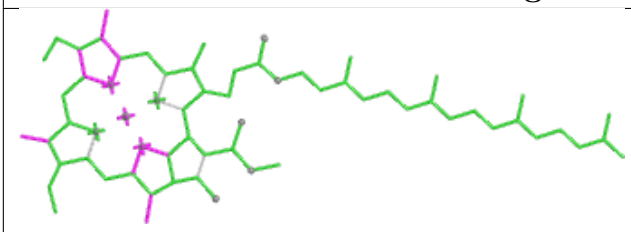


Rings

Ligand CLA B 623



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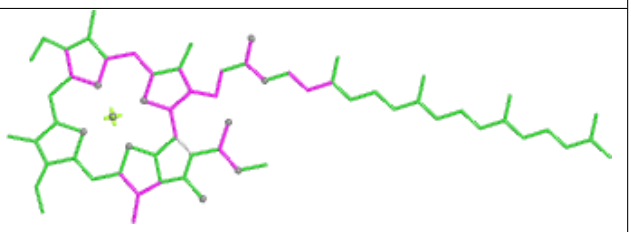
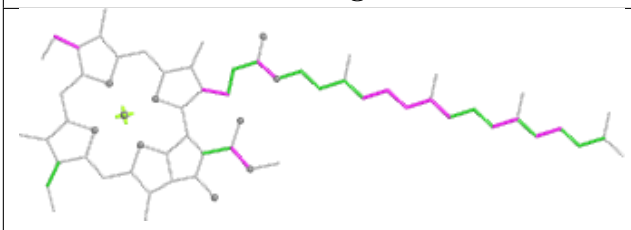


Bond angles



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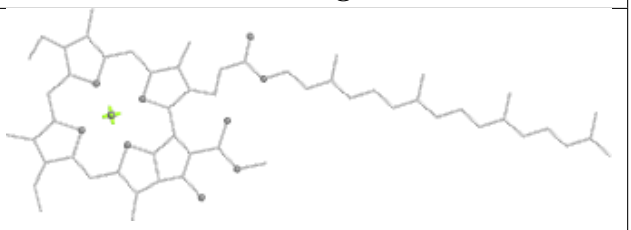
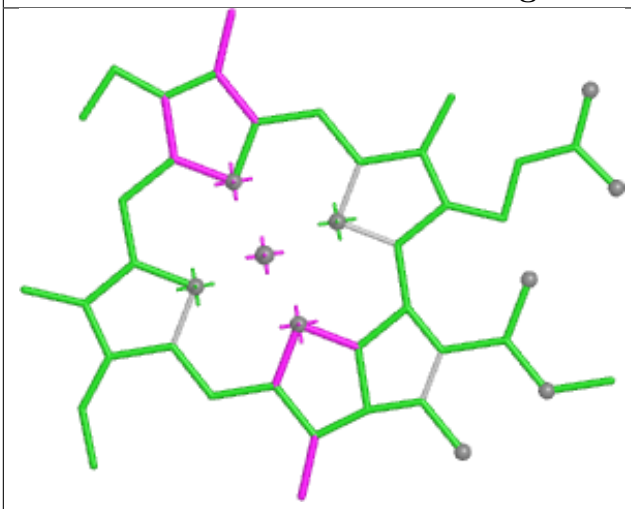


Rings

Ligand CLA 18 308



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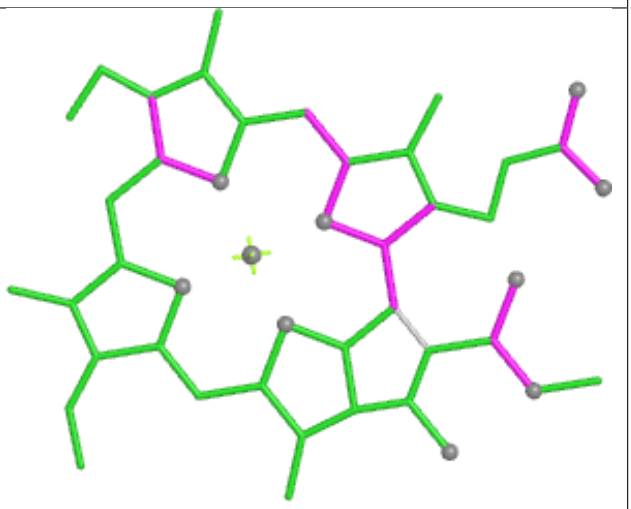
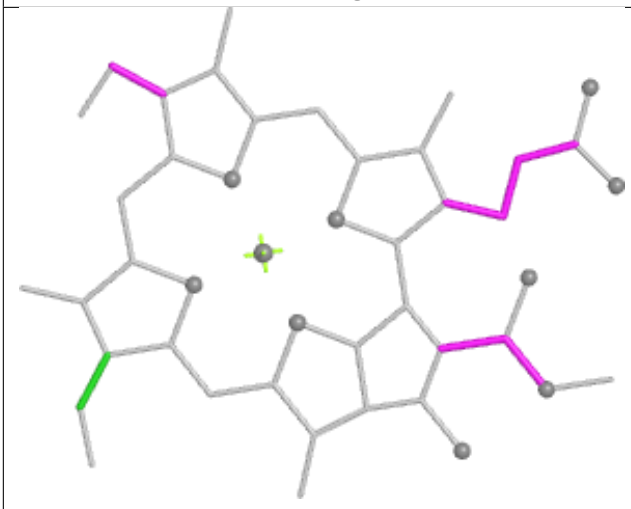


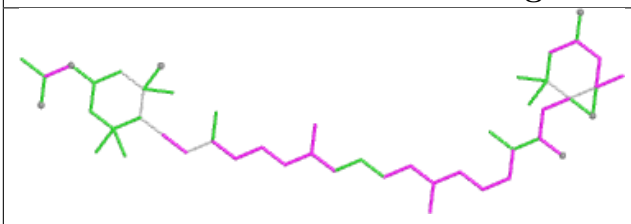
Bond angles



Torsions

Rings

Ligand A86 14 314



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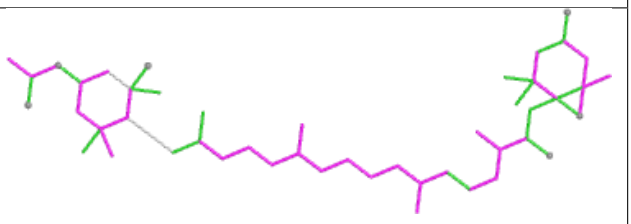
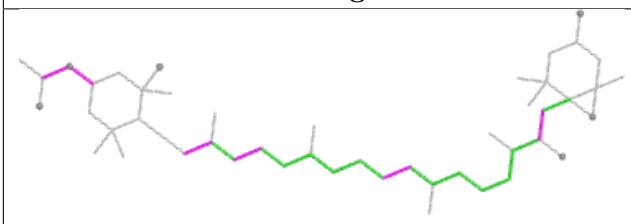


Bond angles



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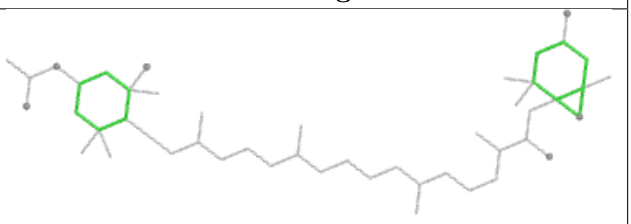
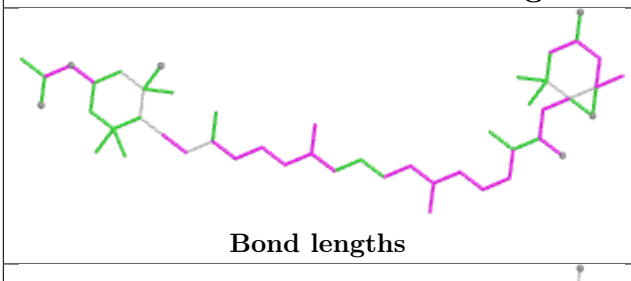


Rings

Ligand A86 21 311



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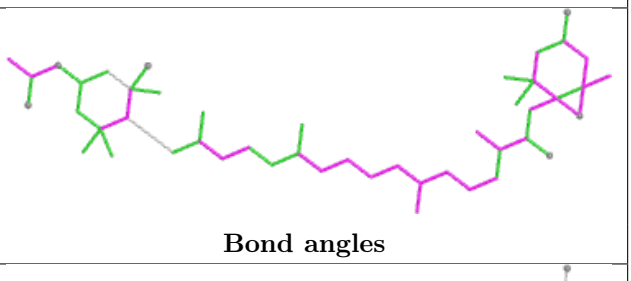
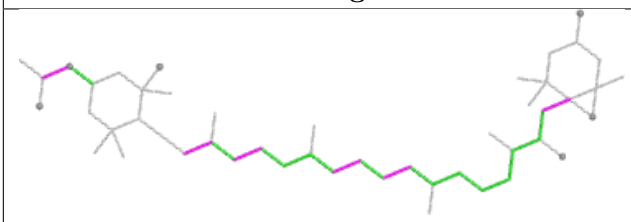


Bond angles



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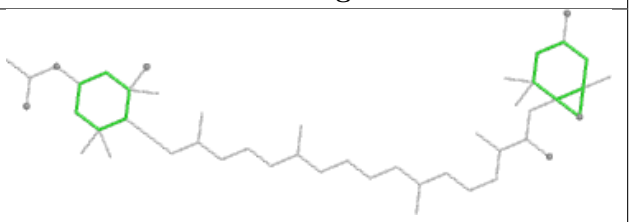
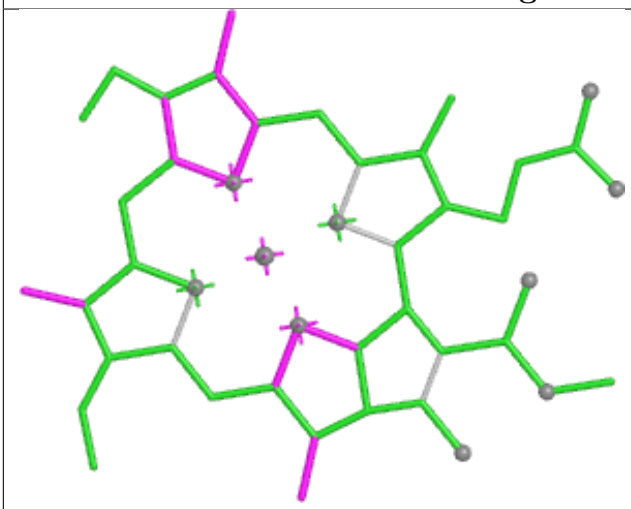


Rings

Ligand CLA 19 308



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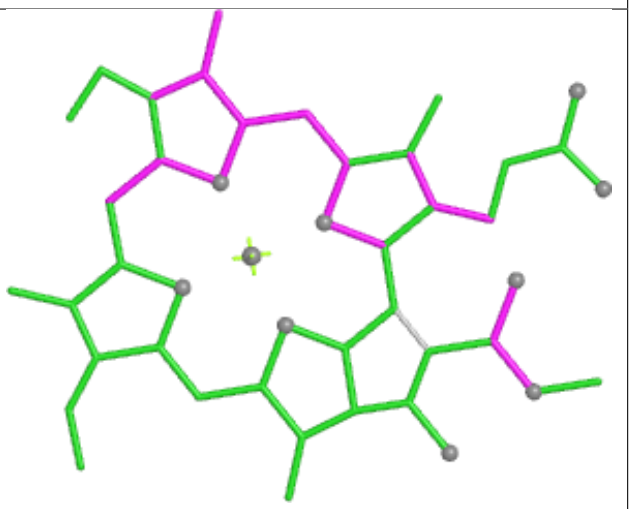
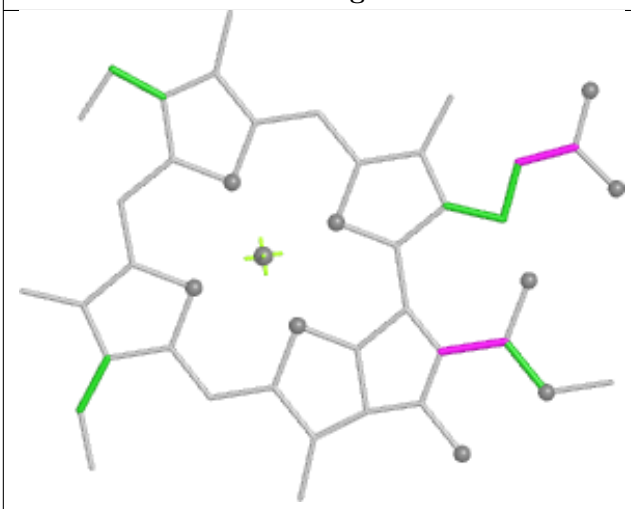
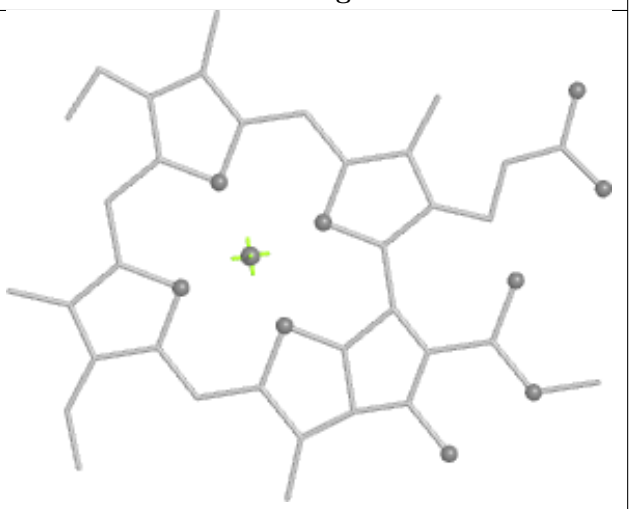


Bond angles

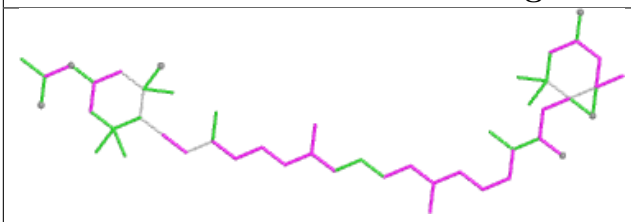


Torsions



Rings

Ligand A86 17 313



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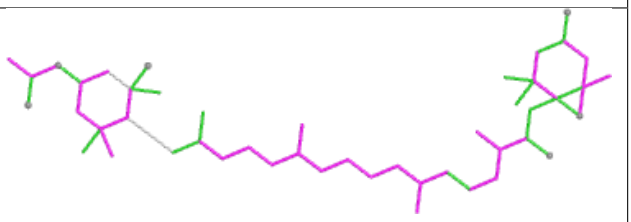

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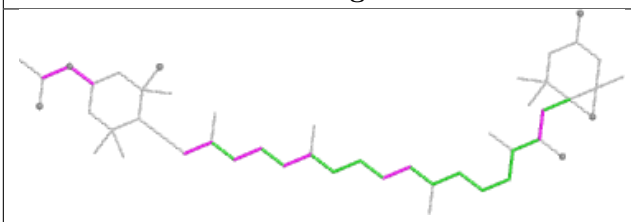

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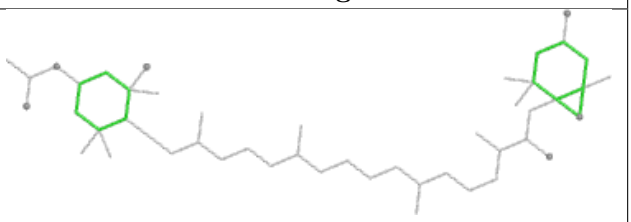
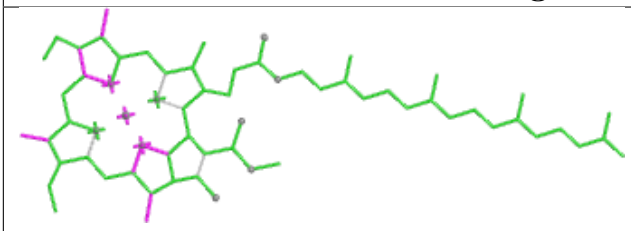


Rings

Ligand CLA c 506



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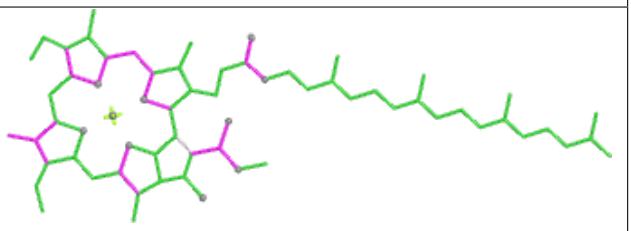

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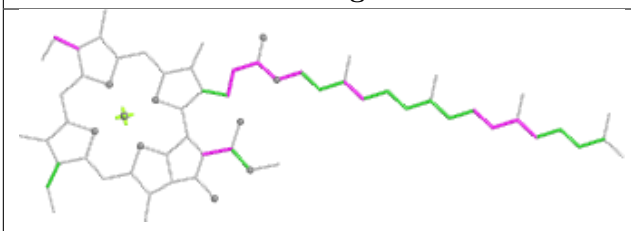

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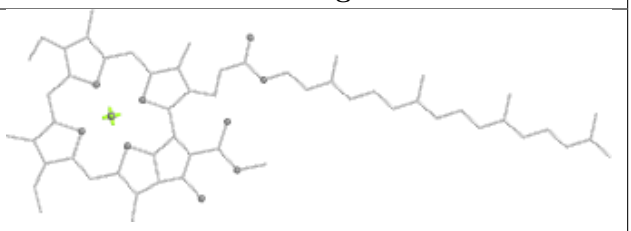
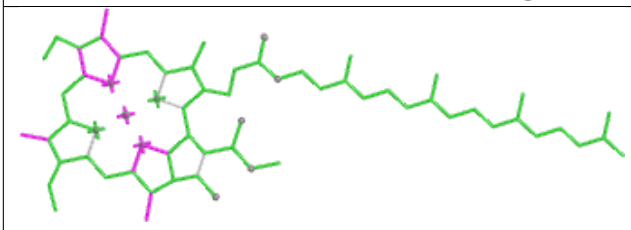


Rings

Ligand CLA 11 315



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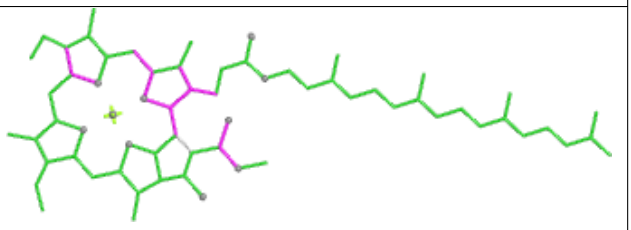

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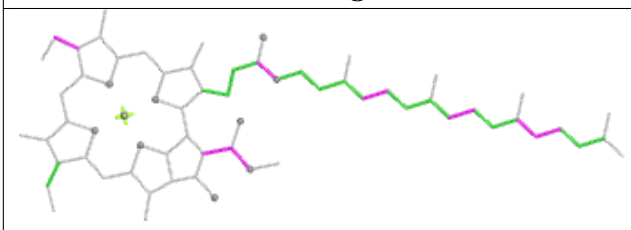

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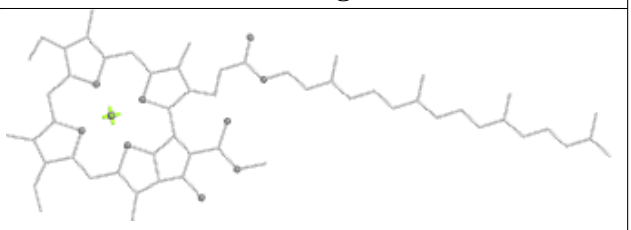

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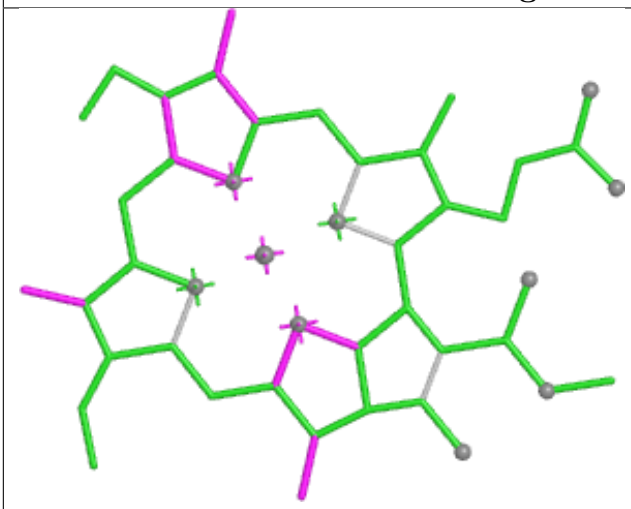

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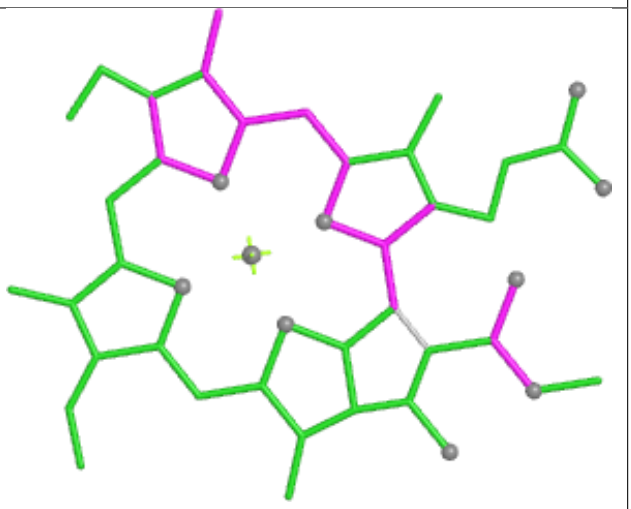

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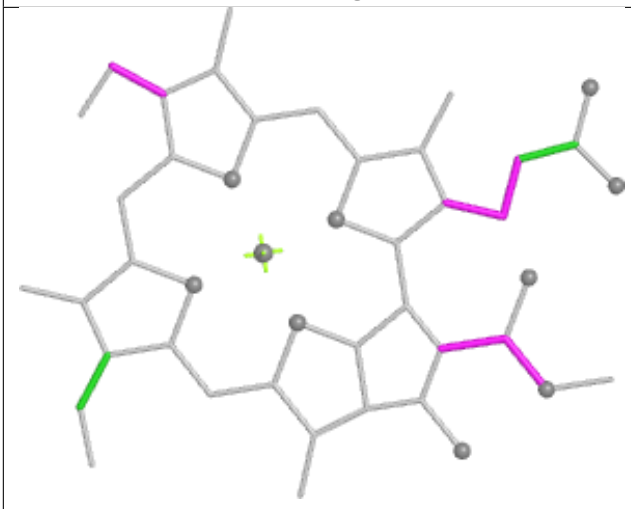
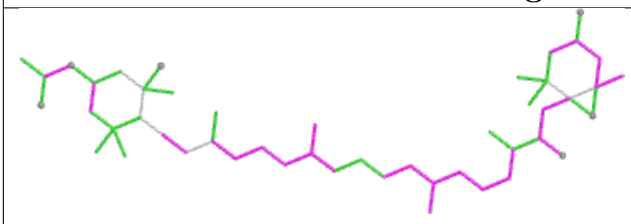


Torsions

Rings

Ligand A86 15 312



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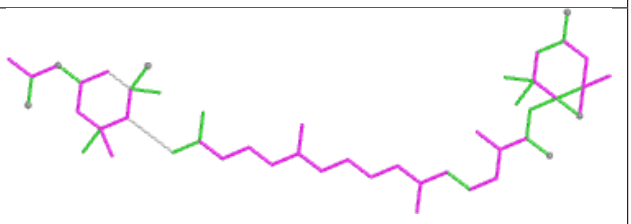

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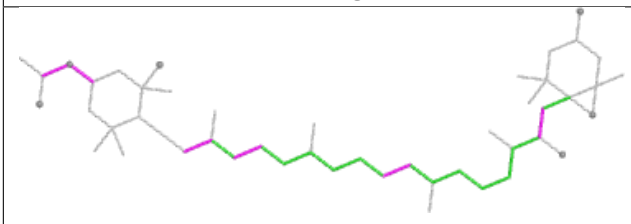

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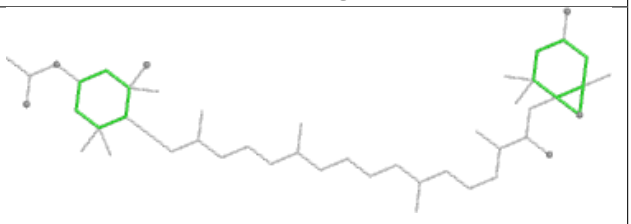
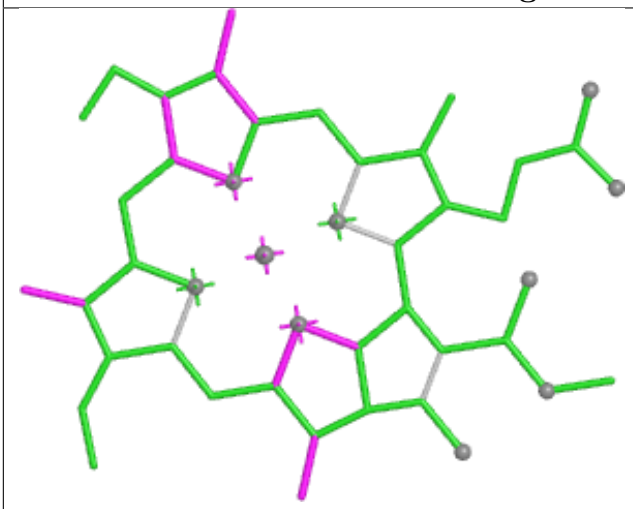


Rings

Ligand CLA 14 307



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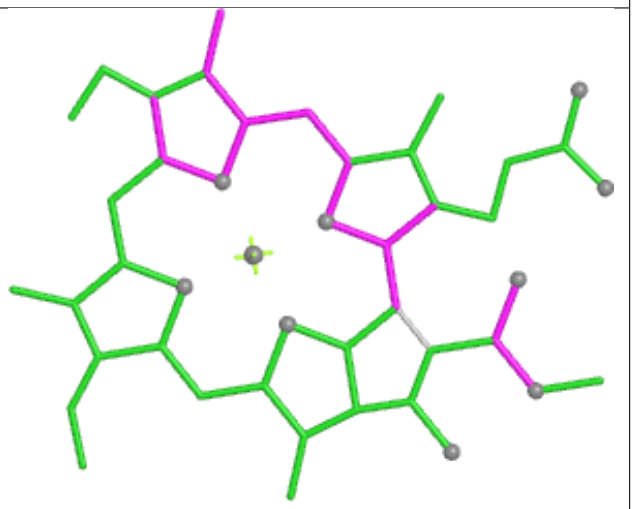

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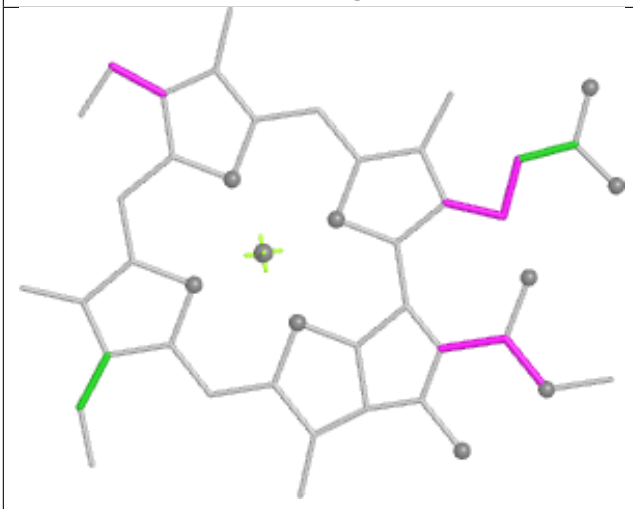
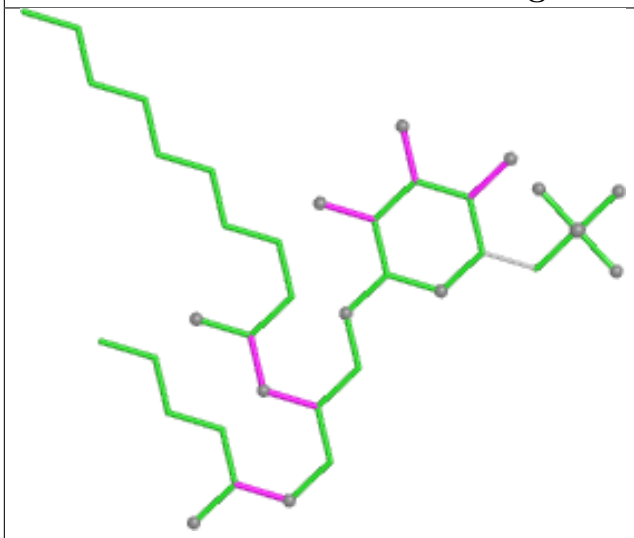


Torsions

Rings

Ligand SQD b 620



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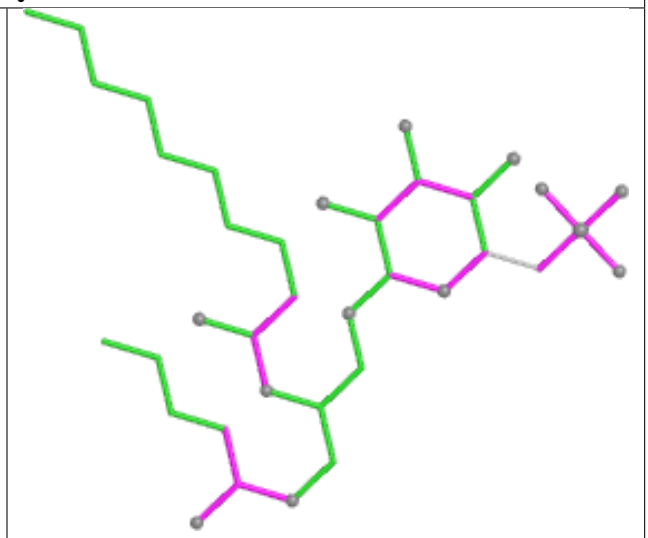

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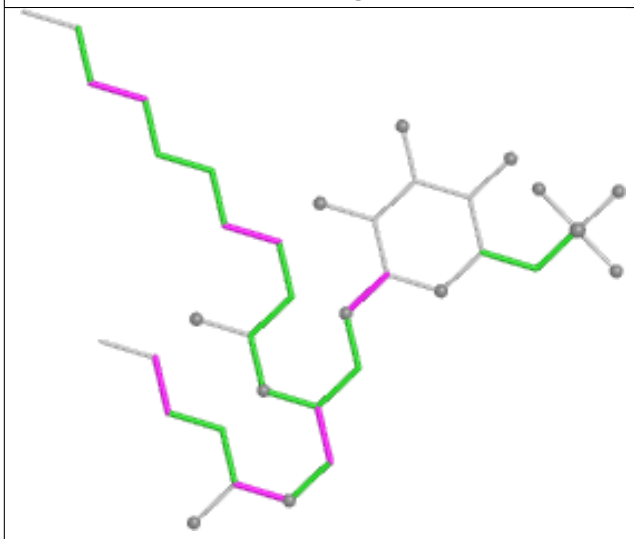

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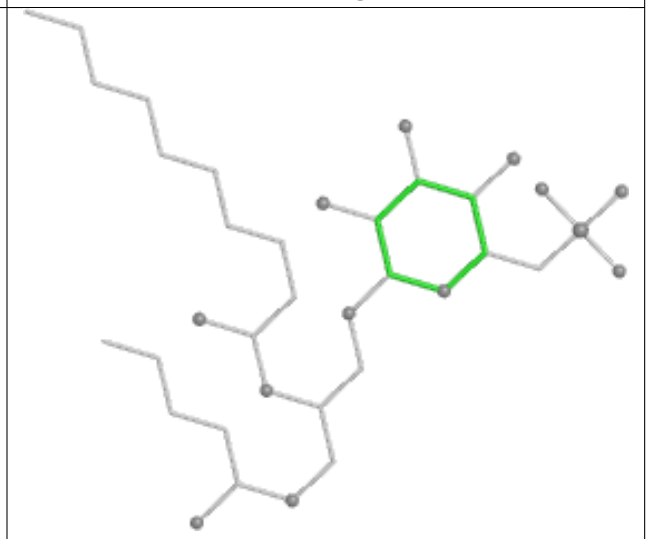
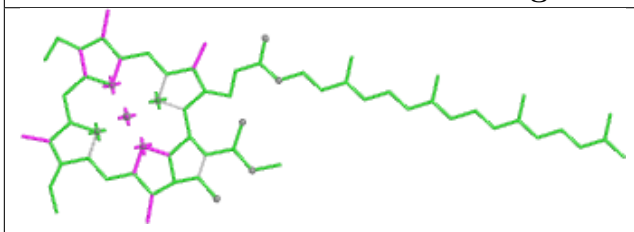


Rings

Ligand CLA c 510



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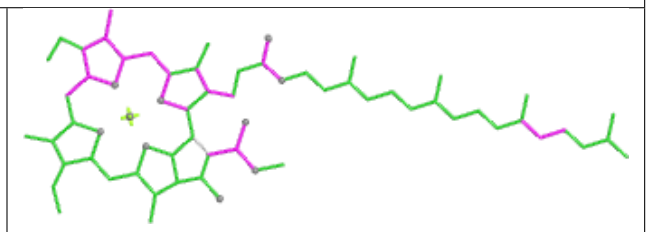

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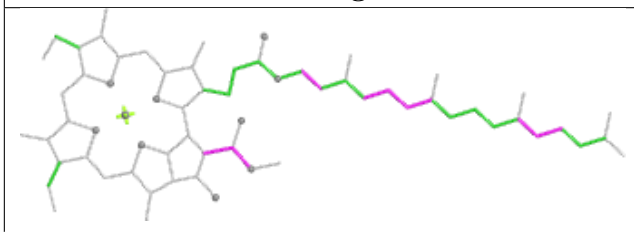

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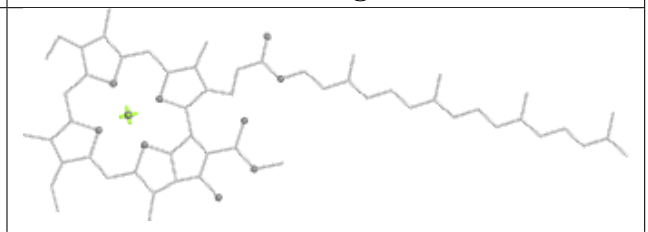
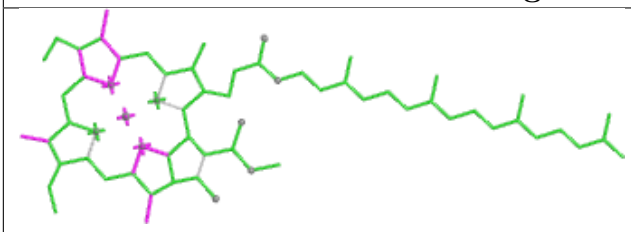


Rings

Ligand CLA A 402



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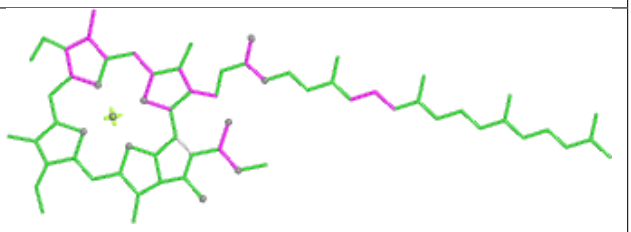

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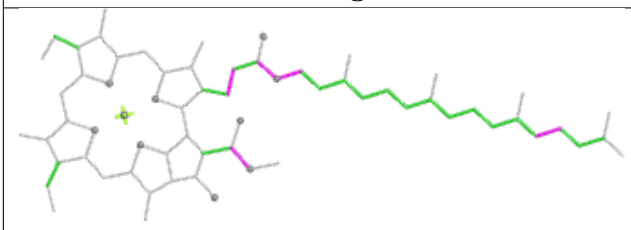

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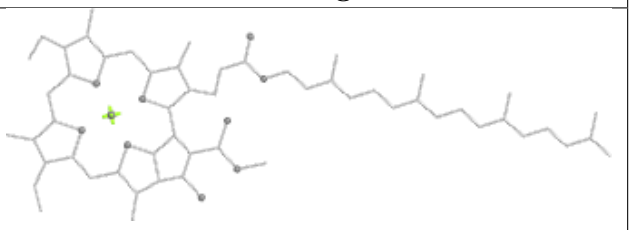
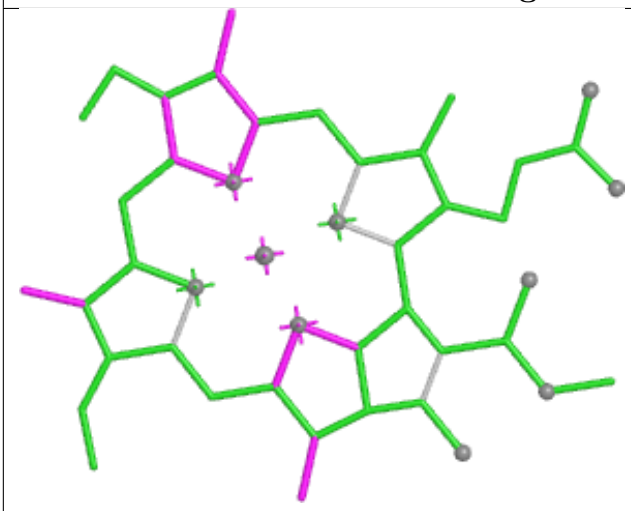


Rings

Ligand CLA 19 305



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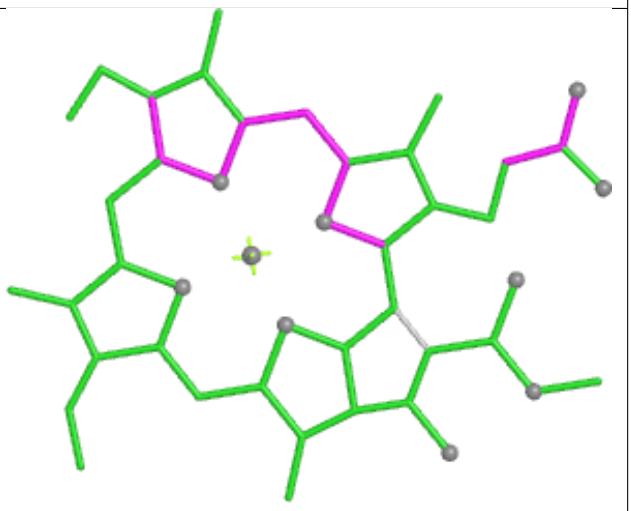

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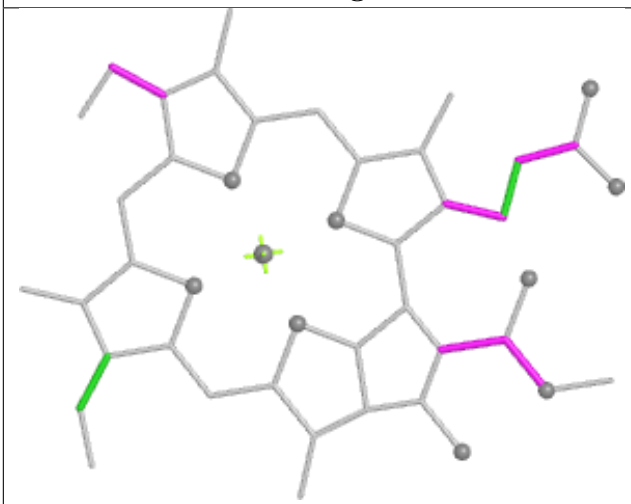

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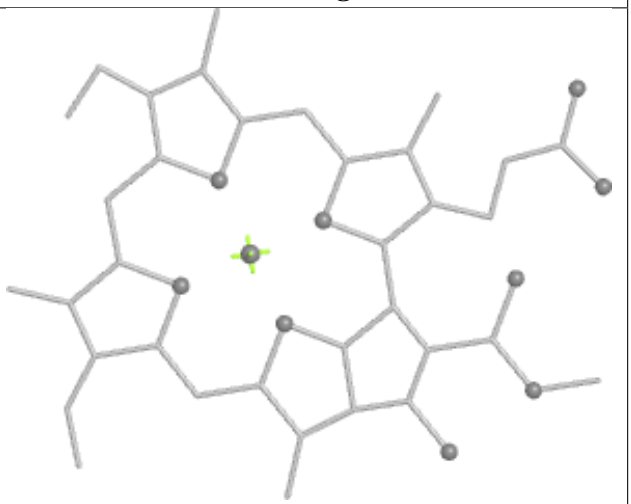
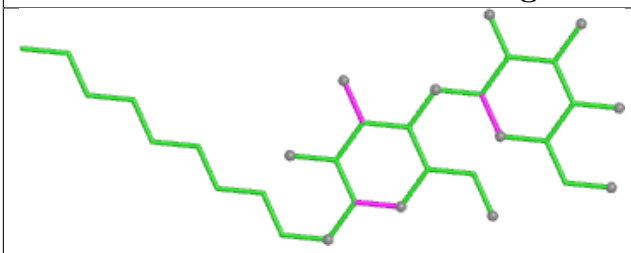


Rings

Ligand LMU B 625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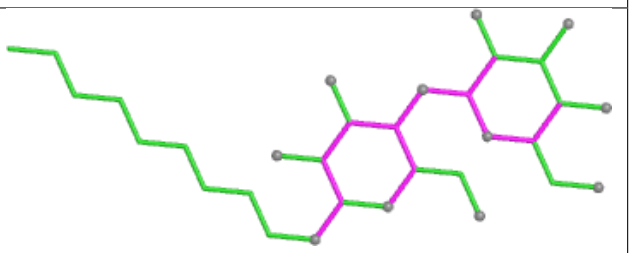
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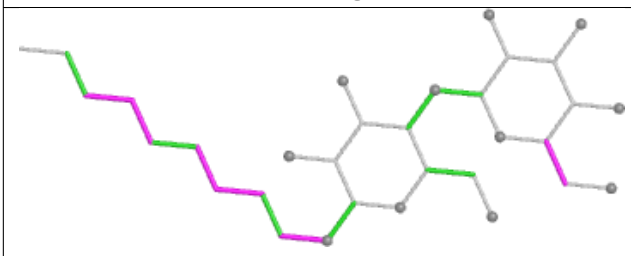
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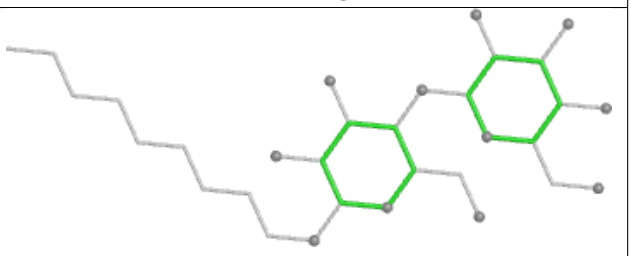
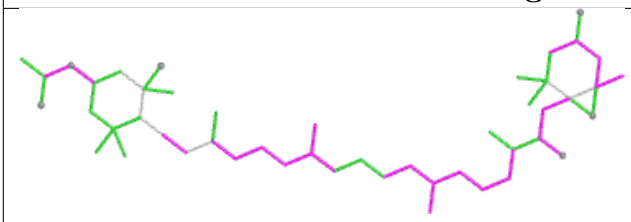

Rings

Ligand A86 21 314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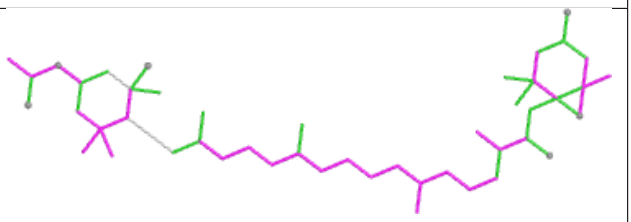
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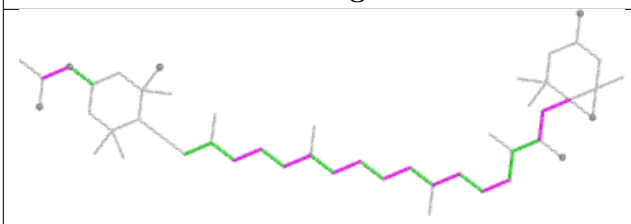
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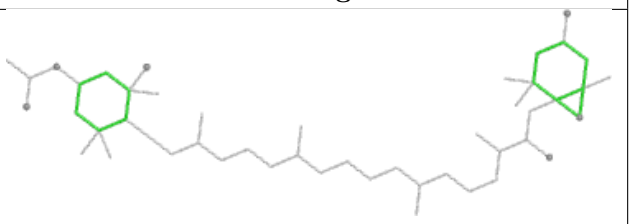
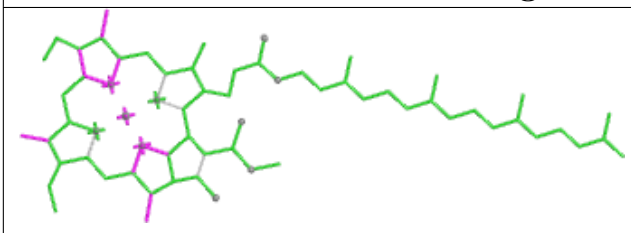

Rings

Ligand CLA 12 311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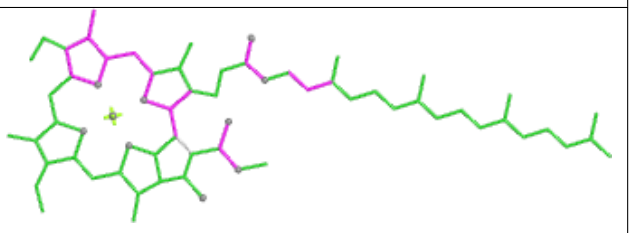
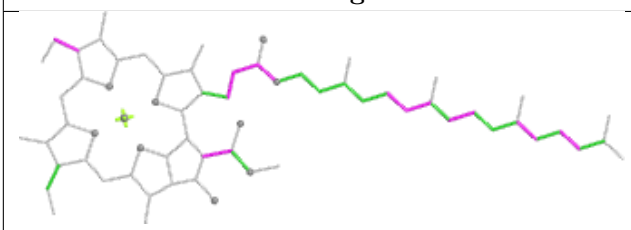

Bond angles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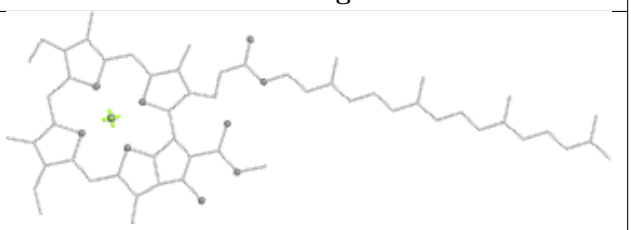
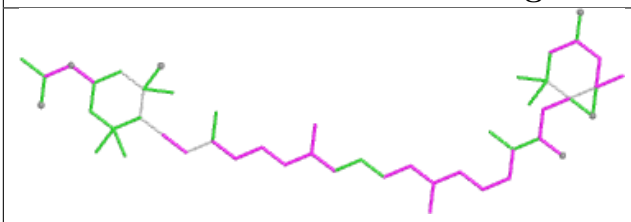

Rings

Ligand A86 18 302



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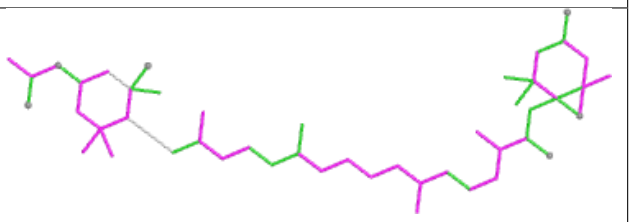
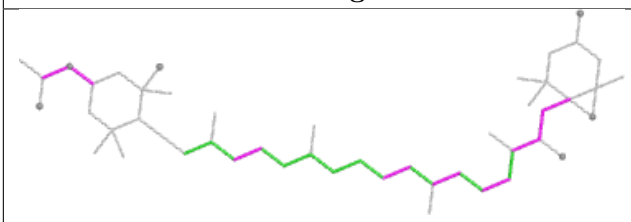
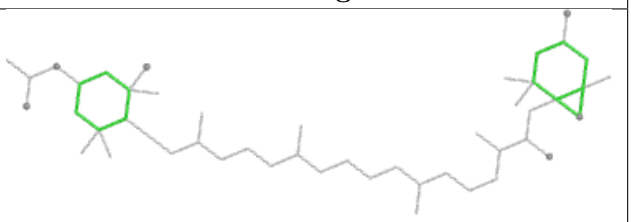


Bond angles

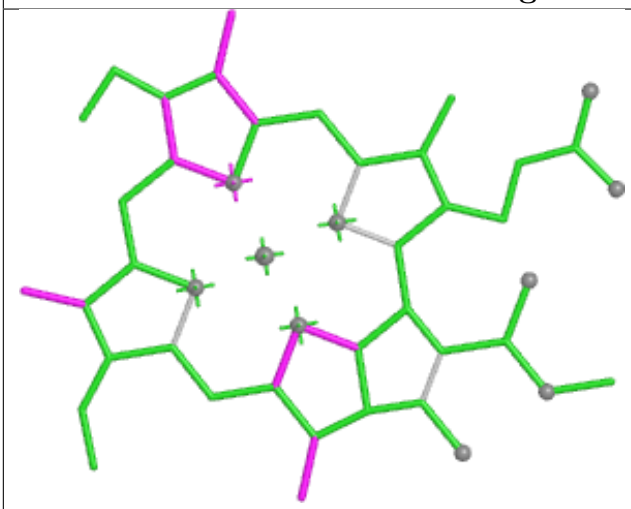


Torsions



Rings

Ligand CLA 15 306



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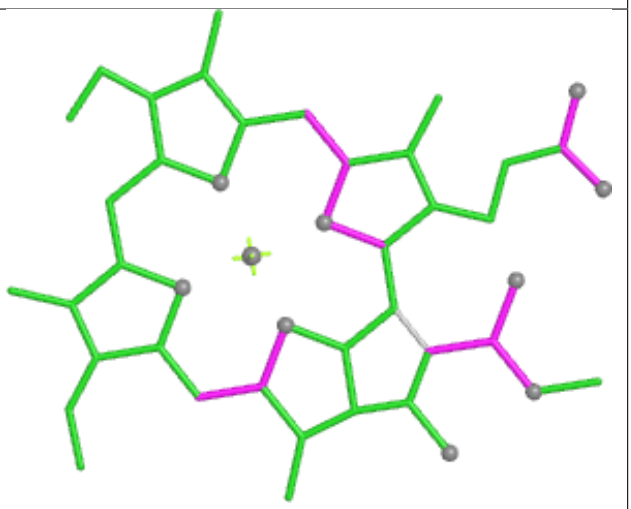

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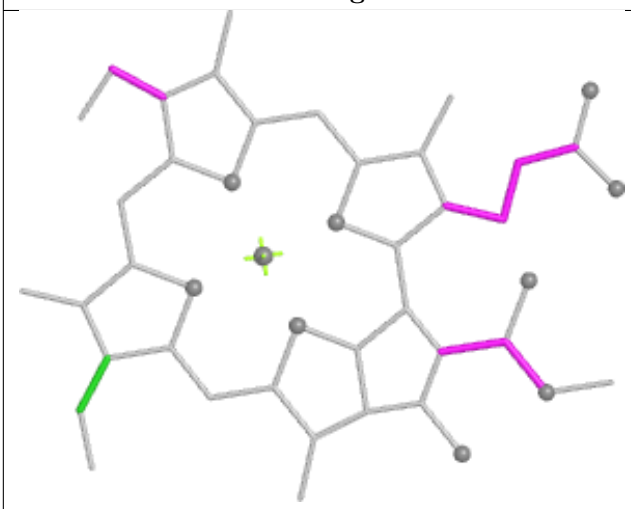

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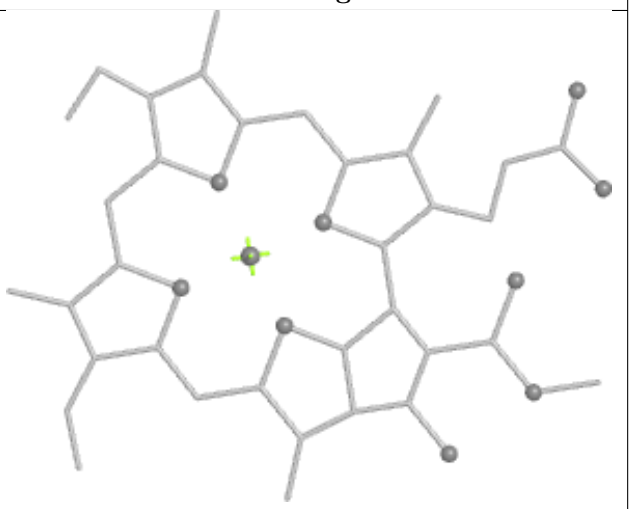
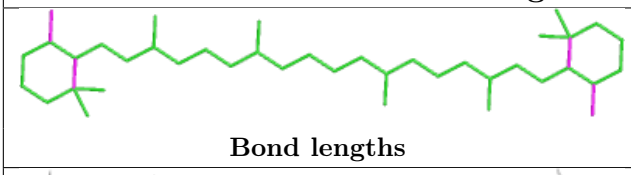


Rings

Ligand BCR c 516



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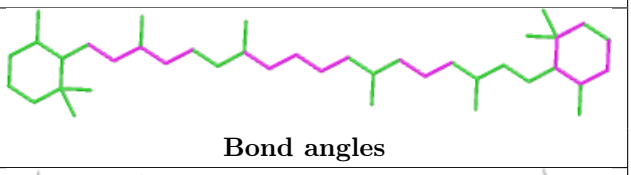

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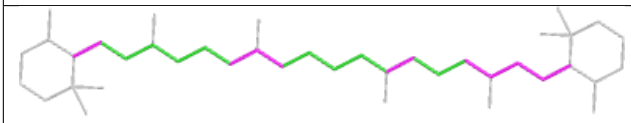

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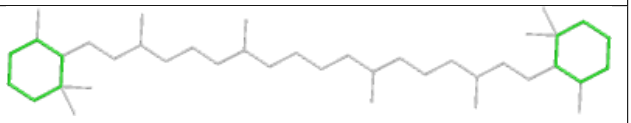
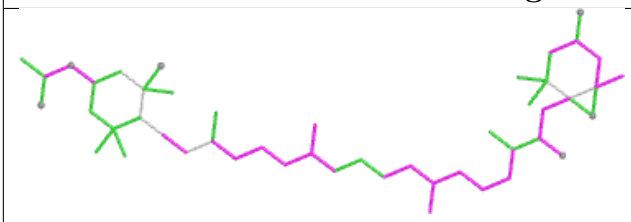


Rings

Ligand A86 14 315



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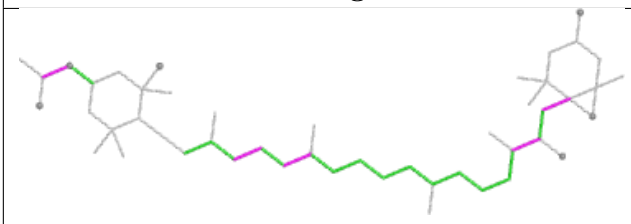

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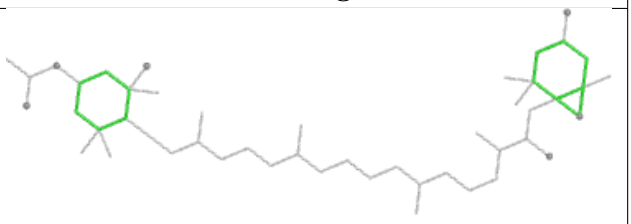
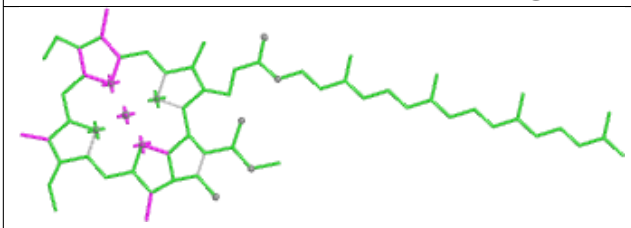


Rings

Ligand CLA b 622



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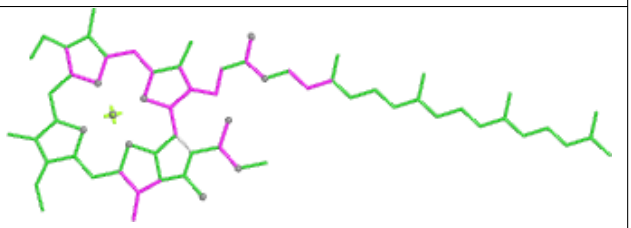

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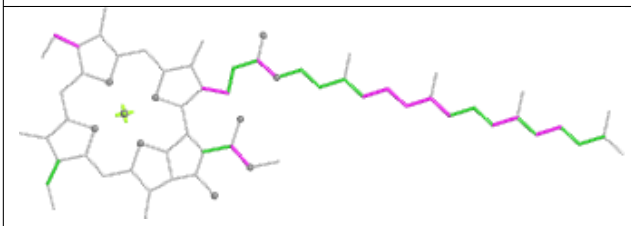

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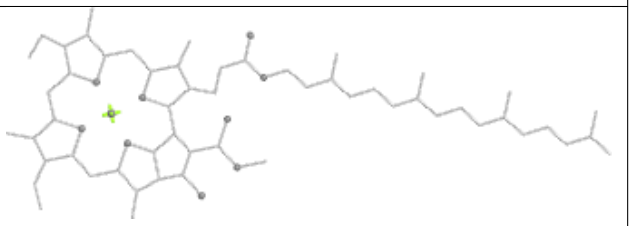
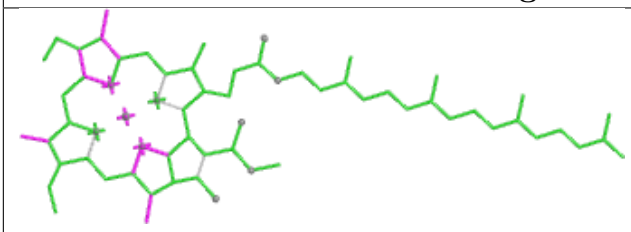


Rings

Ligand CLA 16 302



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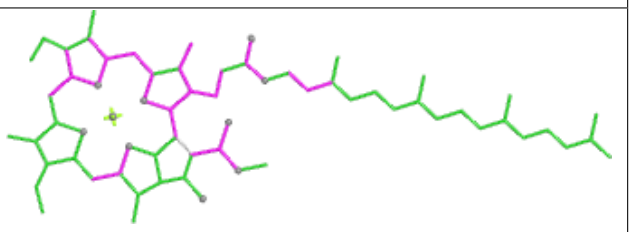

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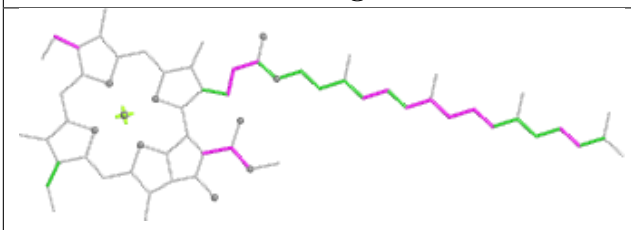

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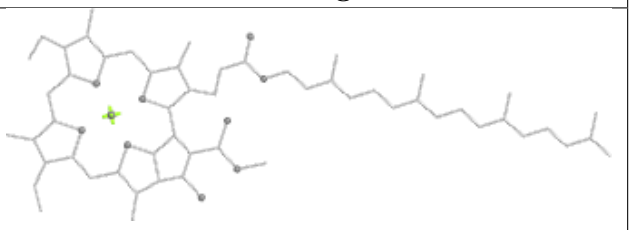
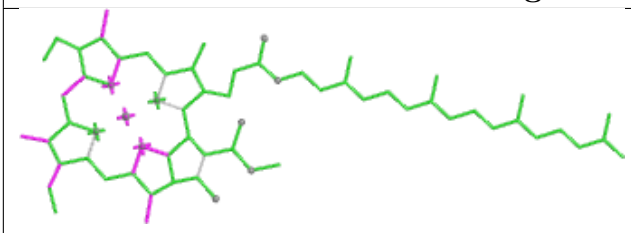


Rings

Ligand CLA C 505



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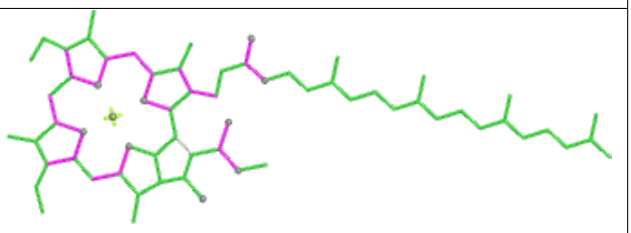

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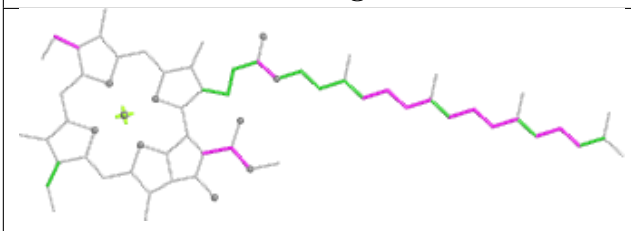

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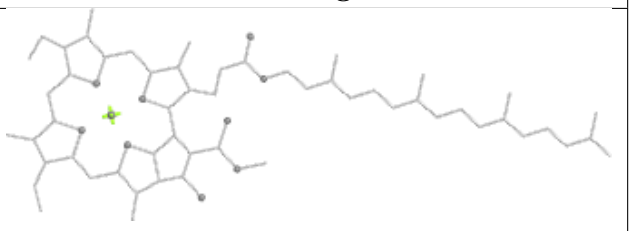

Rings

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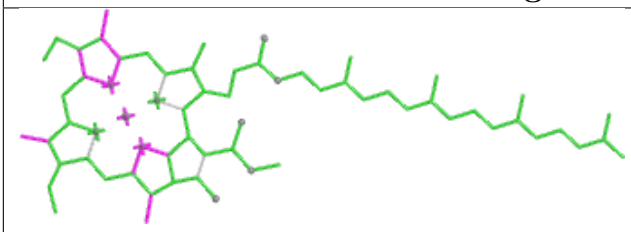

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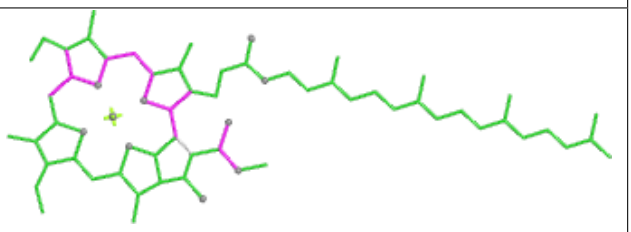

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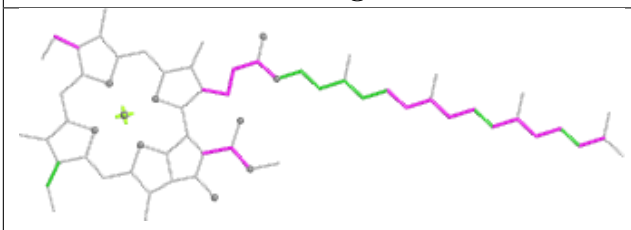

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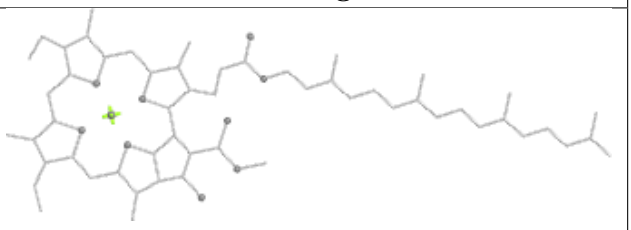
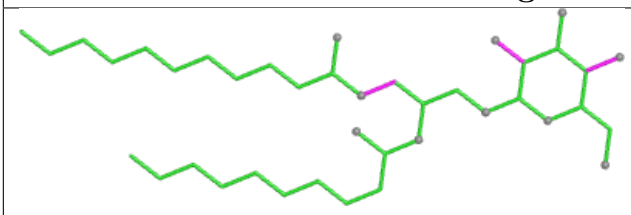
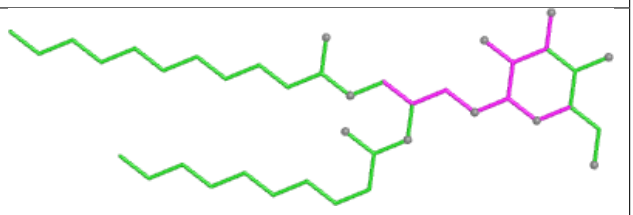
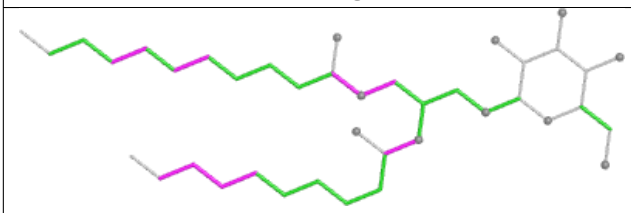
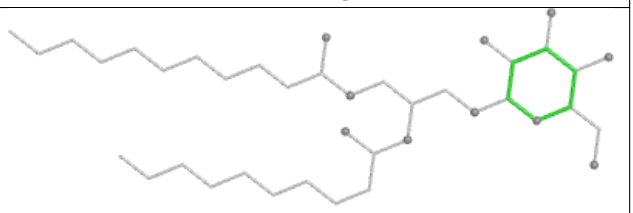
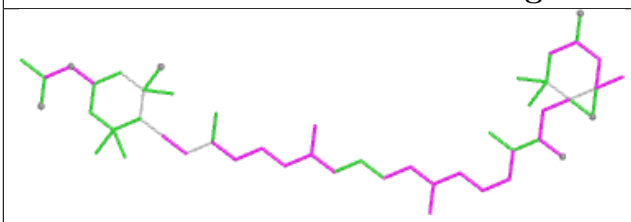
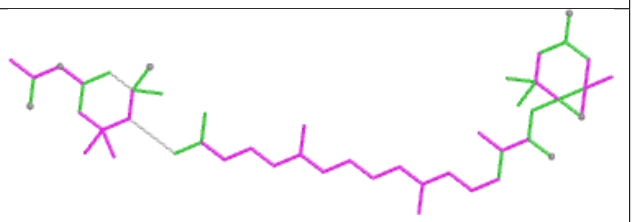
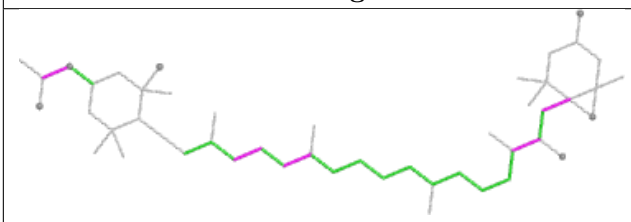
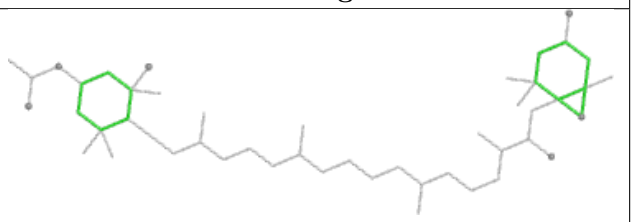
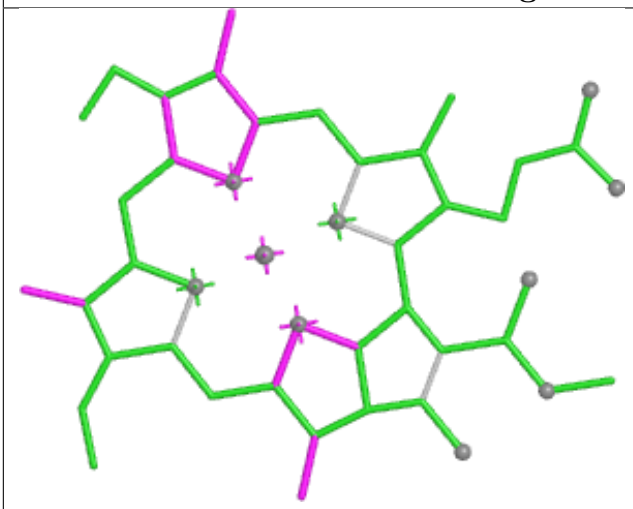


Rings

Ligand LMG m 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 18 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 19 306



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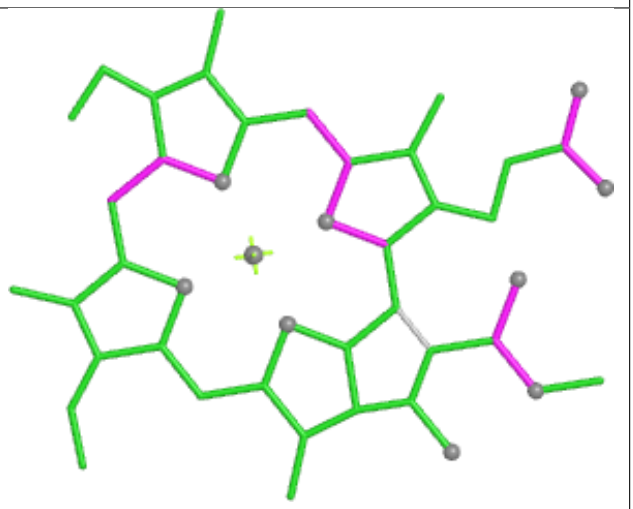
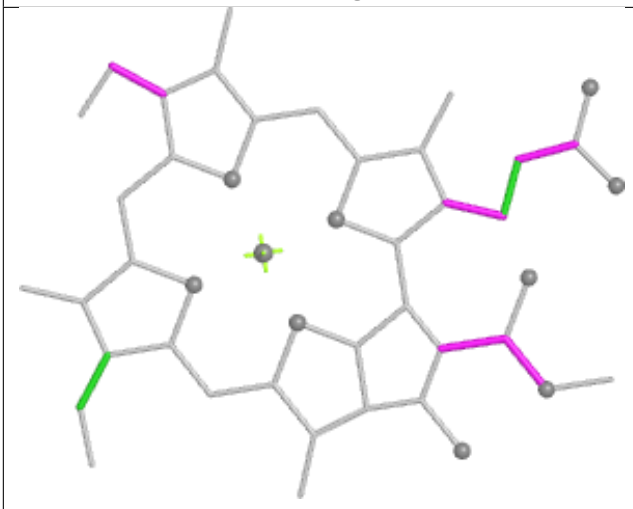


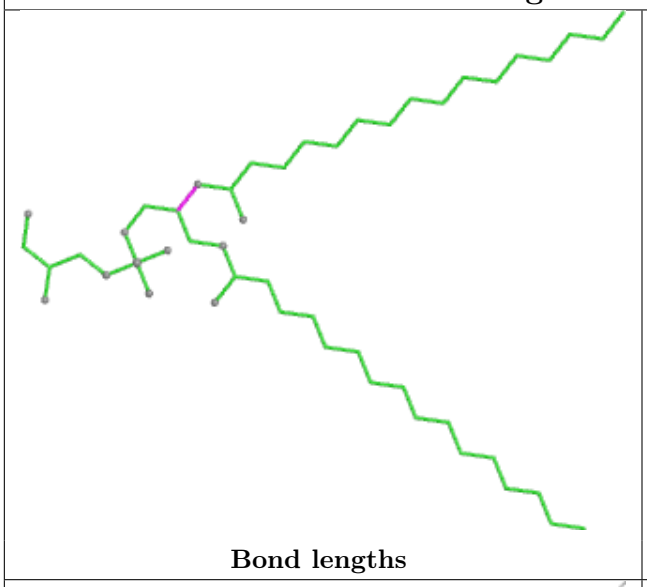
Bond angles



Torsions

Rings

Ligand LHG L 102



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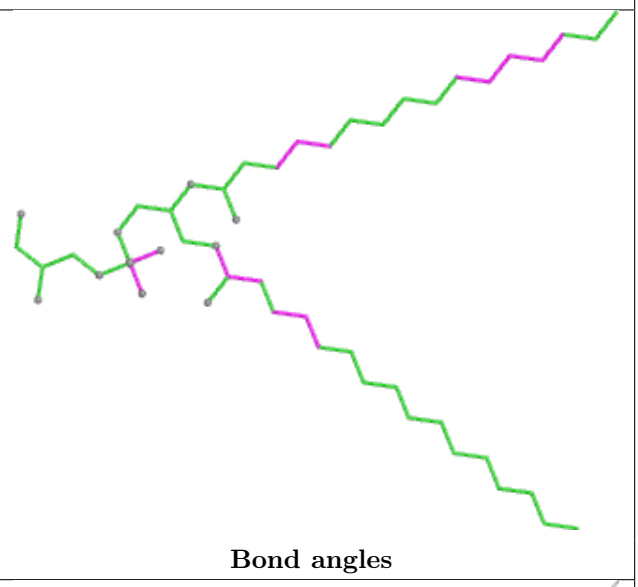

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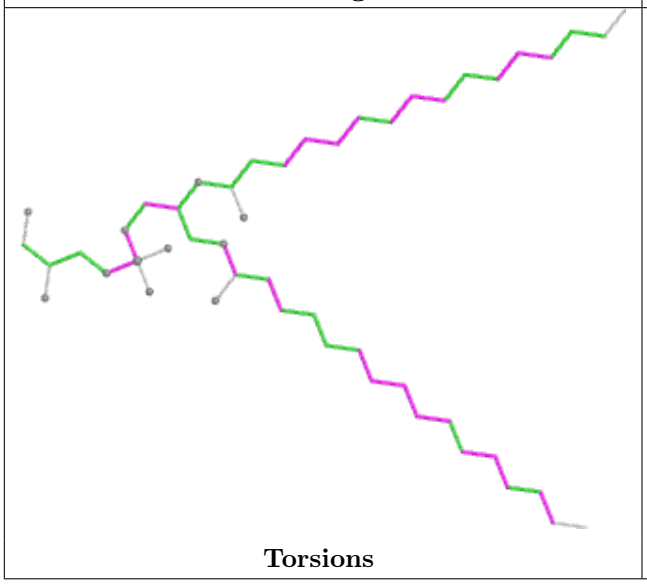

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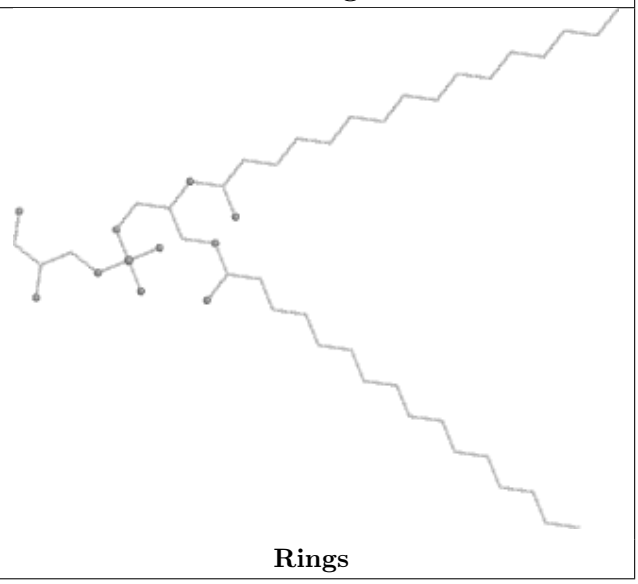
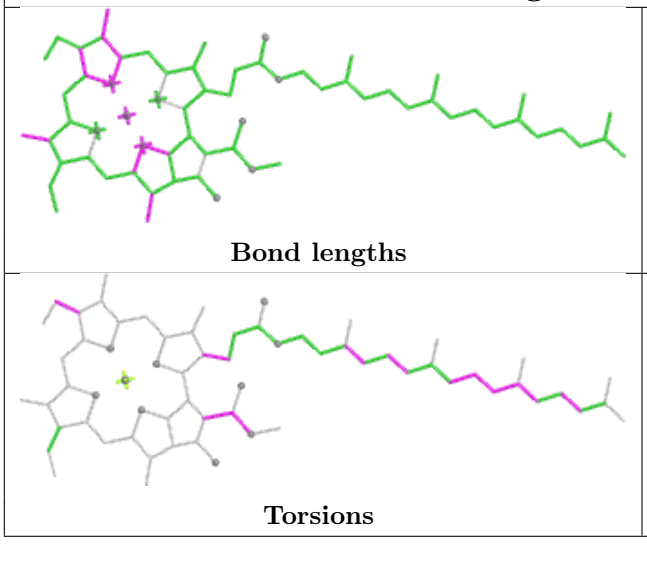


Rings

Ligand CLA w 102



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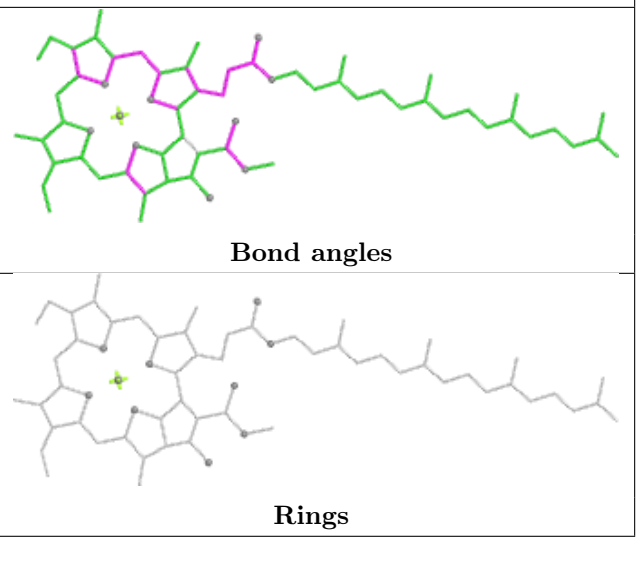
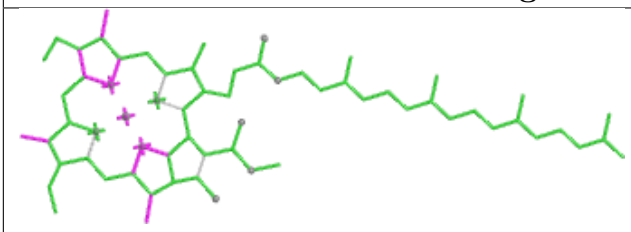


Bond angles

Torsions

Rings

Ligand CLA 11 307



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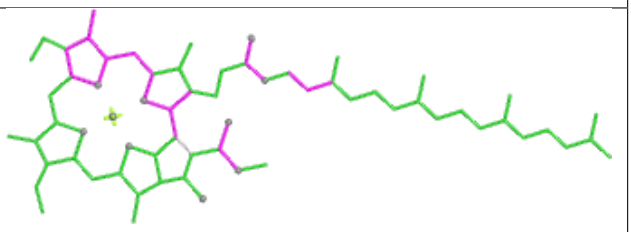
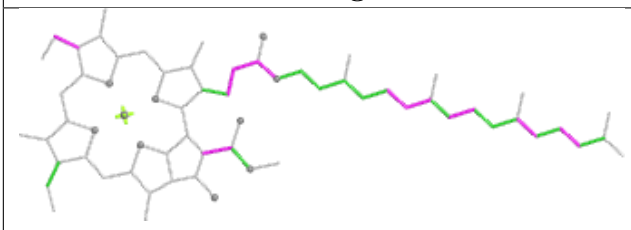


Bond angles



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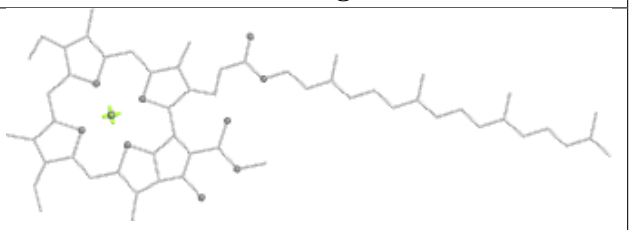
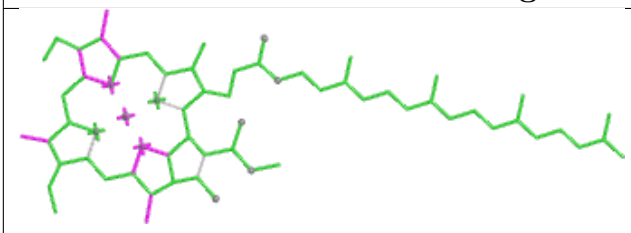


Rings

Ligand CLA 18 301



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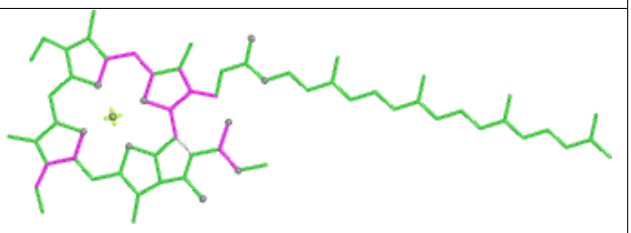
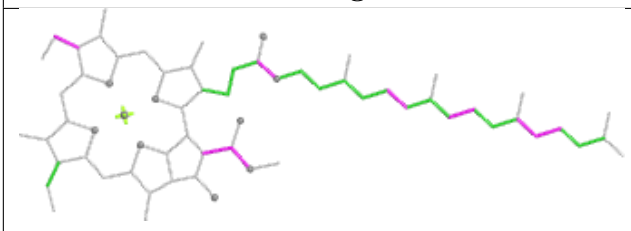


Bond angles



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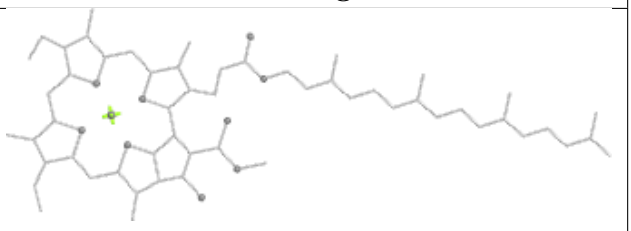
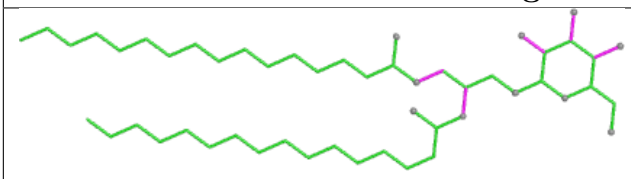


Rings

Ligand LMG b 619



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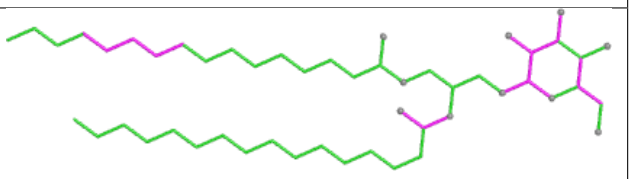
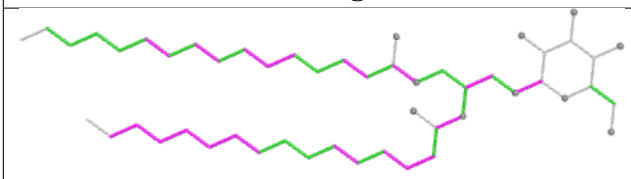


Bond angles



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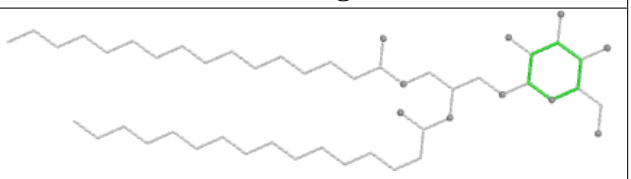
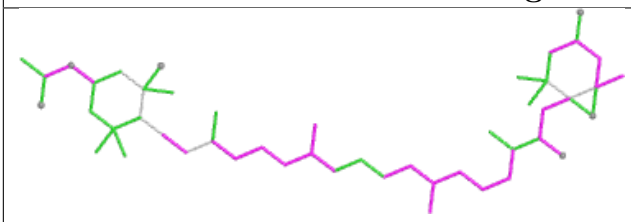


Rings

Ligand A86 11 310



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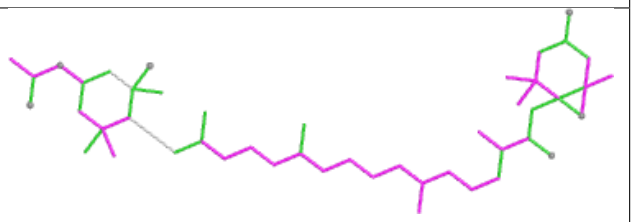

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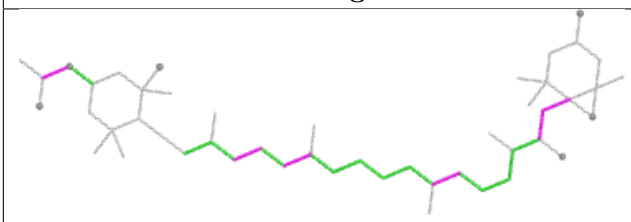

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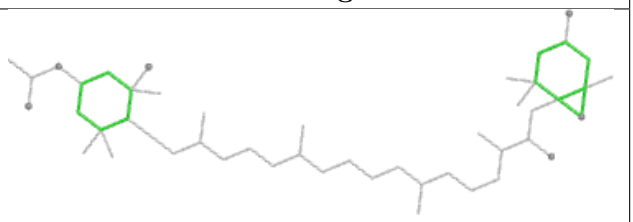
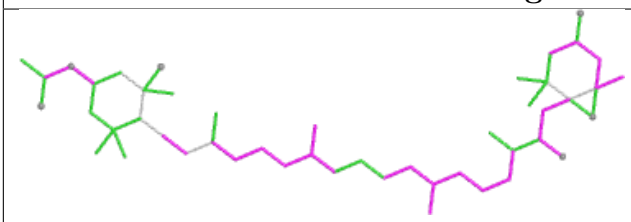


Rings

Ligand A86 12 304



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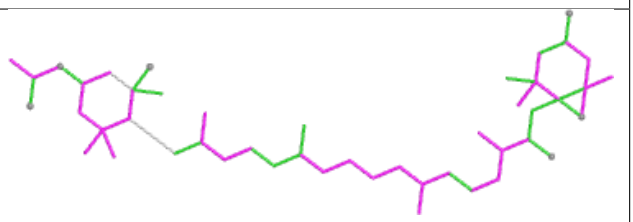

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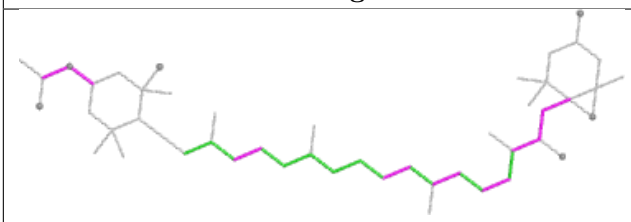

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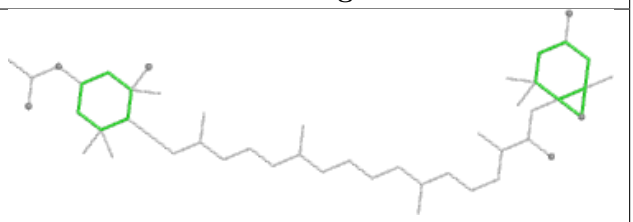
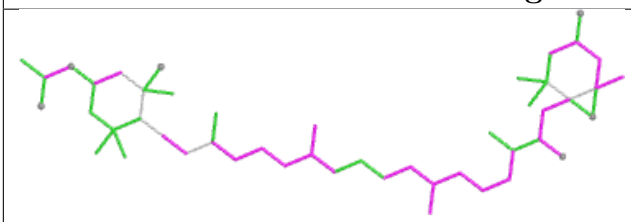


Rings

Ligand A86 20 212



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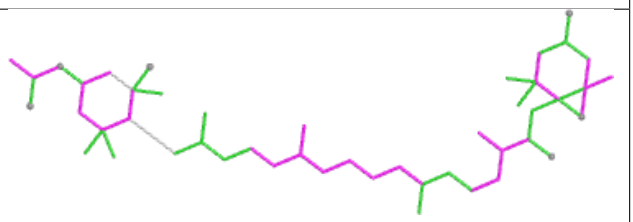

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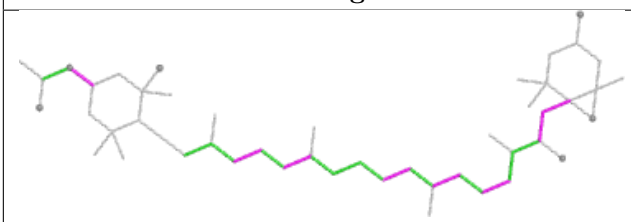

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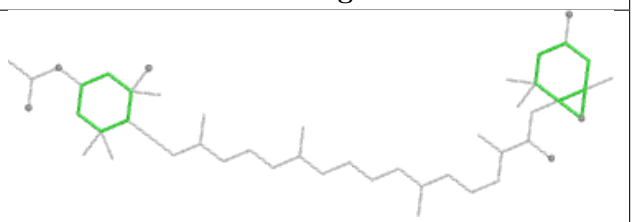
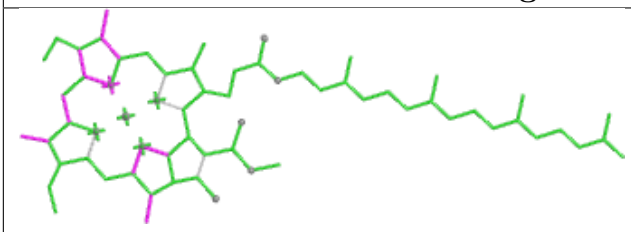


Rings

Ligand CLA 18 305



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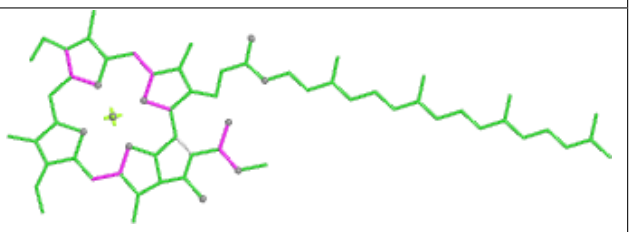

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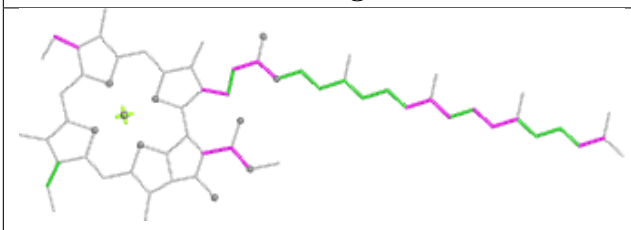

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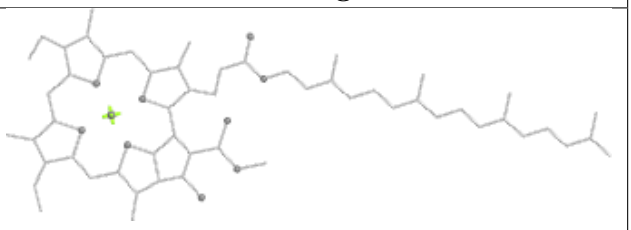

Rings

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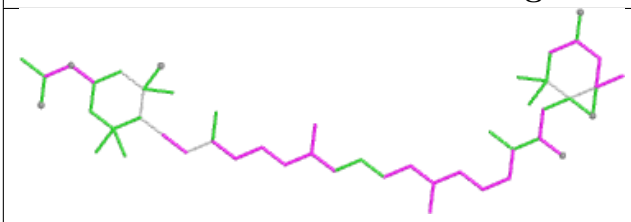

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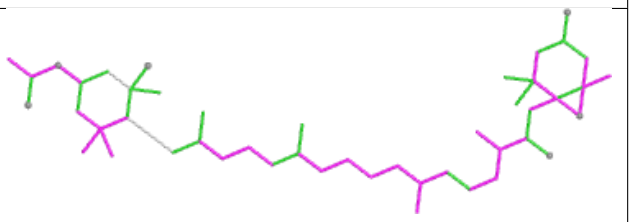

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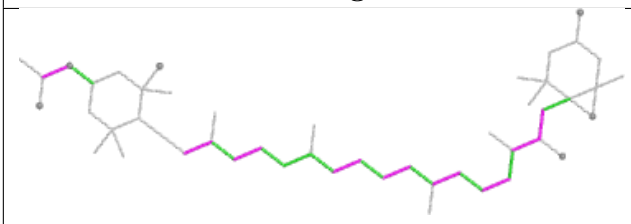

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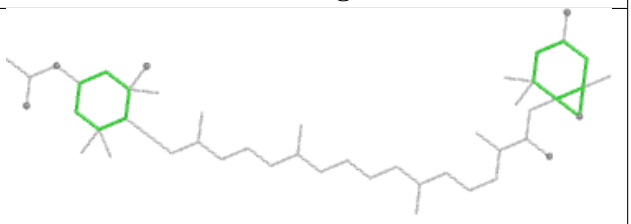
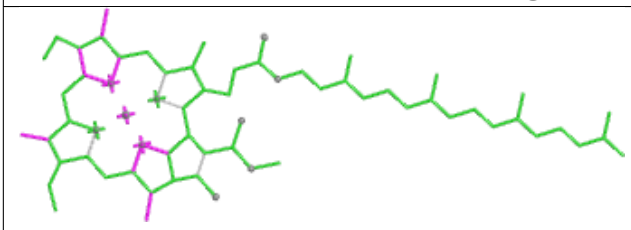


Rings

Ligand CLA C 513



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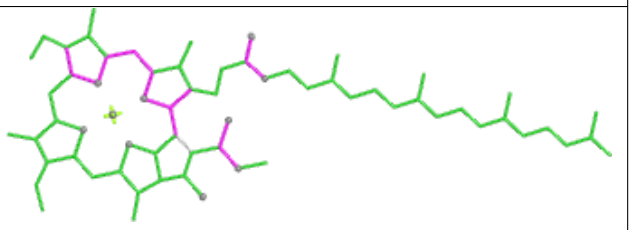

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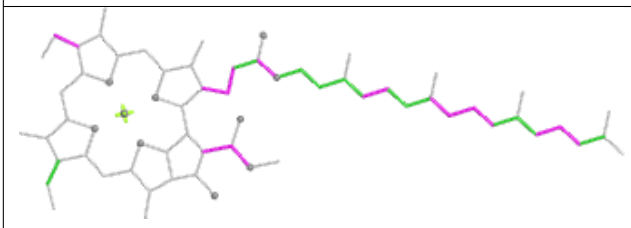

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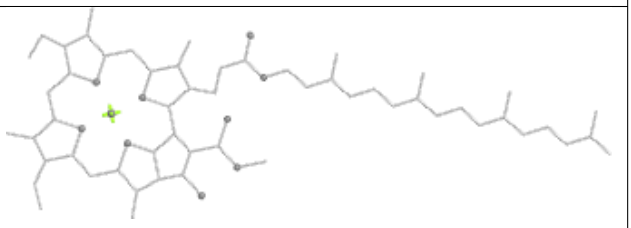
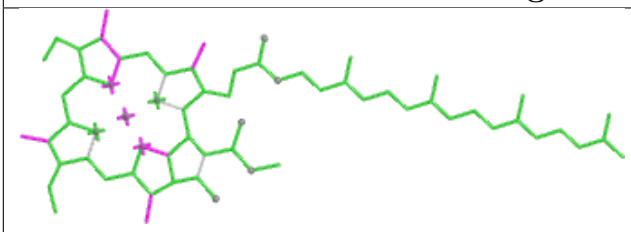


Rings

Ligand CLA b 612



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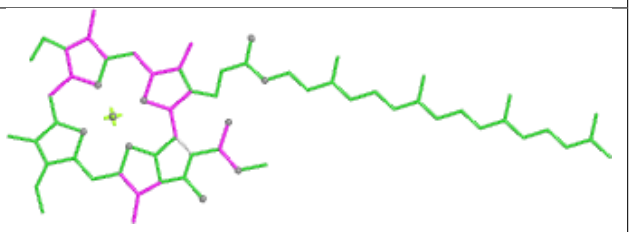

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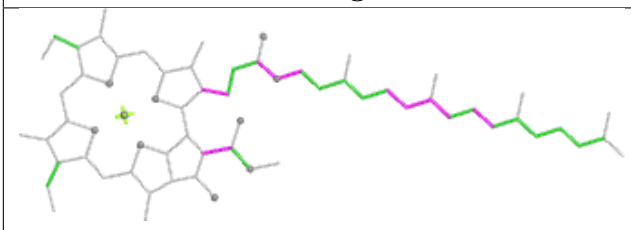

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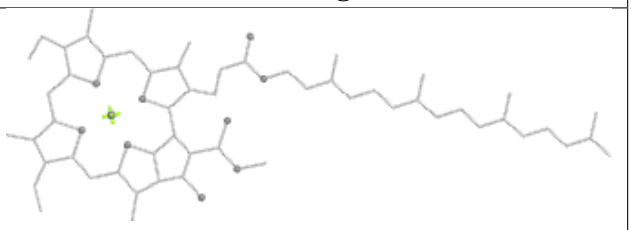
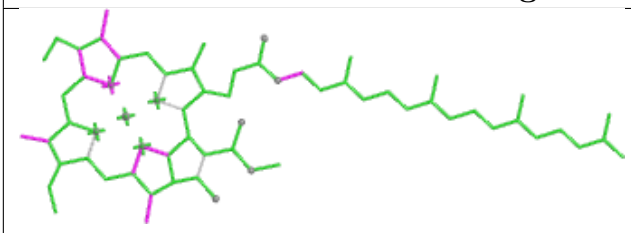


Rings

Ligand CLA 21 306



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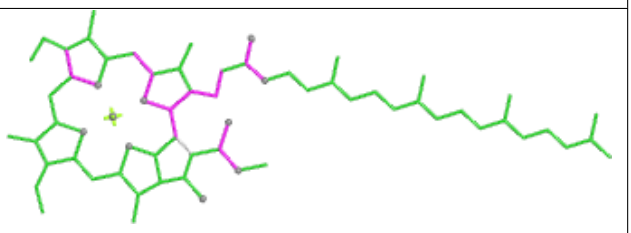

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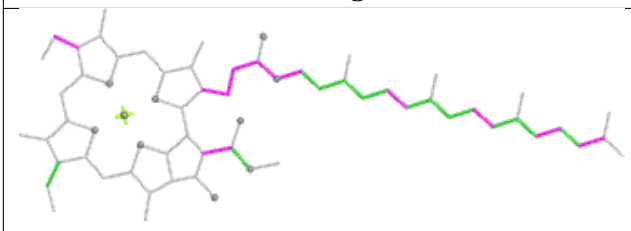

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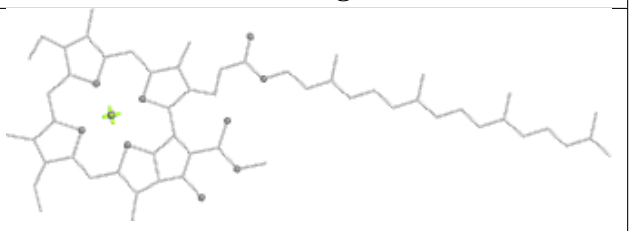
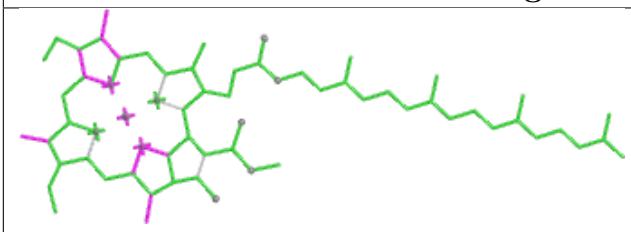


Rings

Ligand CLA B 609



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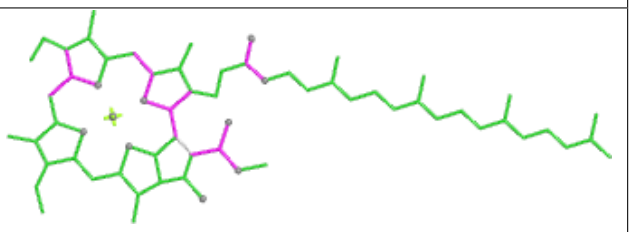
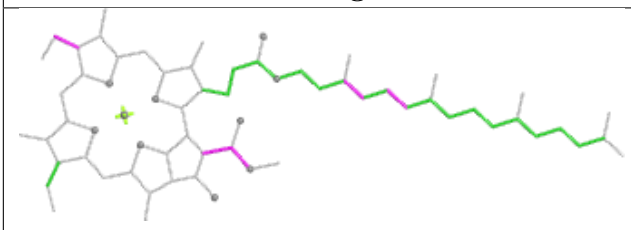


Bond angles



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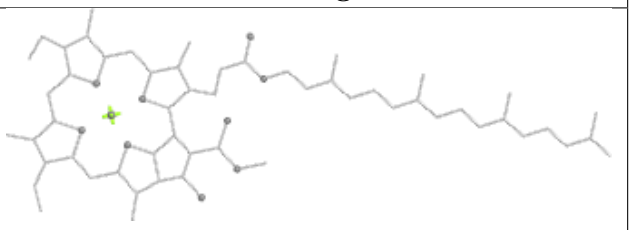
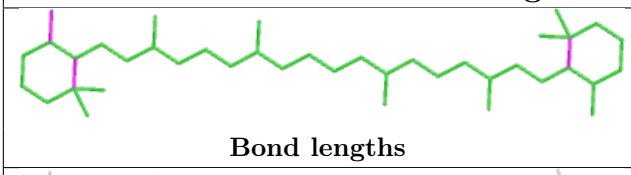


Rings

Ligand BCR F 101



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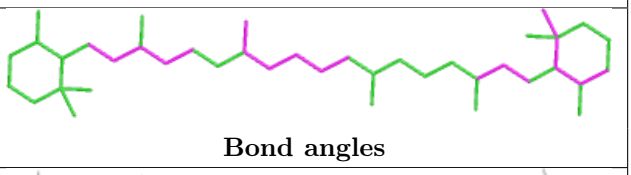
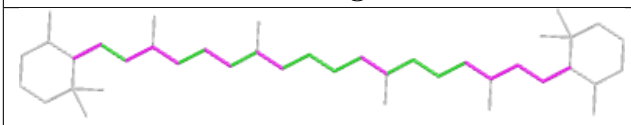


Bond angles



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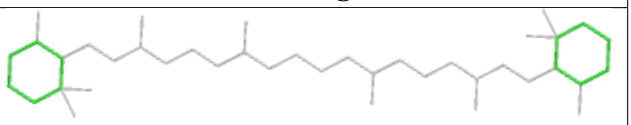
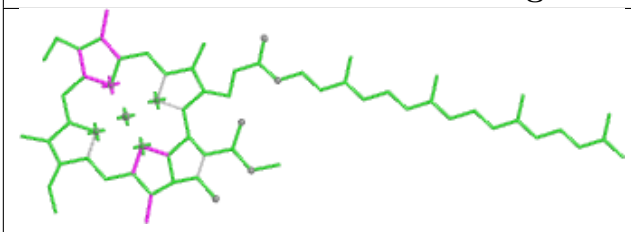


Rings

Ligand CLA Z 102



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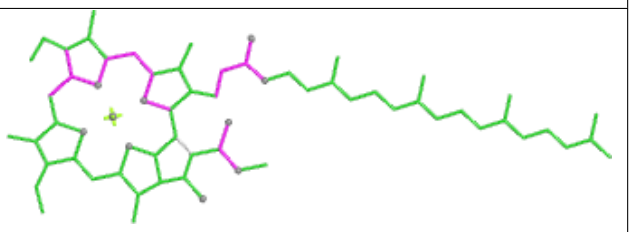
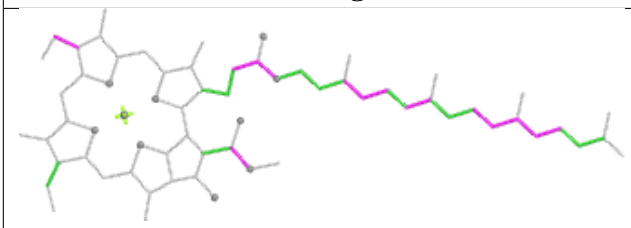


Bond angles



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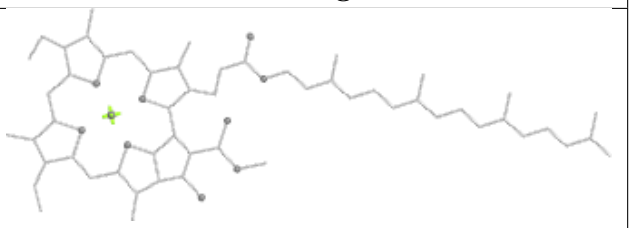
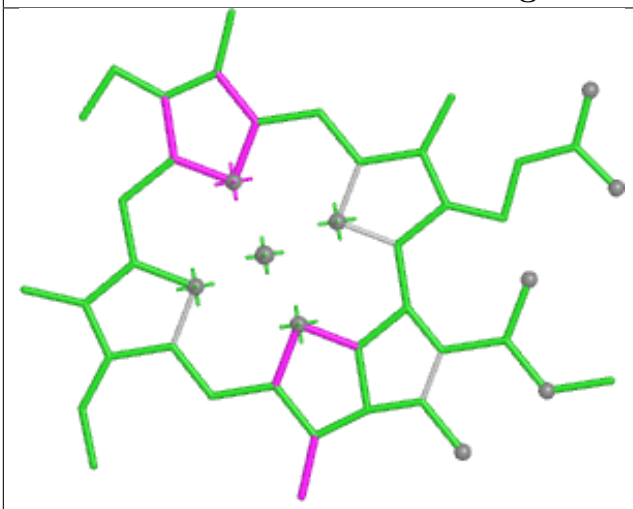


Rings

Ligand CLA 21 305



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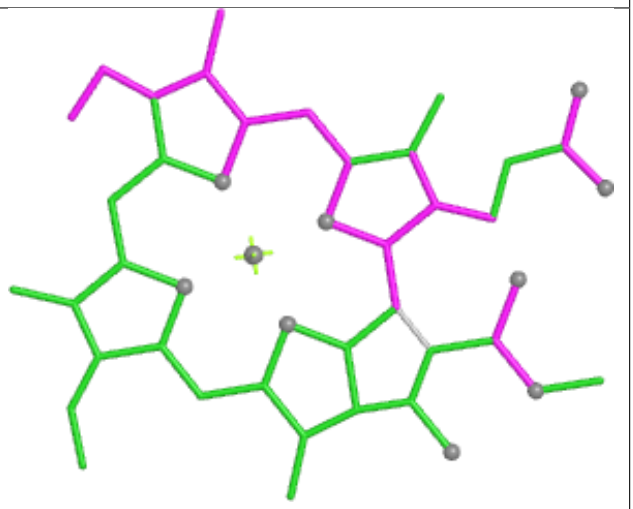

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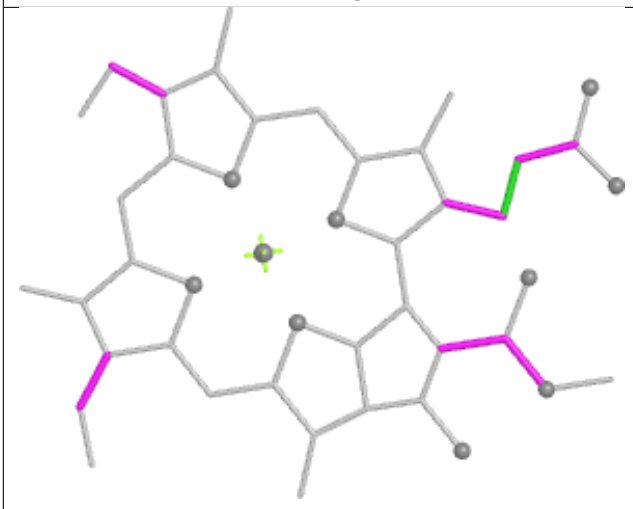
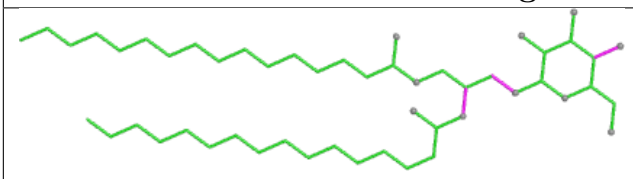


Torsions

Rings

Ligand LMG D 408



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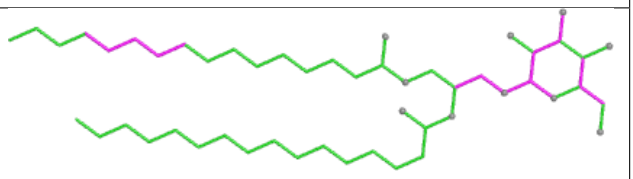
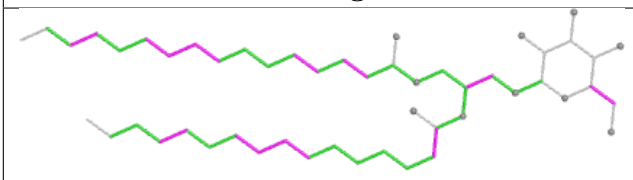
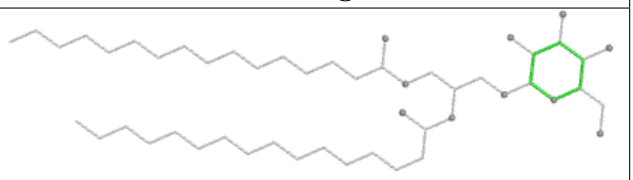


Bond angles

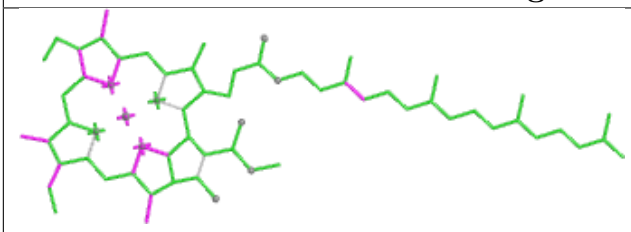


Torsions



Rings

Ligand CLA b 606



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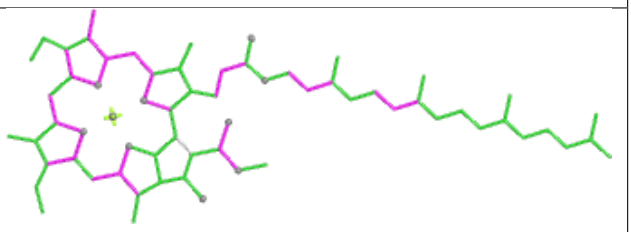
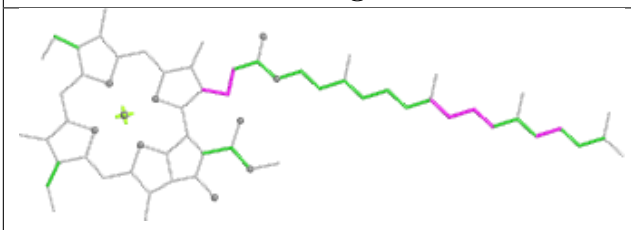
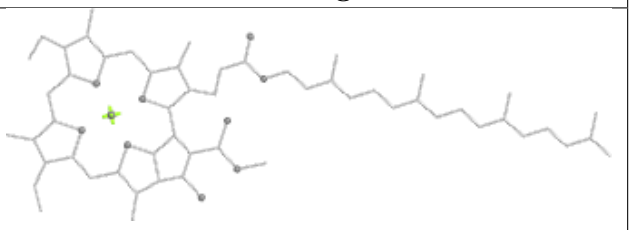


Bond angles

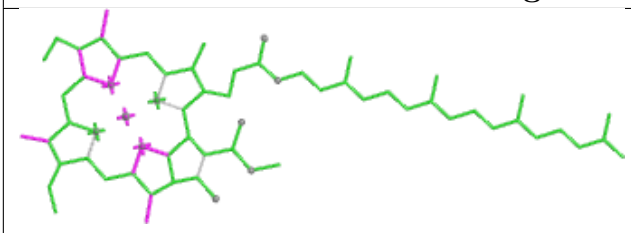


Torsions



Rings

Ligand CLA D 402



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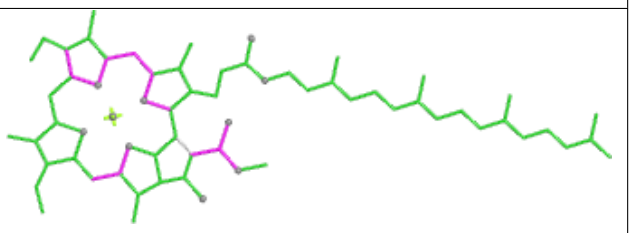
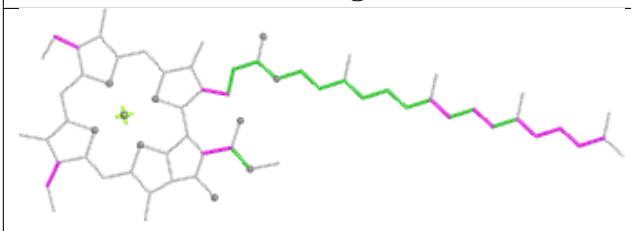


Bond angles



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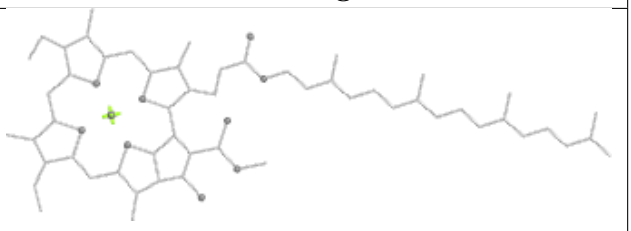
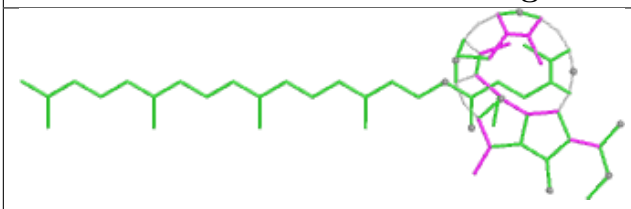


Rings

Ligand PHO D 403



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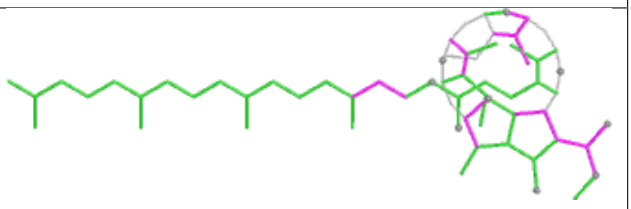

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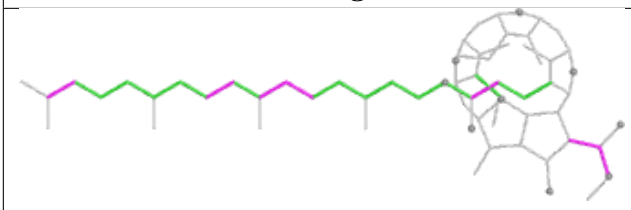

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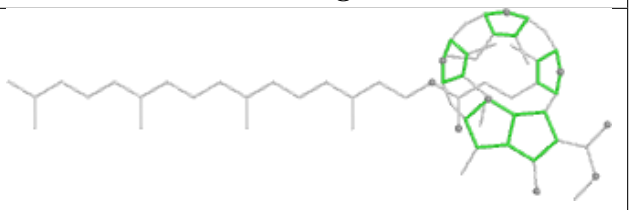
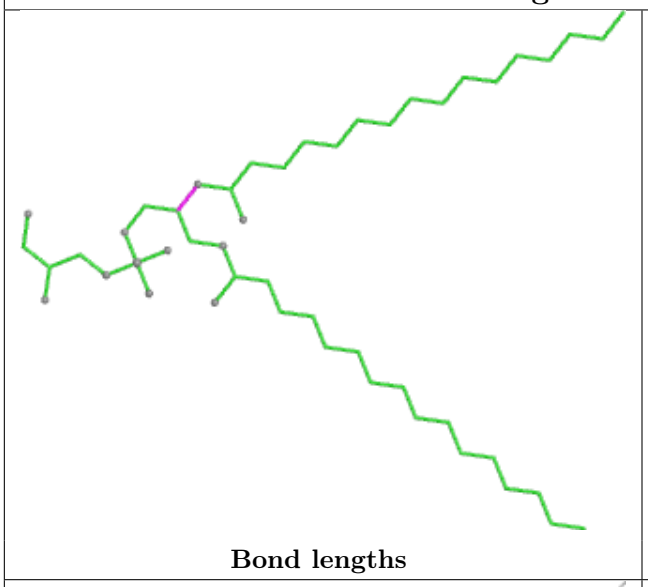


Rings

Ligand LHG l 102



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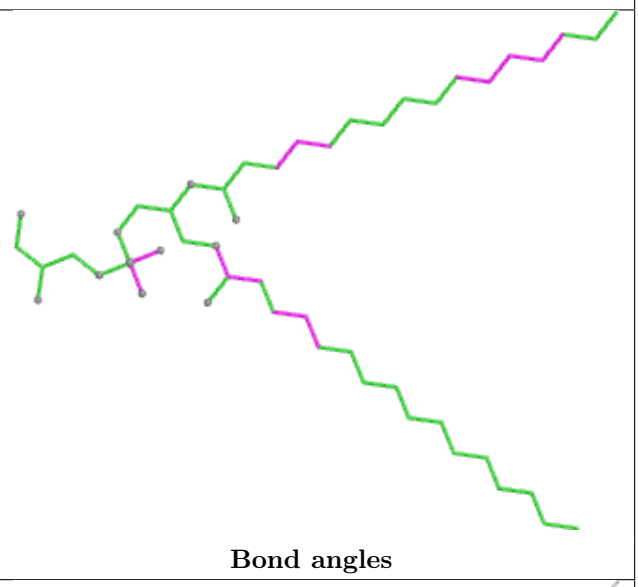

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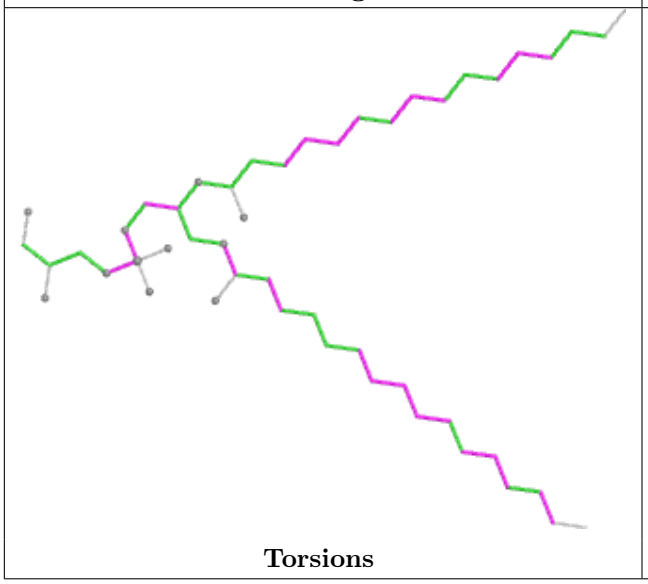

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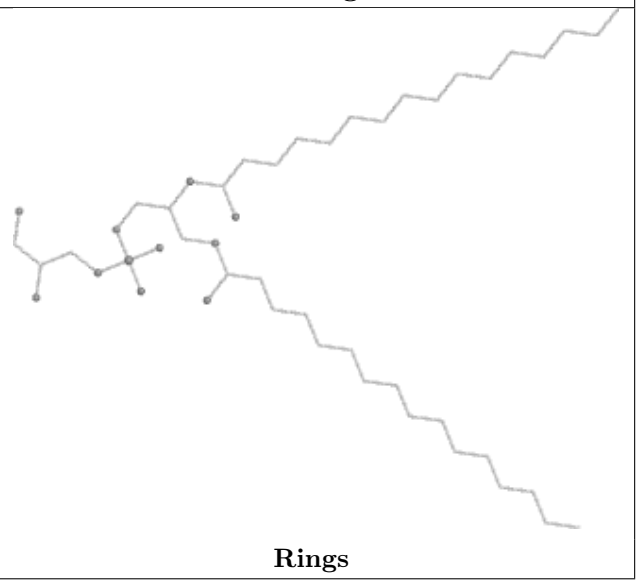
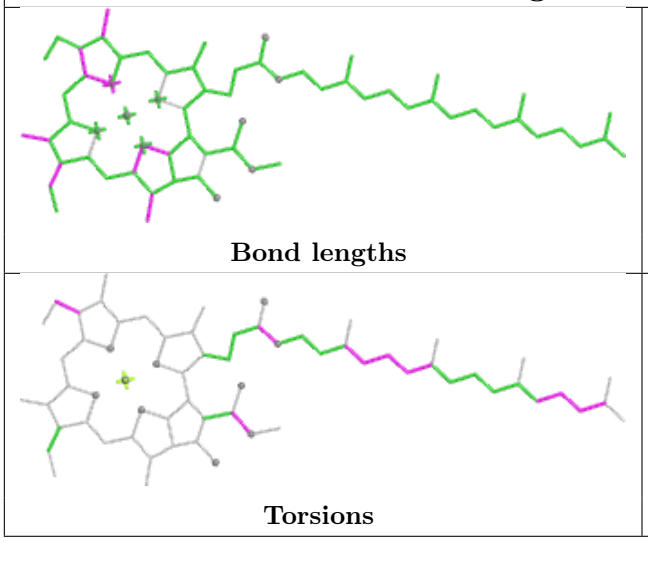


Rings

Ligand CLA b 602



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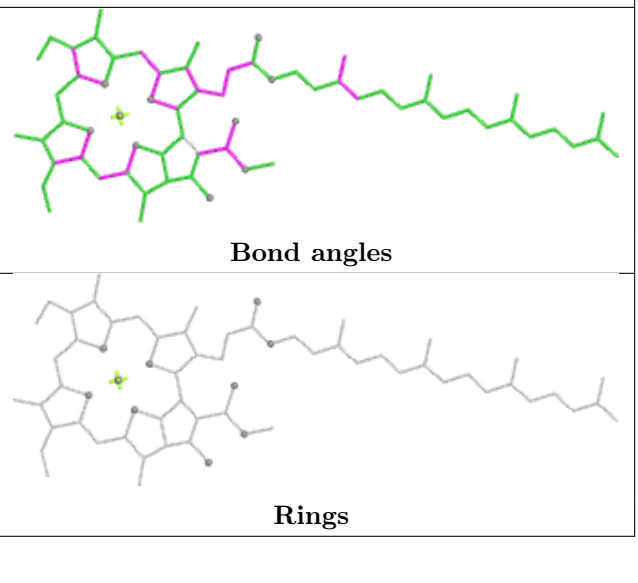
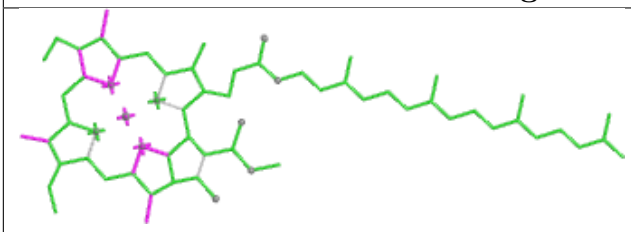


Bond angles

Torsions

Rings

Ligand CLA M 101



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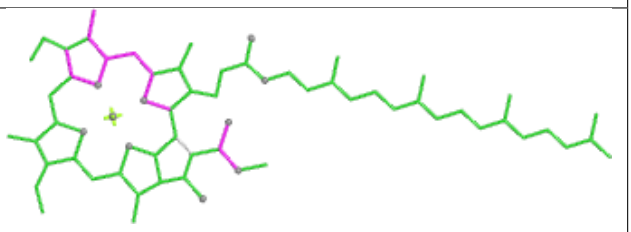
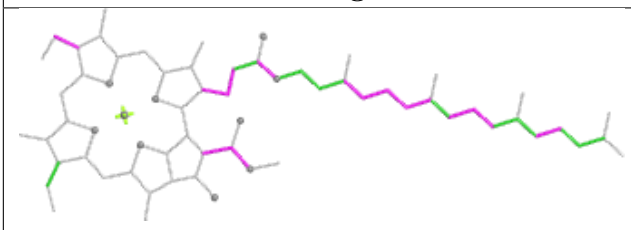


Bond angles



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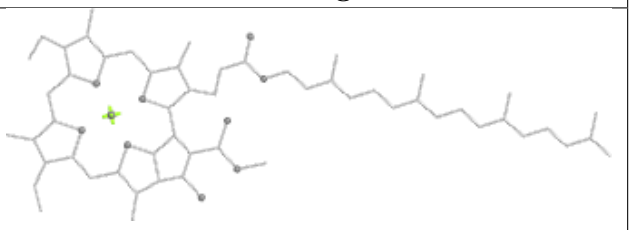
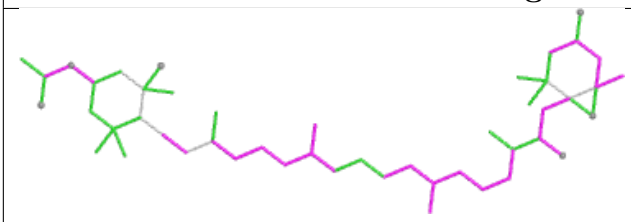


Rings

Ligand A86 18 313



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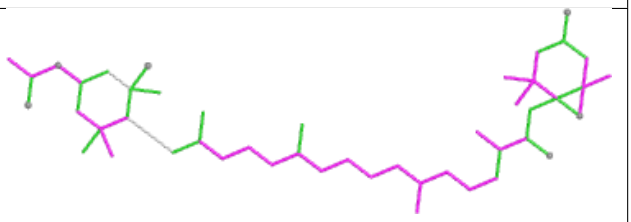

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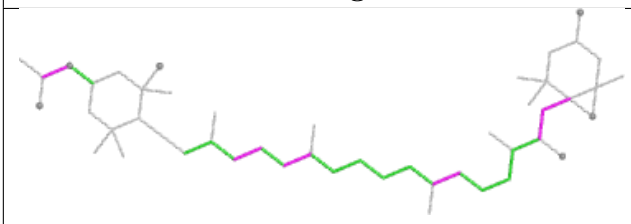

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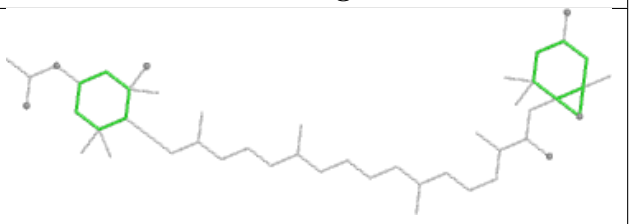
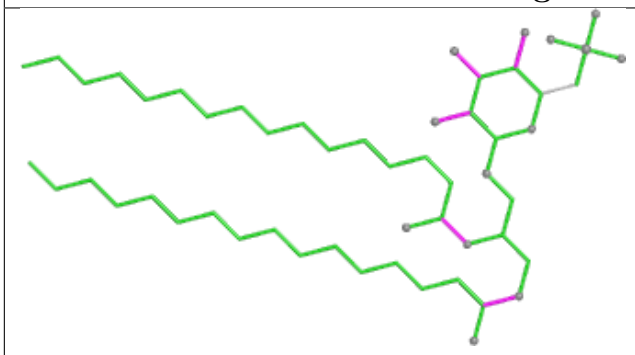


Rings

Ligand SQD l 101



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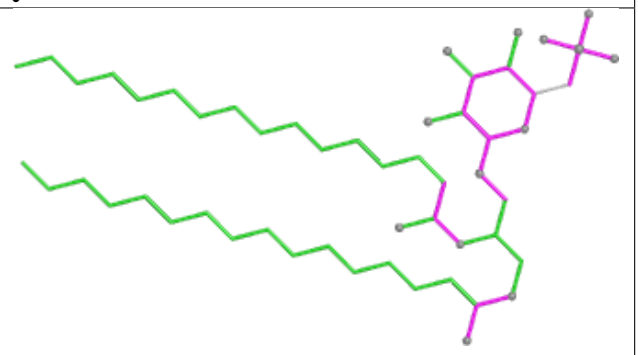

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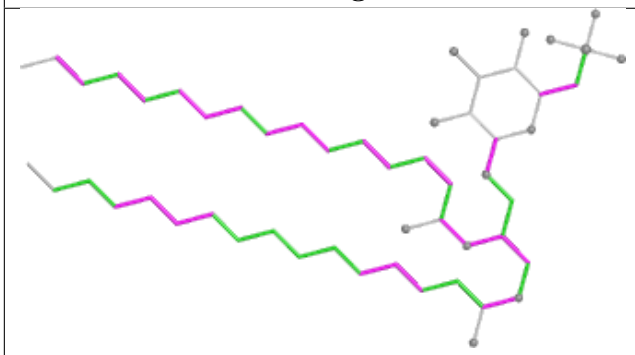

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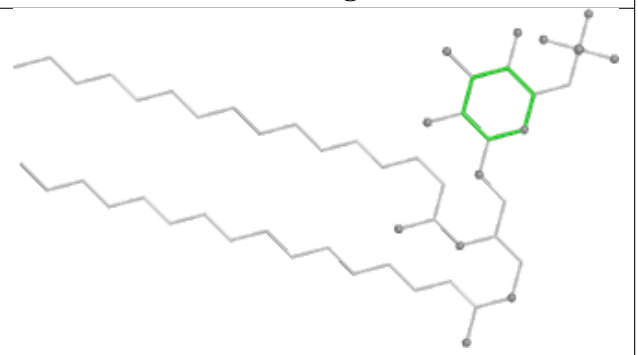
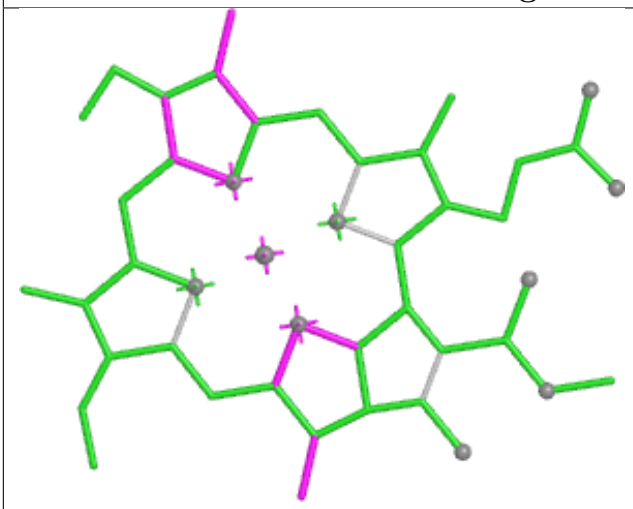


Rings

Ligand CLA 12 314



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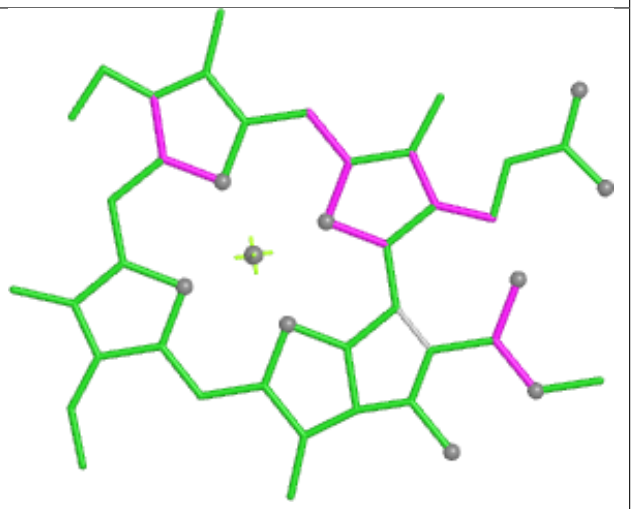

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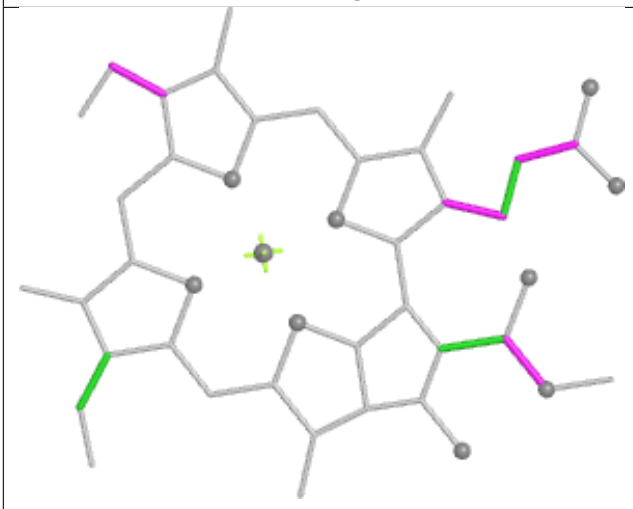
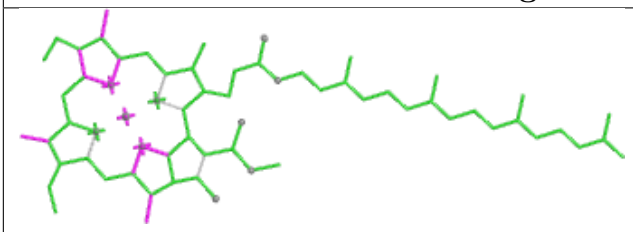


Torsions

Rings

Ligand CLA 18 309



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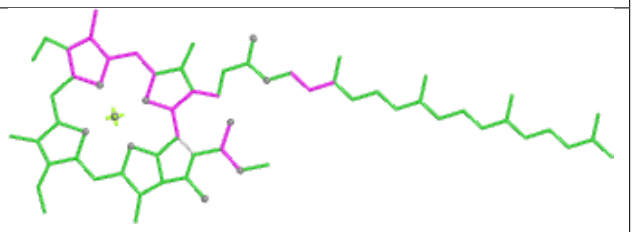

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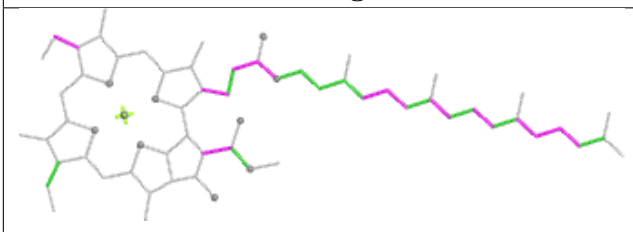

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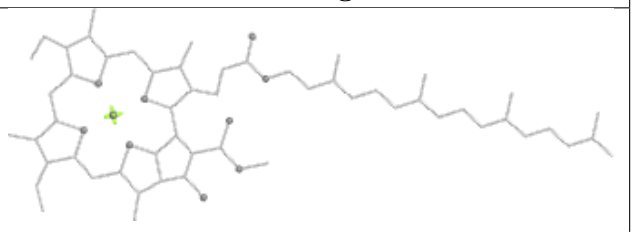
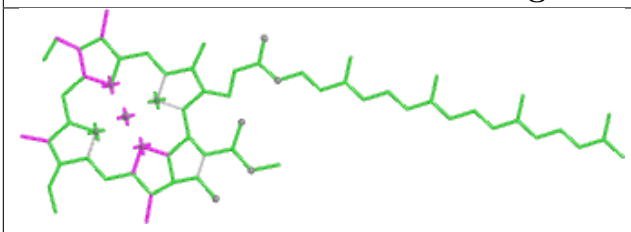


Rings

Ligand CLA a 403



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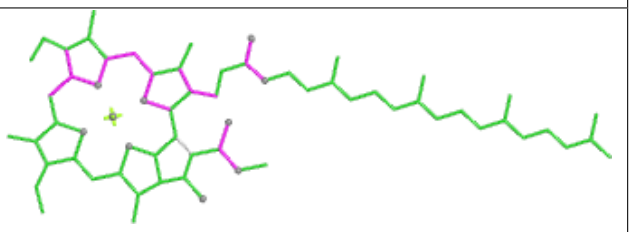

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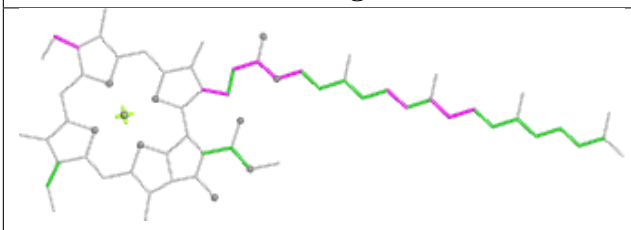

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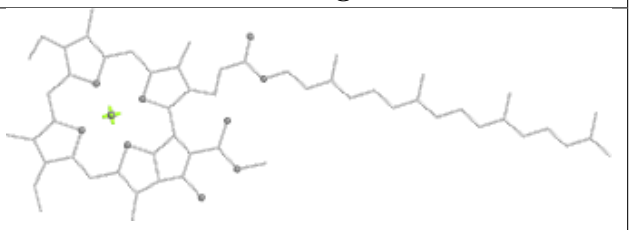
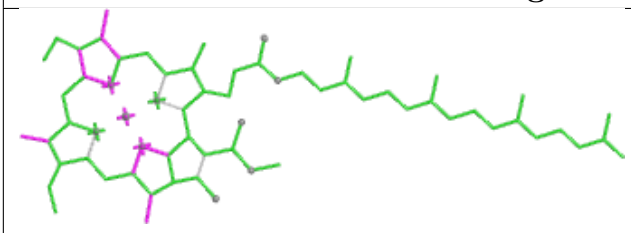


Rings

Ligand CLA b 609



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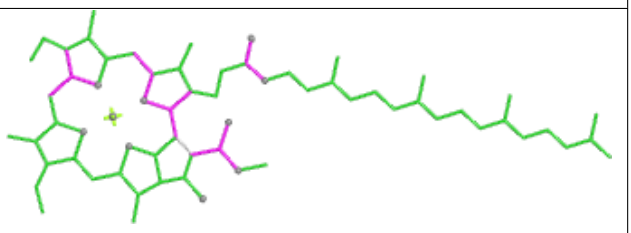
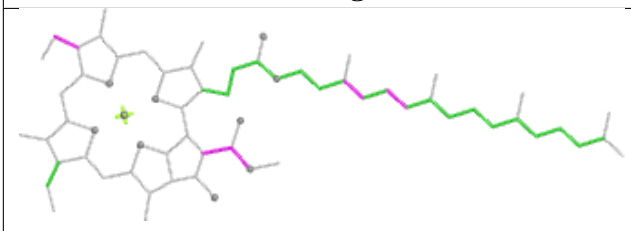


Bond angles



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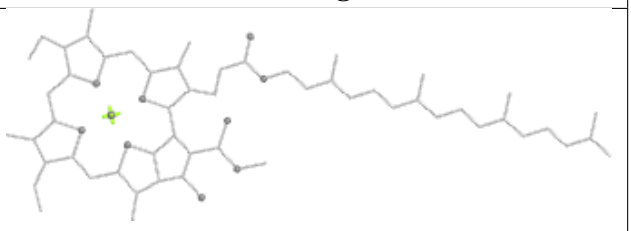
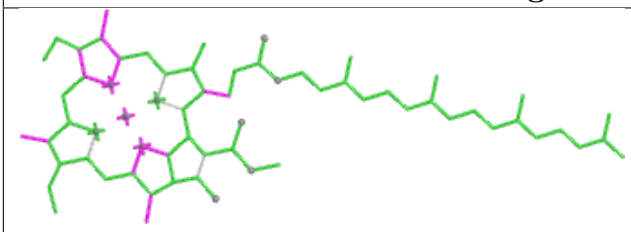


Rings

Ligand CLA d 406



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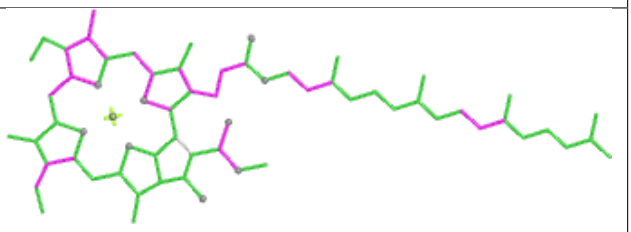
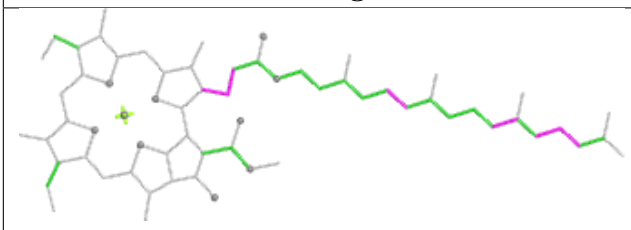


Bond angles



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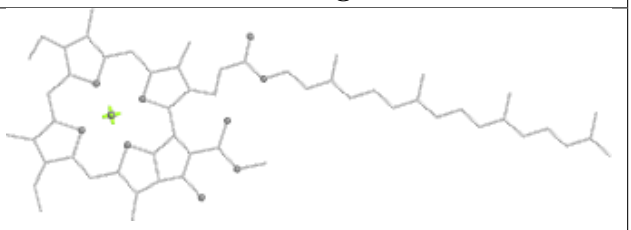
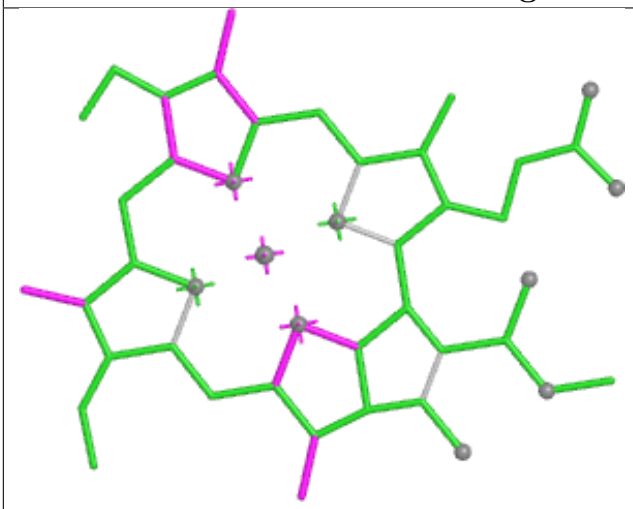


Rings

Ligand CLA 11 309



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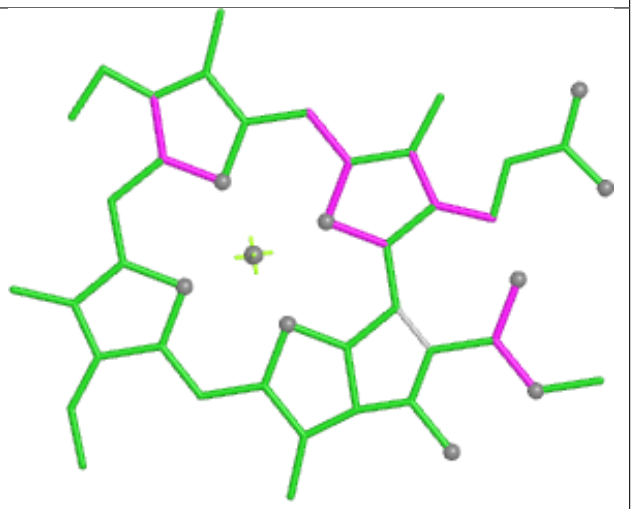
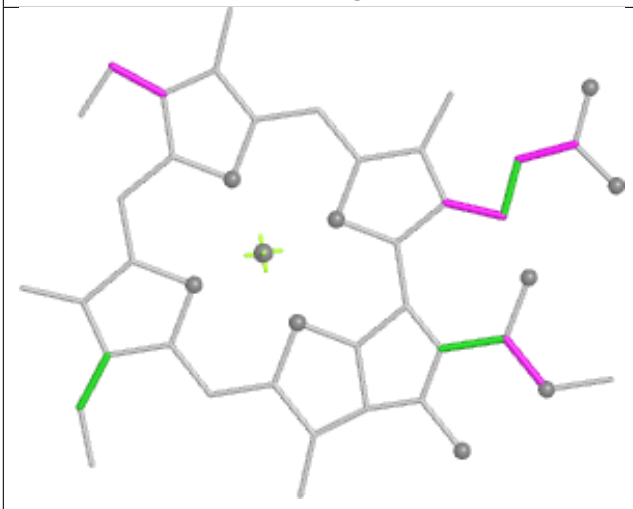


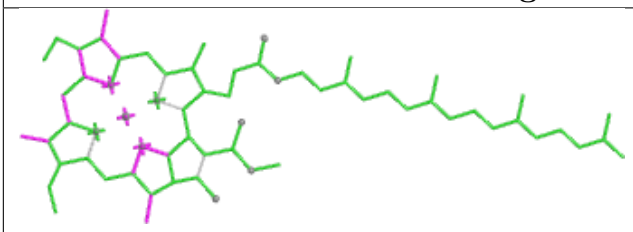
Bond angles



Torsions

Rings

Ligand CLA 11 301



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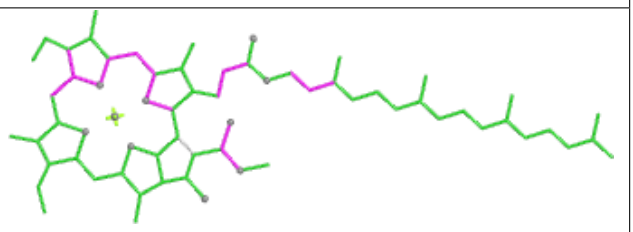
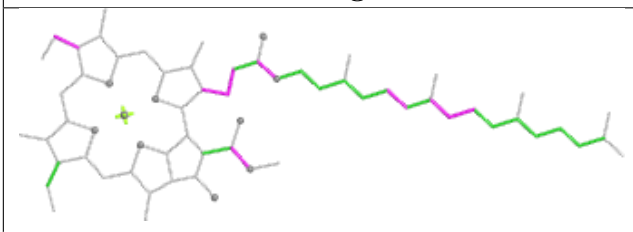


Bond angles



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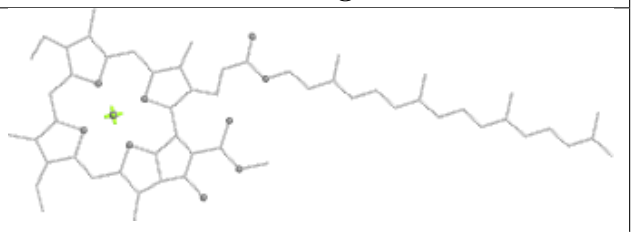

Rings

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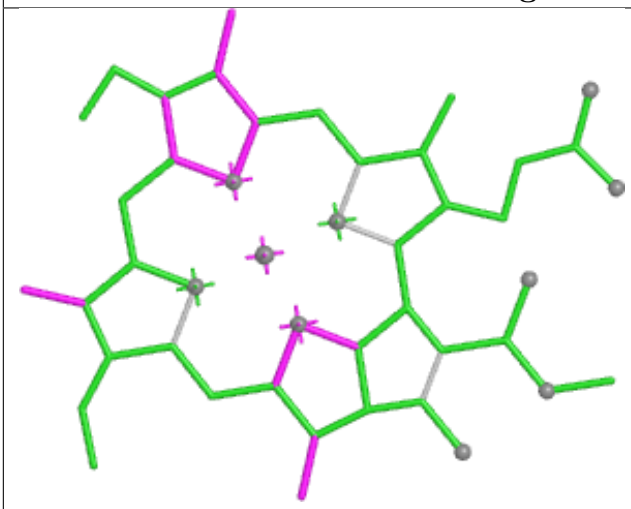
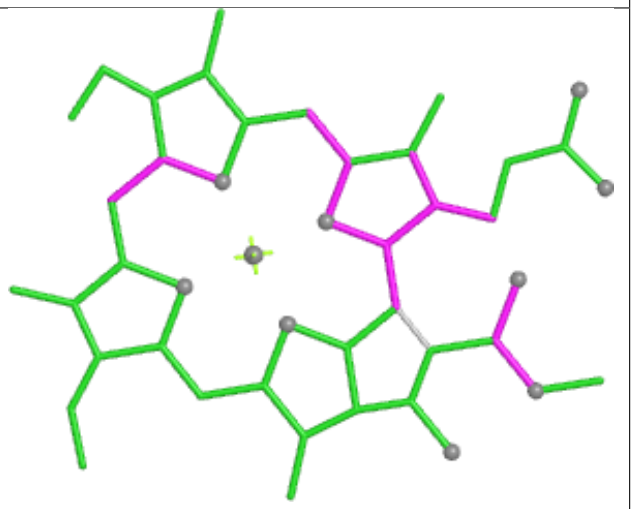


Bond lengths



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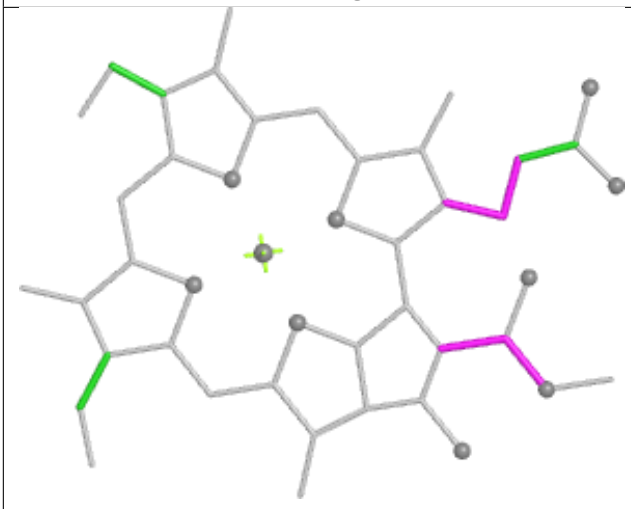

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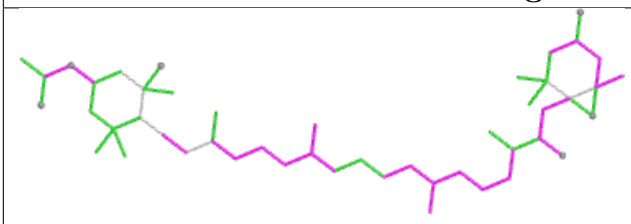

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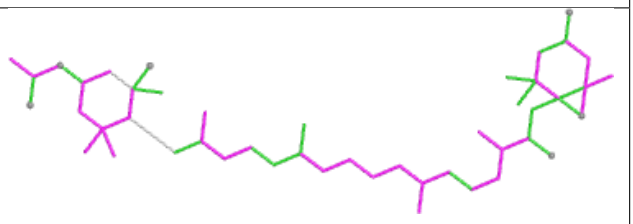

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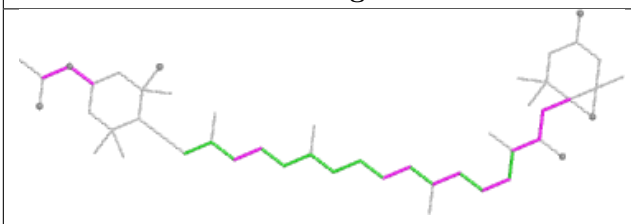

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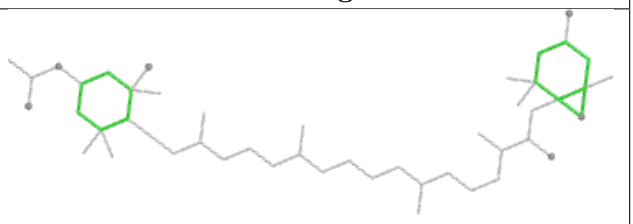

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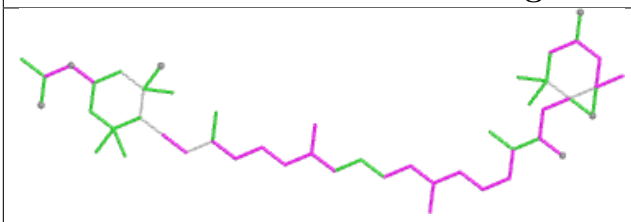

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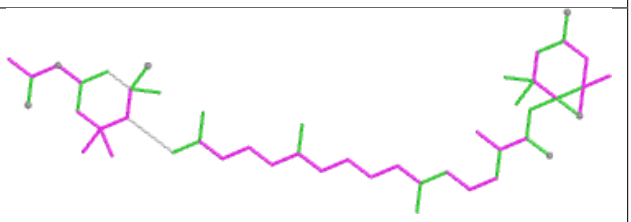

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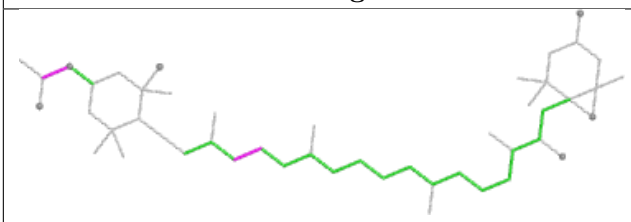

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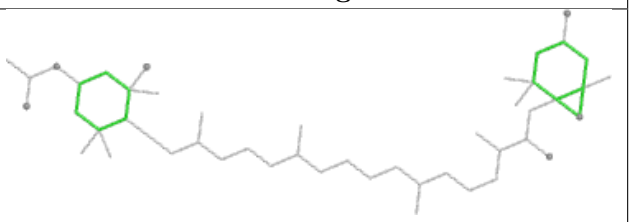

Rings

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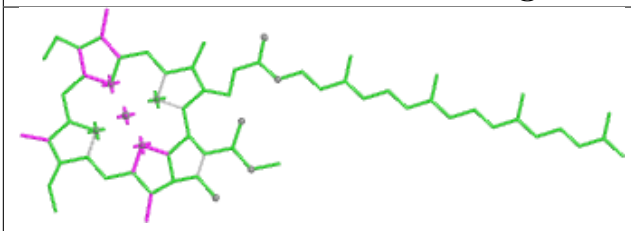

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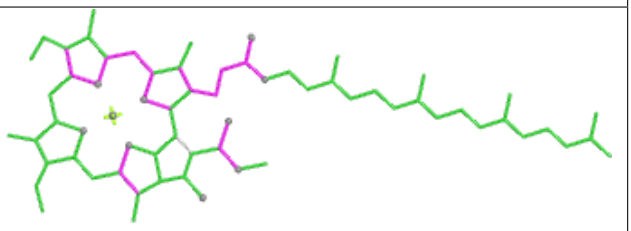

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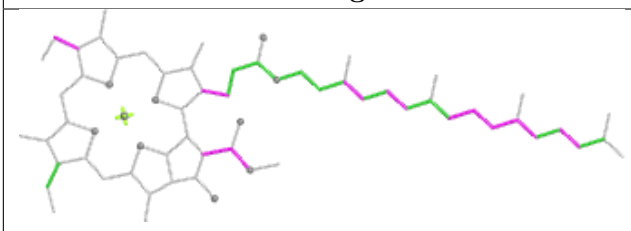

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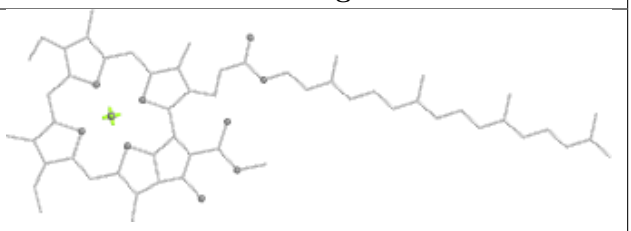

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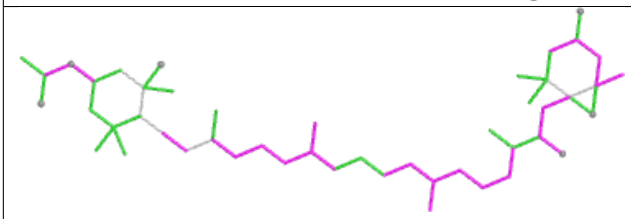

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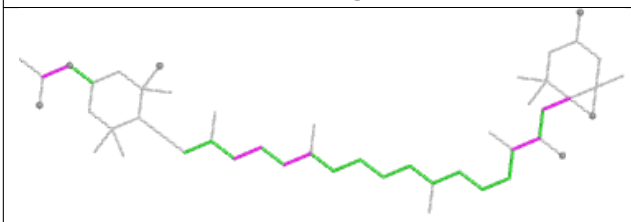

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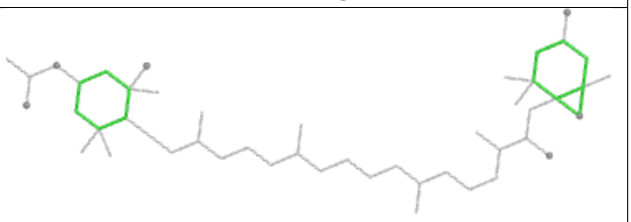

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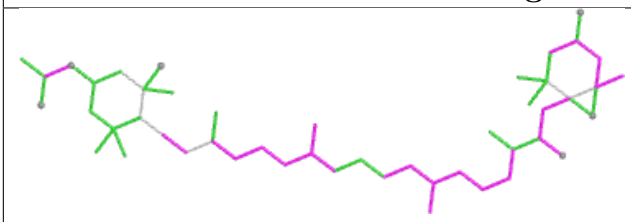

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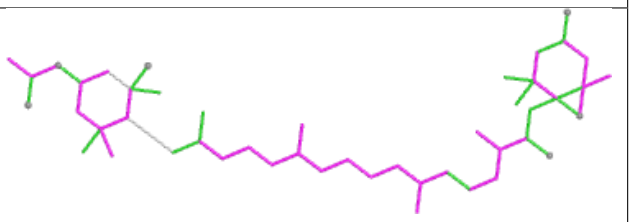

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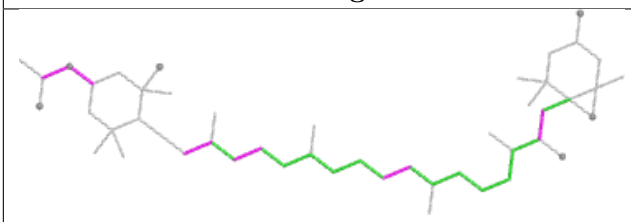

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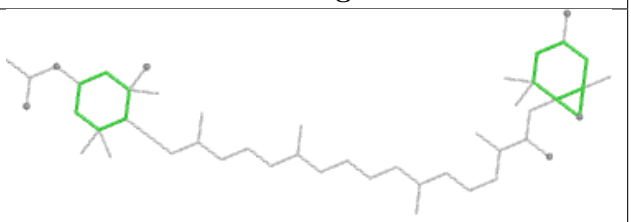

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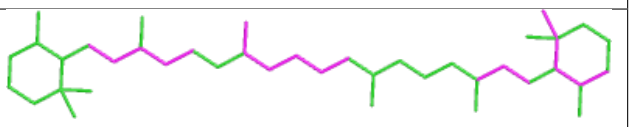

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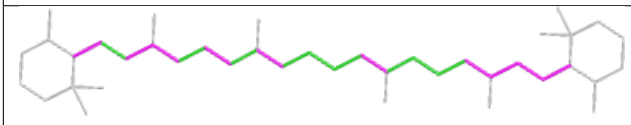

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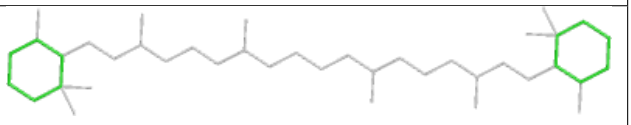

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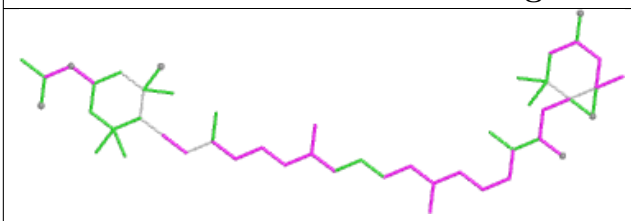

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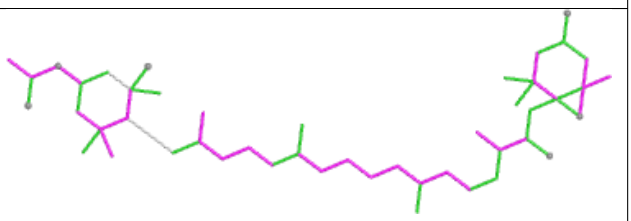

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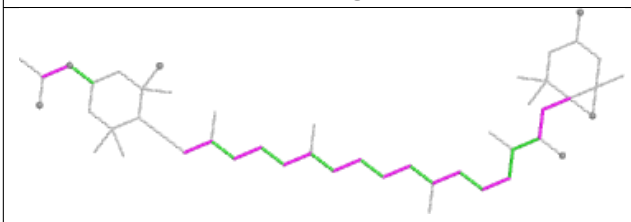

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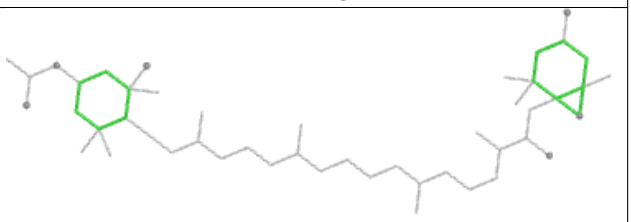

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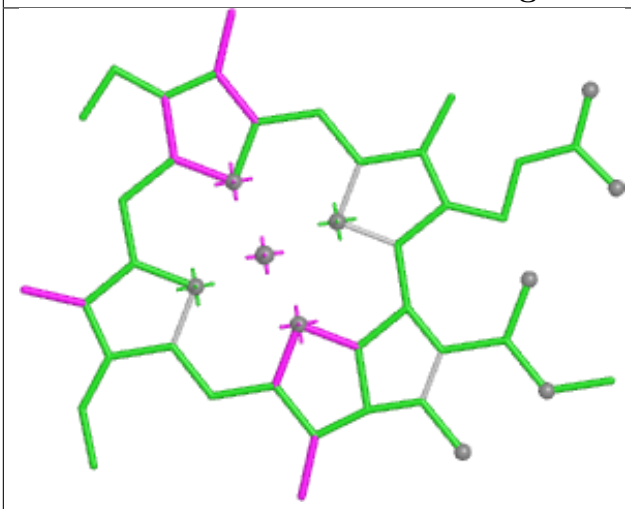

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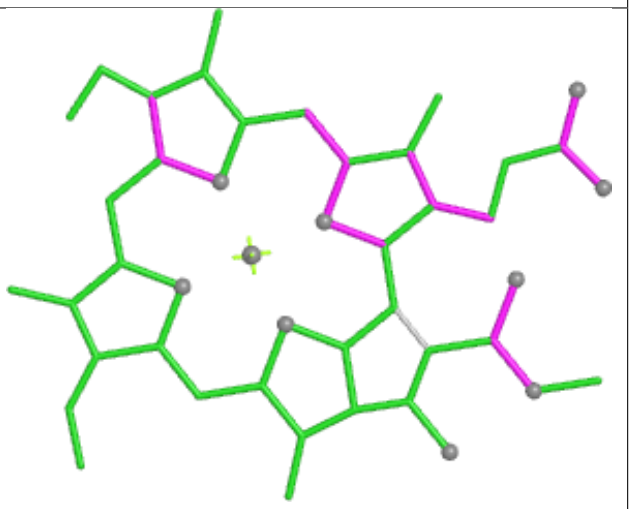

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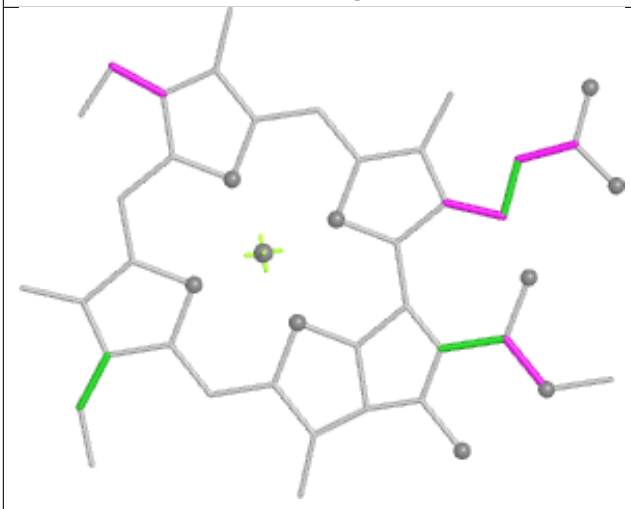

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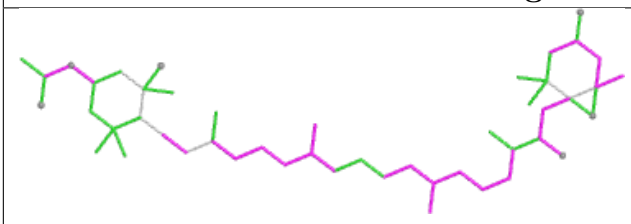

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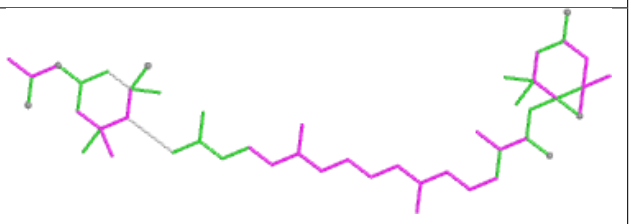

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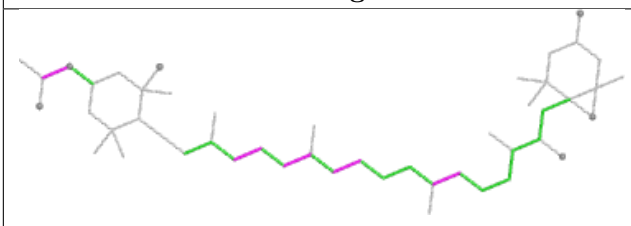

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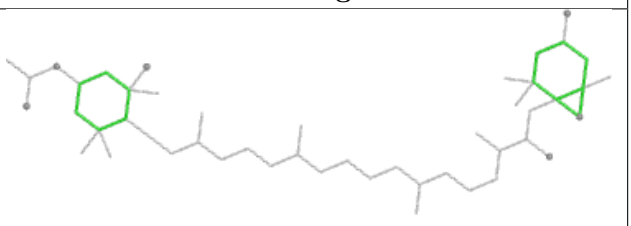

Rings

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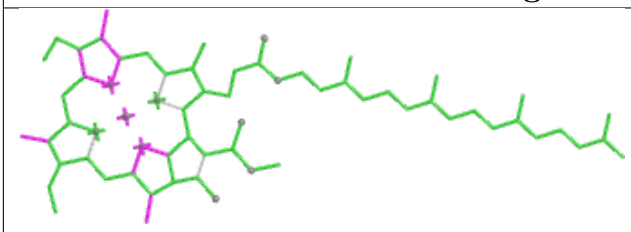

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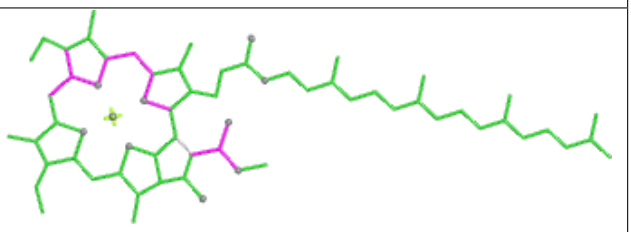

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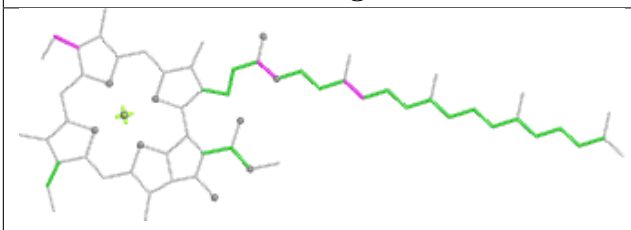

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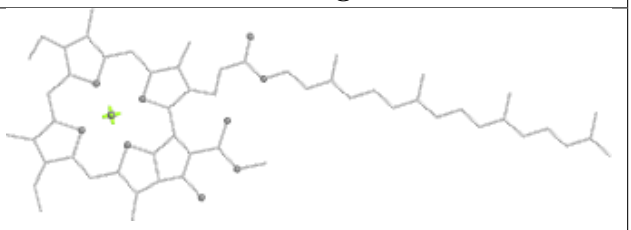

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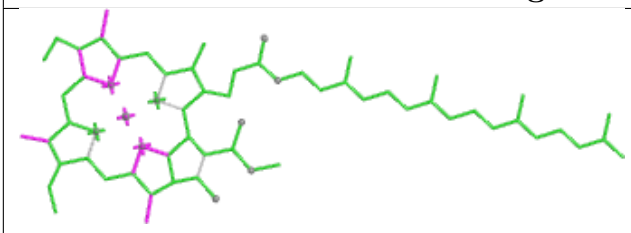

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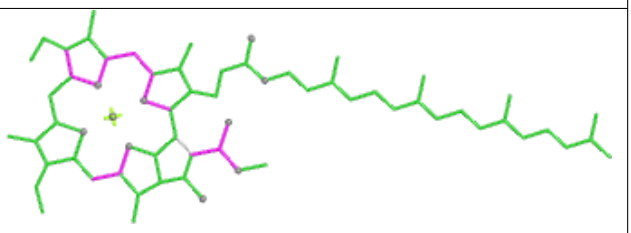

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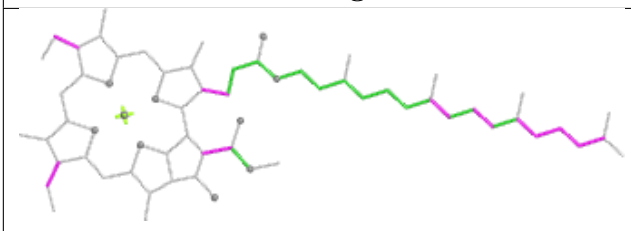

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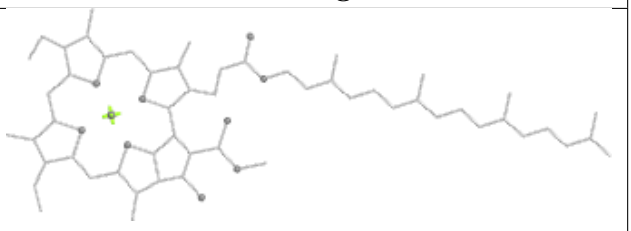

Rings

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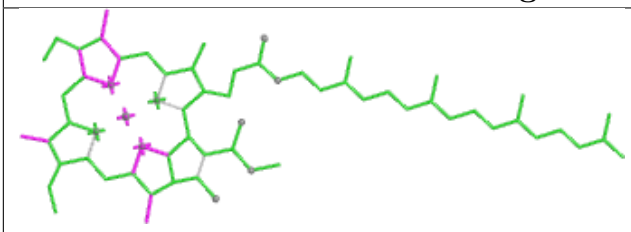

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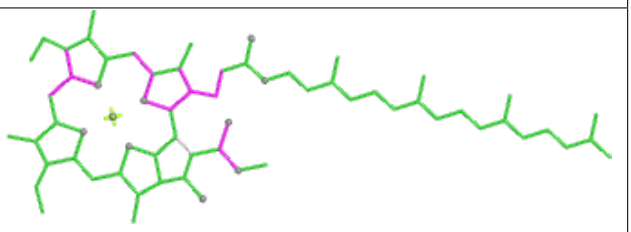

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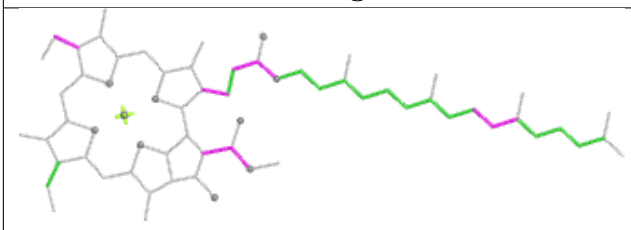

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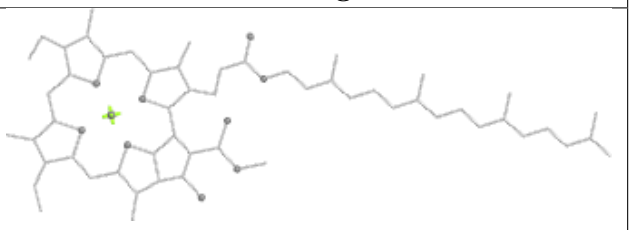
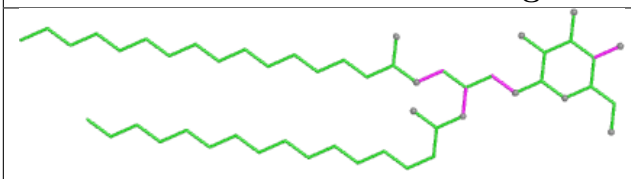


Rings

Ligand LMG b 618



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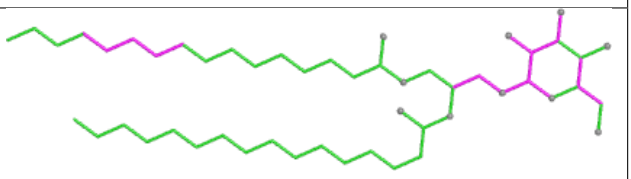
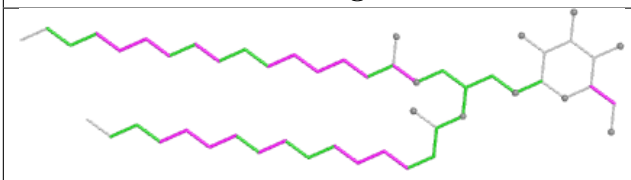


Bond angles



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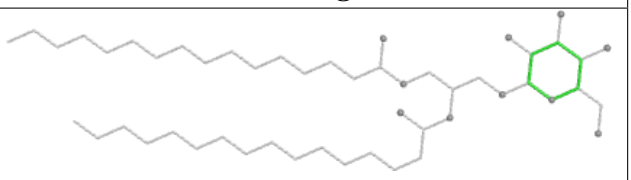

Rings

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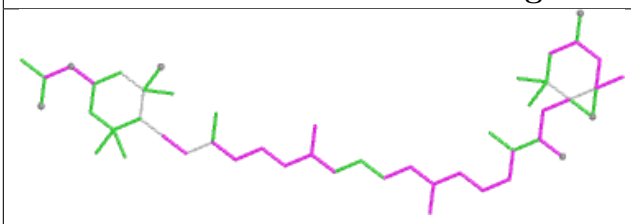

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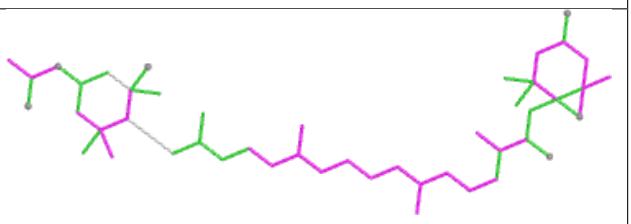
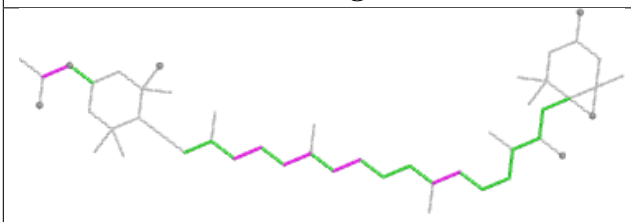


Bond angles



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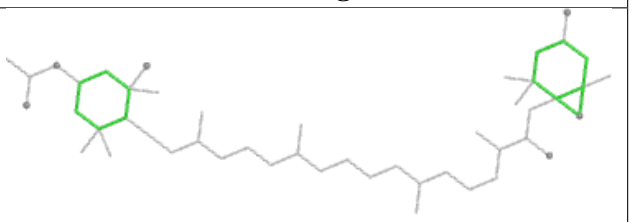
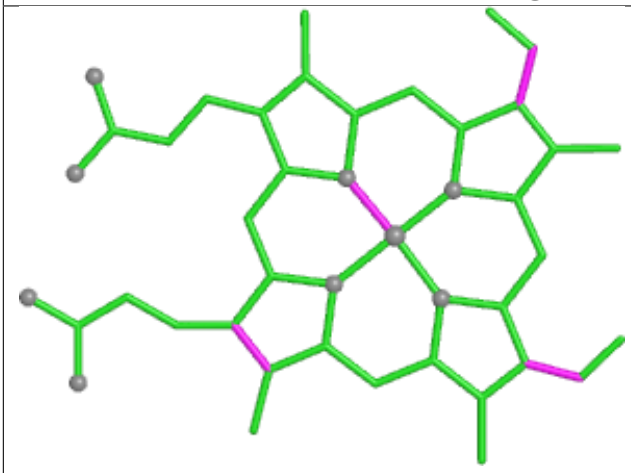


Rings

Ligand HEM f 102



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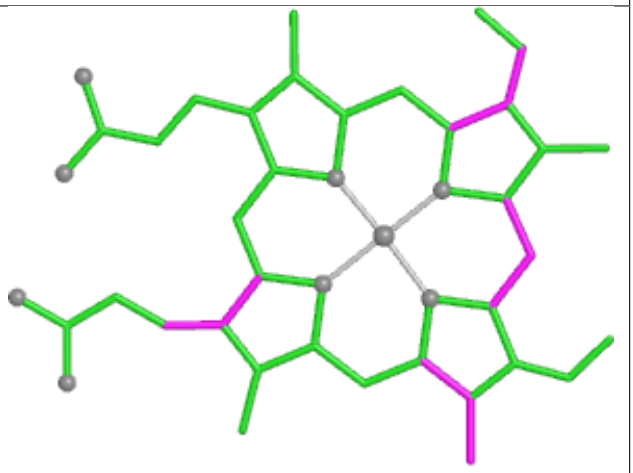
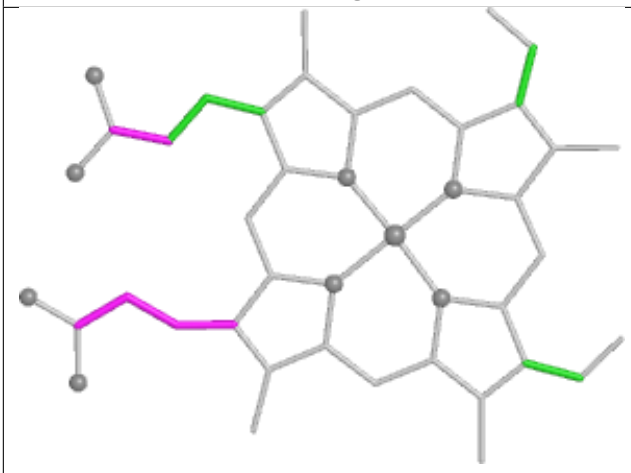
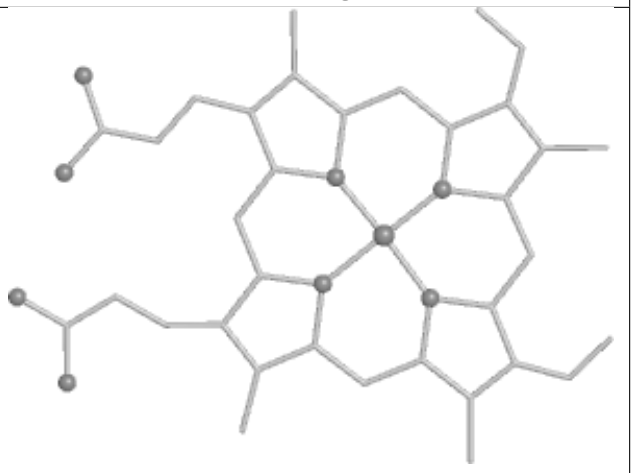


Bond angles

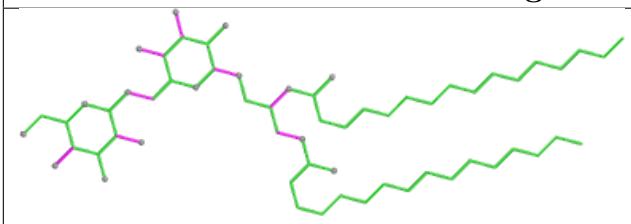


Torsions



Rings

Ligand DGD c 517



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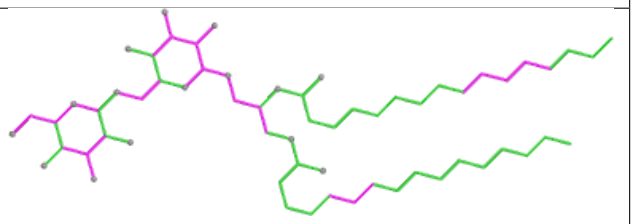

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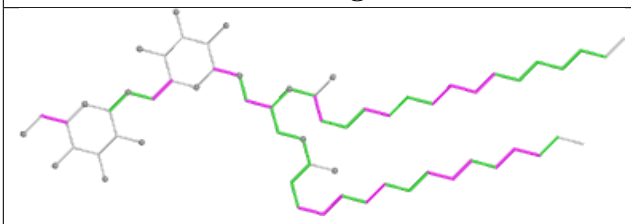

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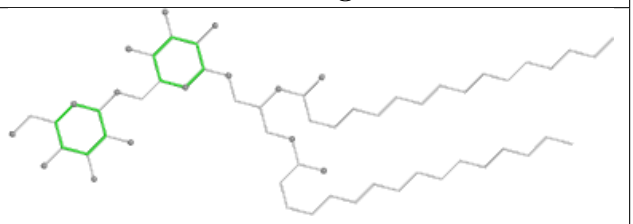
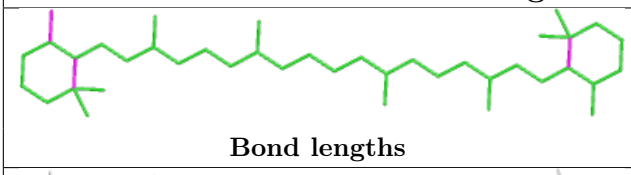


Rings

Ligand BCR c 515



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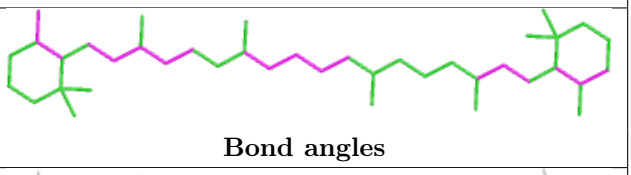

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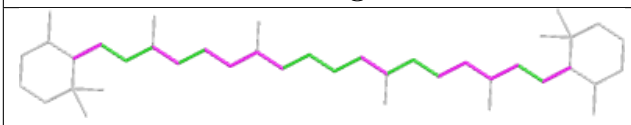

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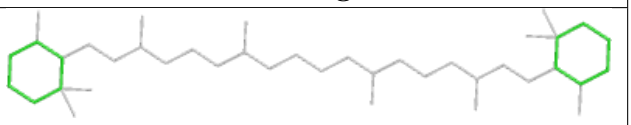
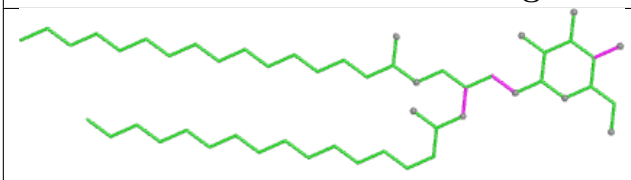


Rings

Ligand LMG d 410



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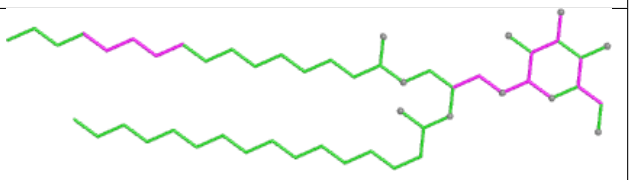

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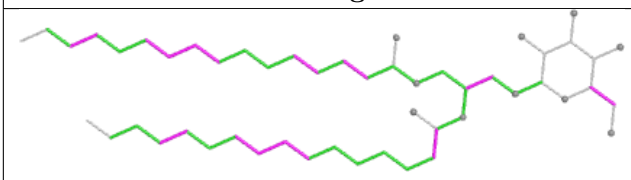

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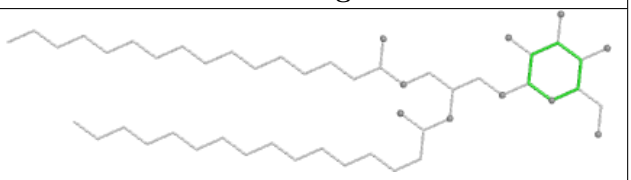
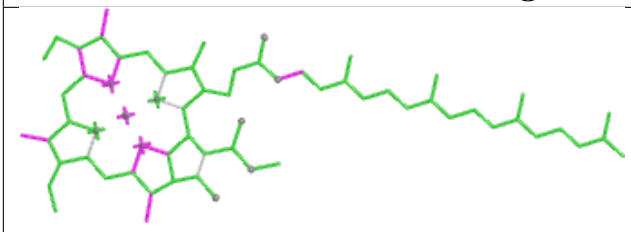


Rings

Ligand CLA 14 309



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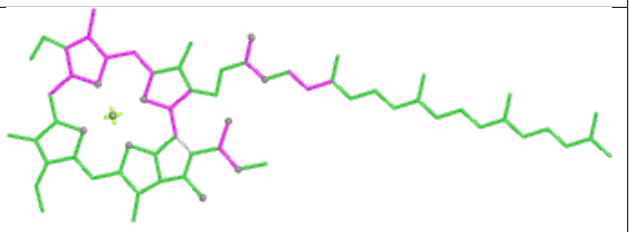
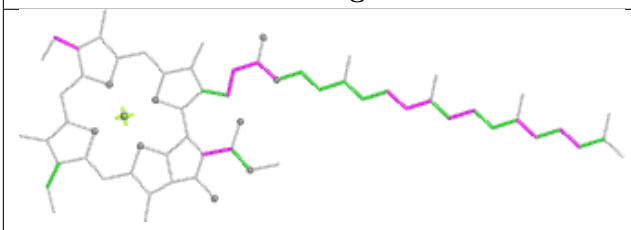


Bond angles



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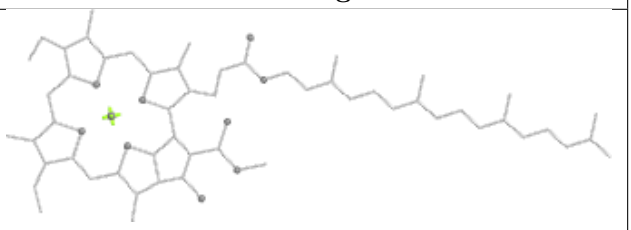
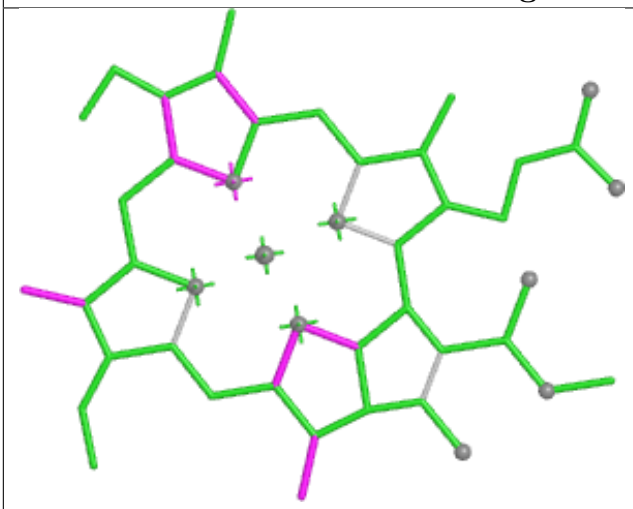


Rings

Ligand CLA 15 304



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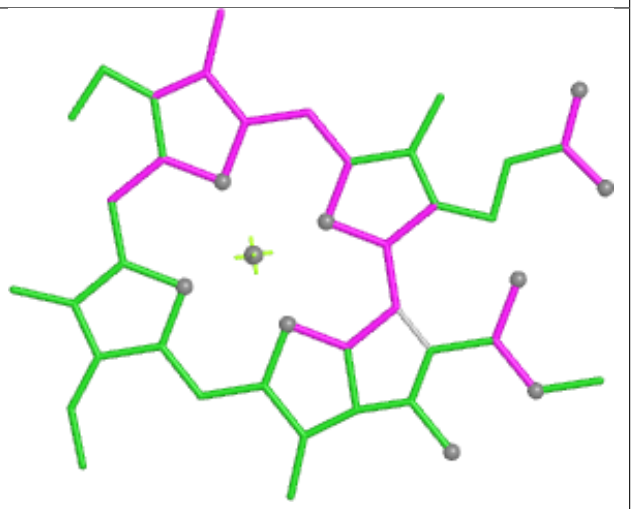

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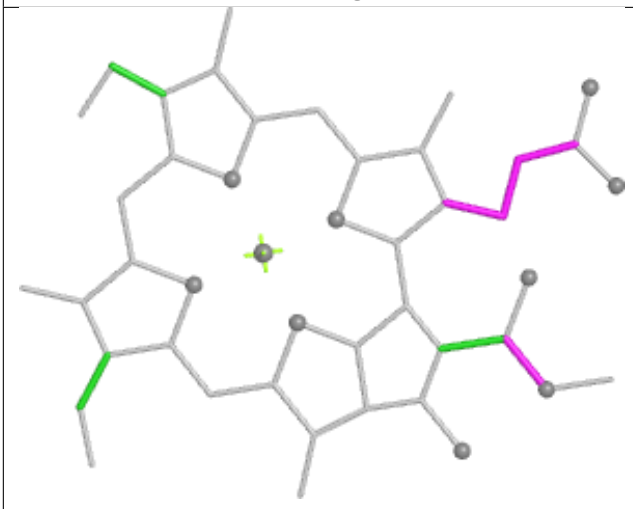
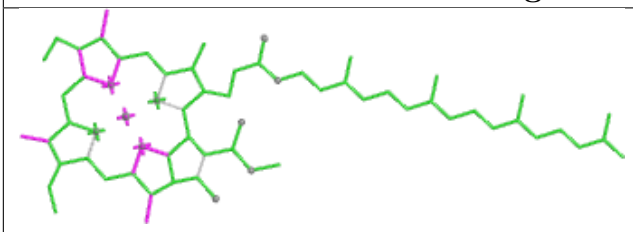


Torsions

Rings

Ligand CLA C 520



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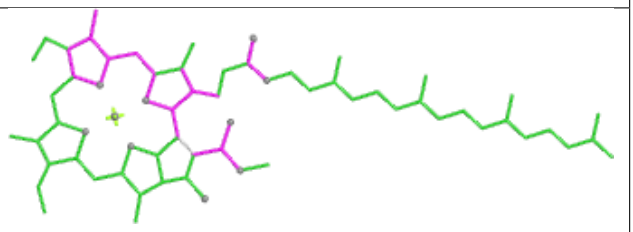

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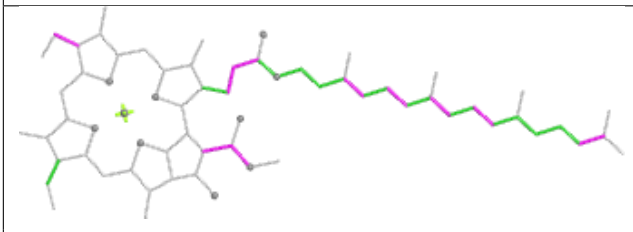

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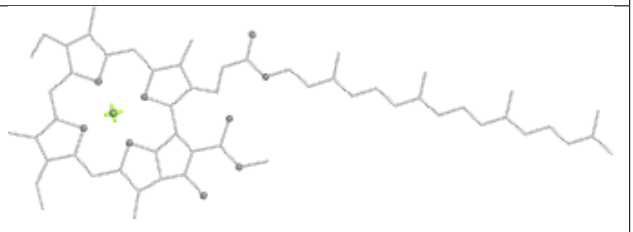
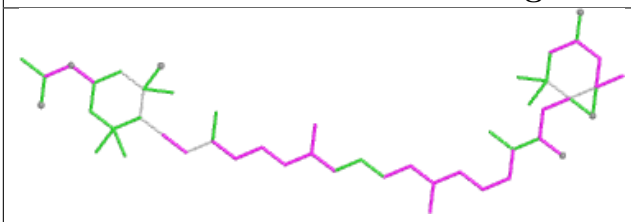


Rings

Ligand A86 17 316



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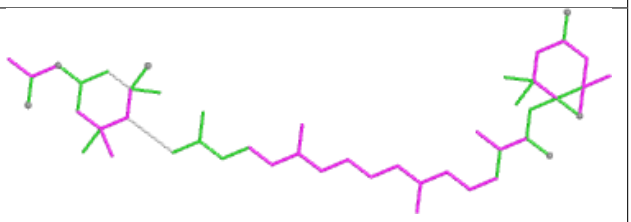

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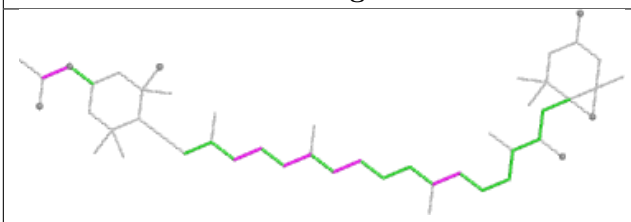

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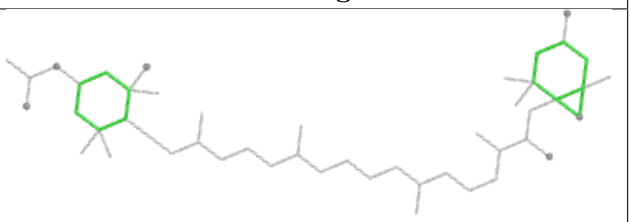
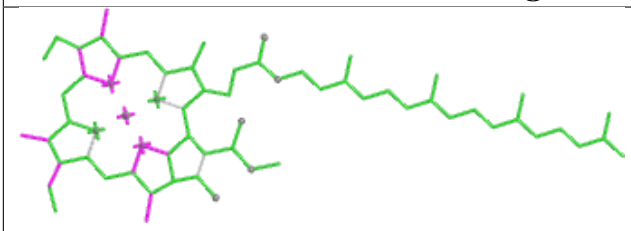


Rings

Ligand CLA B 615



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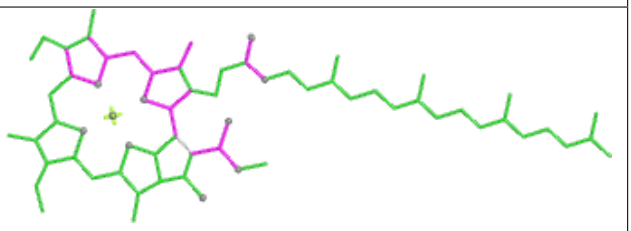

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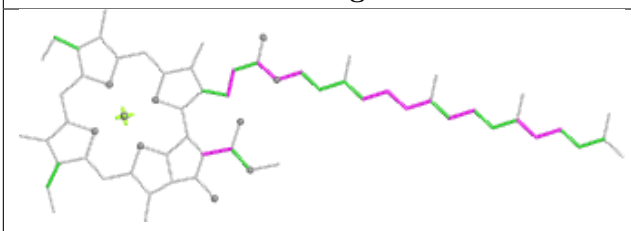

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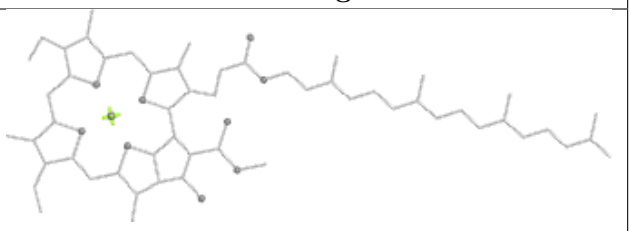
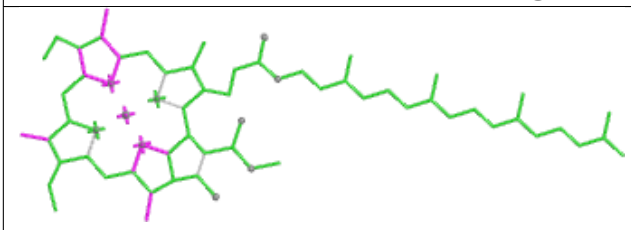


Rings

Ligand CLA c 504



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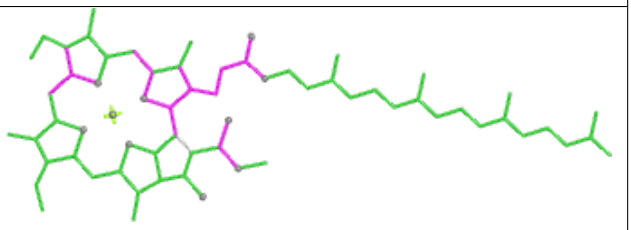

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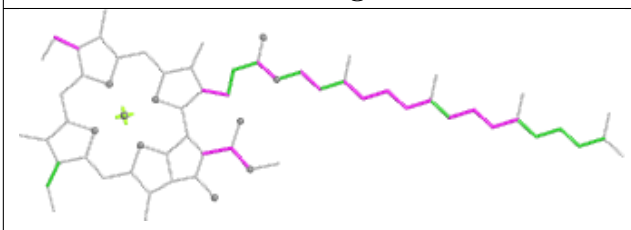

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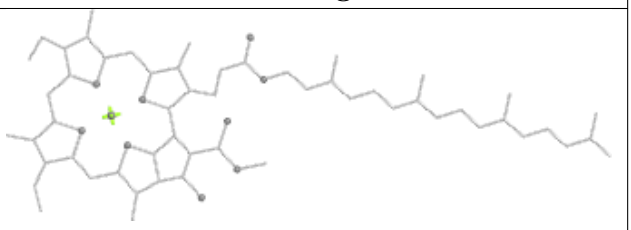
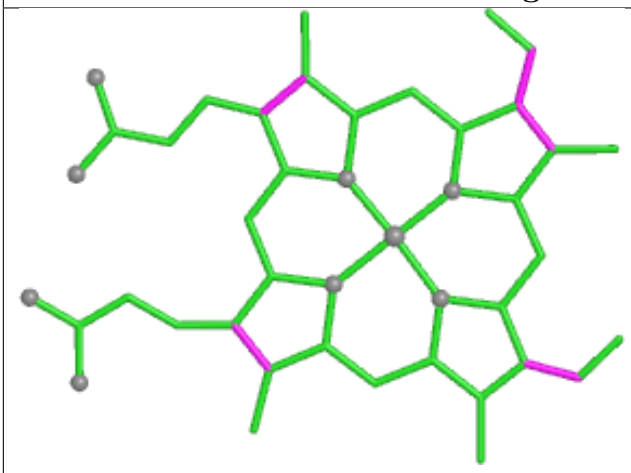


Rings

Ligand HEM v 201



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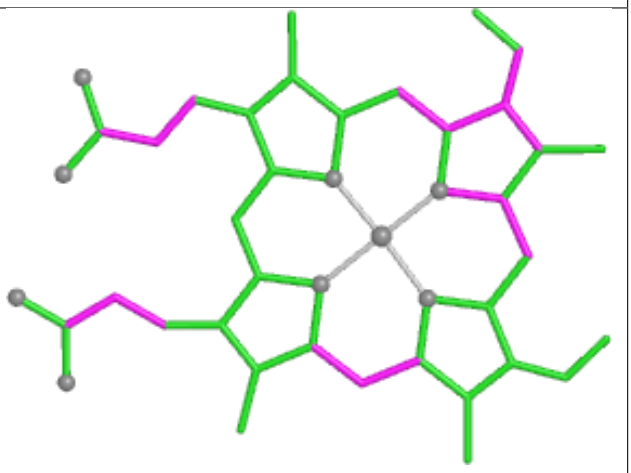

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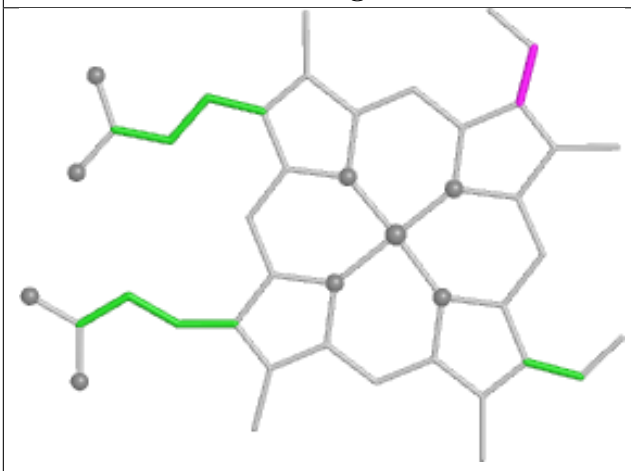

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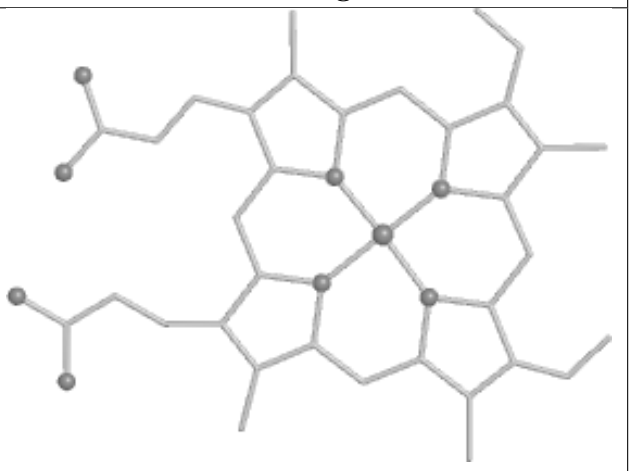
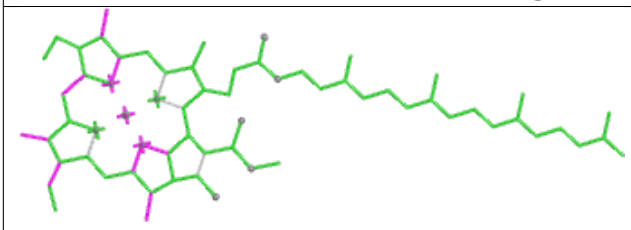


Rings

Ligand CLA c 508



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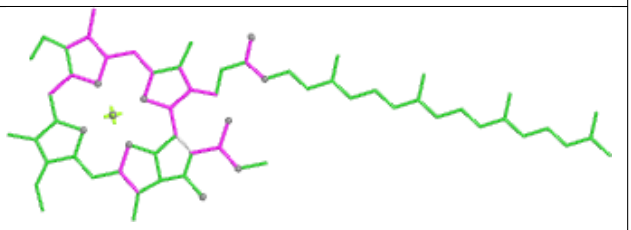
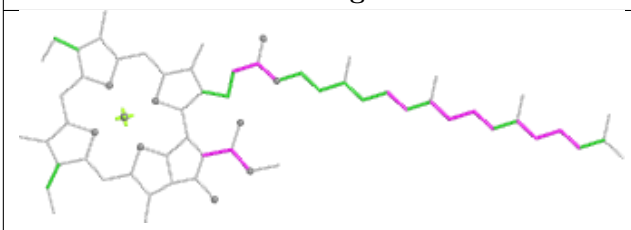


Bond angles



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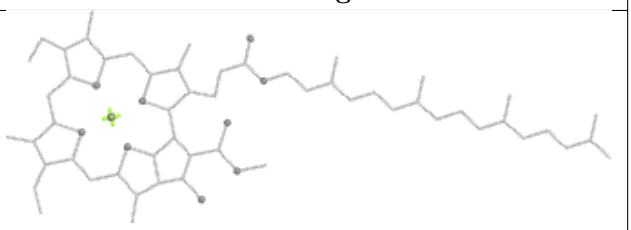
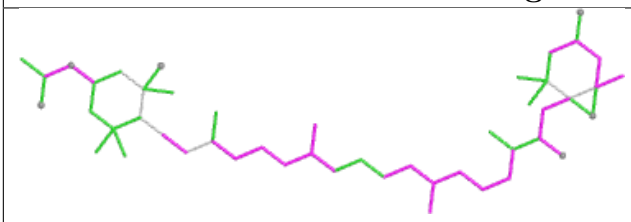


Rings

Ligand A86 13 311



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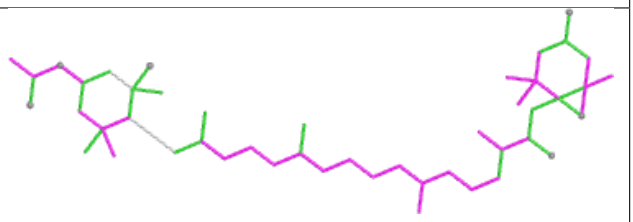
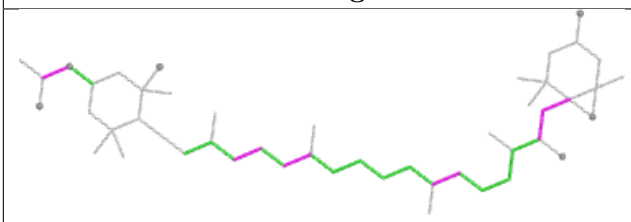


Bond angles



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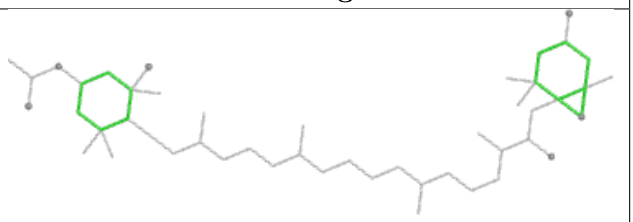
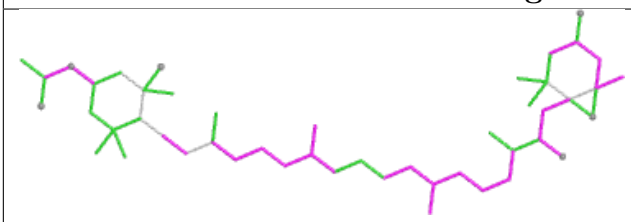


Rings

Ligand A86 12 315



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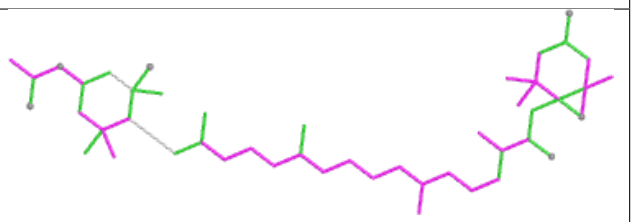
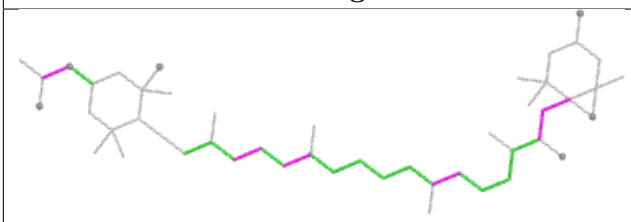


Bond angles



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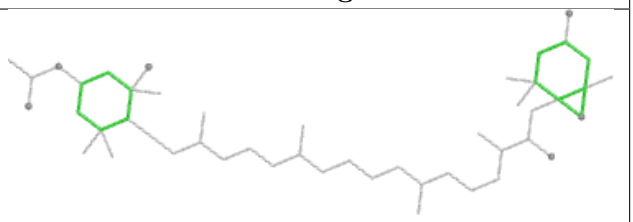
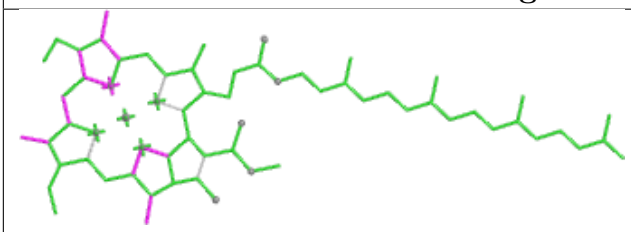


Rings

Ligand CLA 14 303



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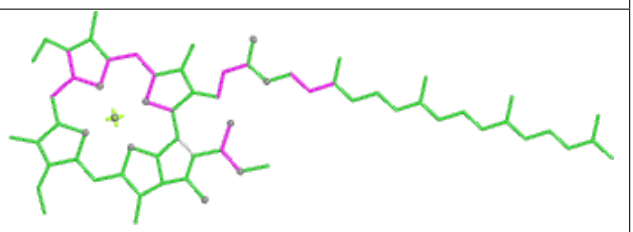

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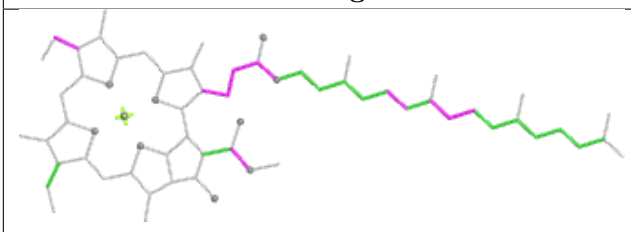

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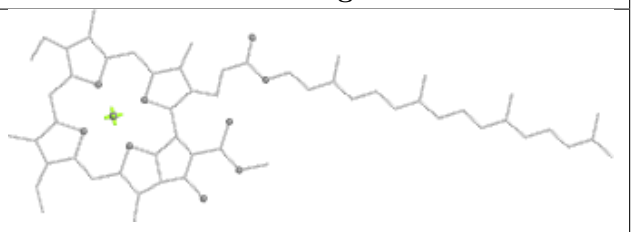

Rings

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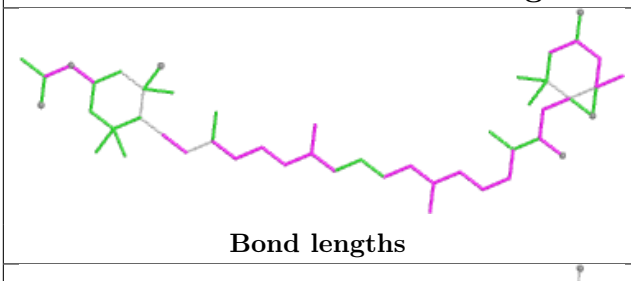

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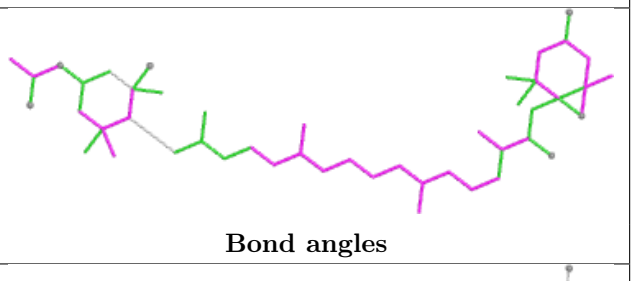

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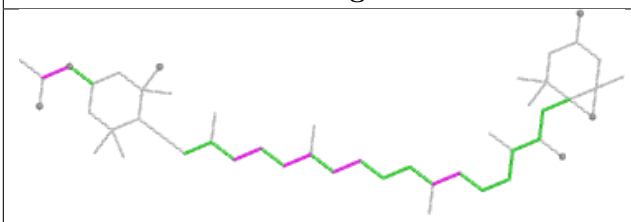

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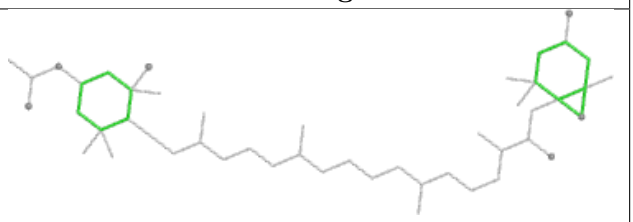

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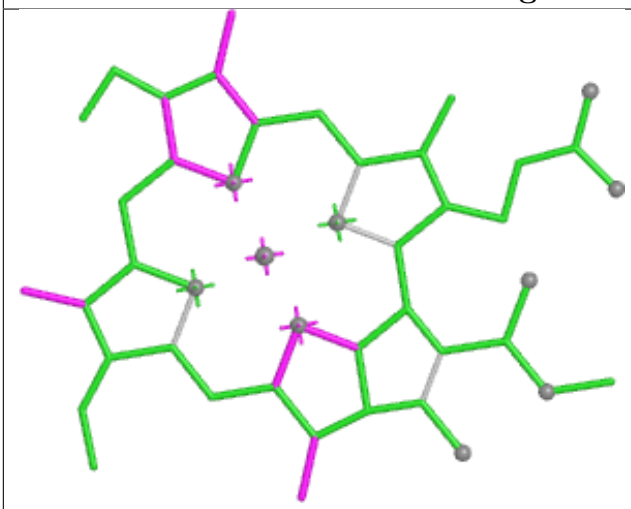

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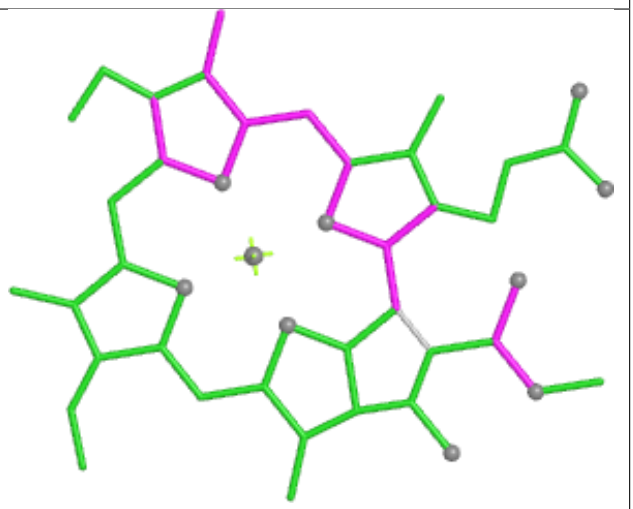

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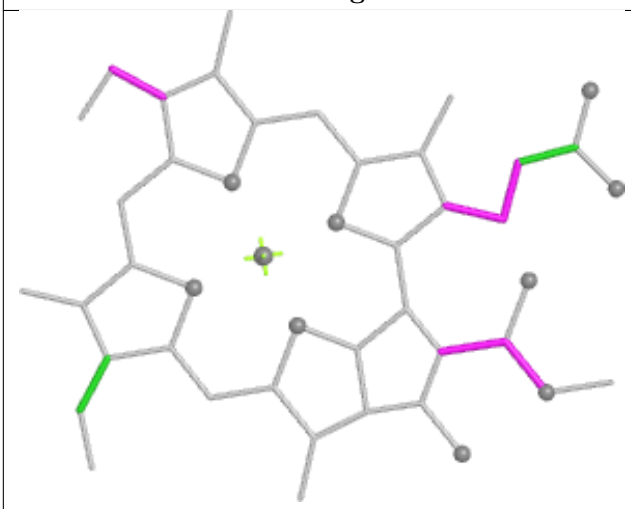

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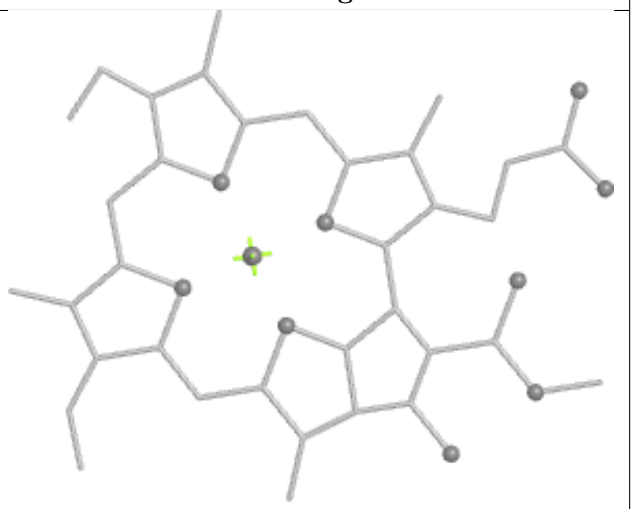

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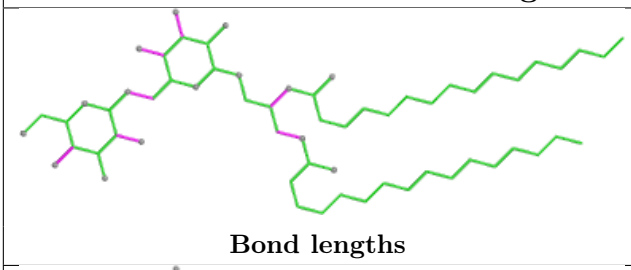

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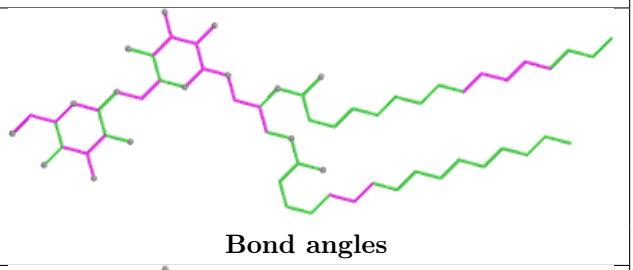

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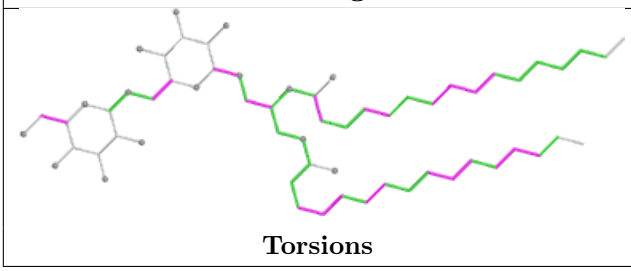

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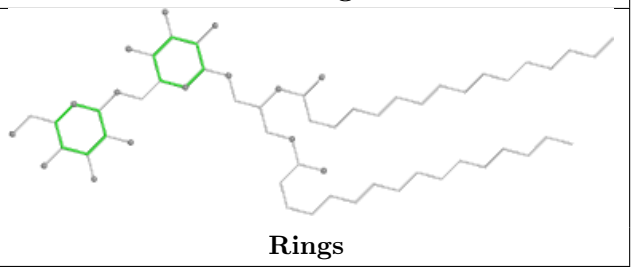

Rings

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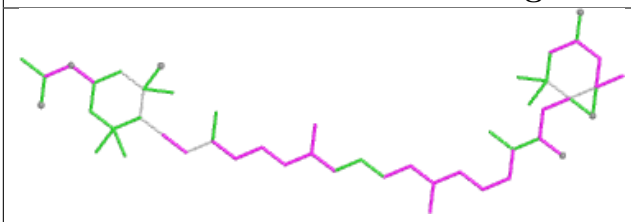

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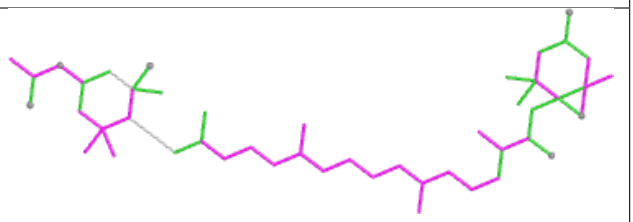

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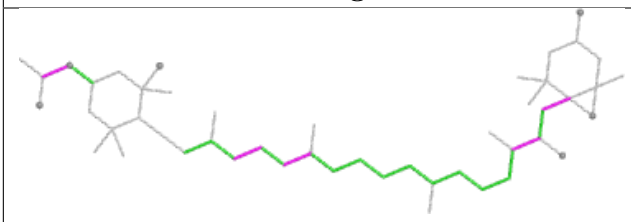

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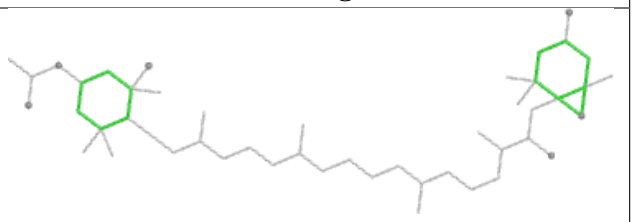

Rings

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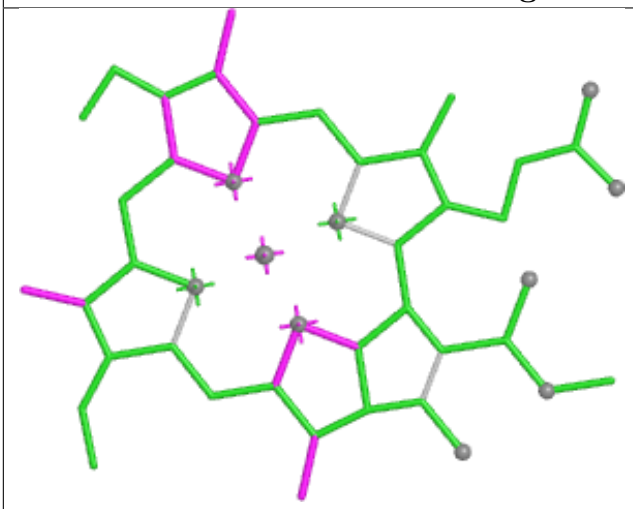

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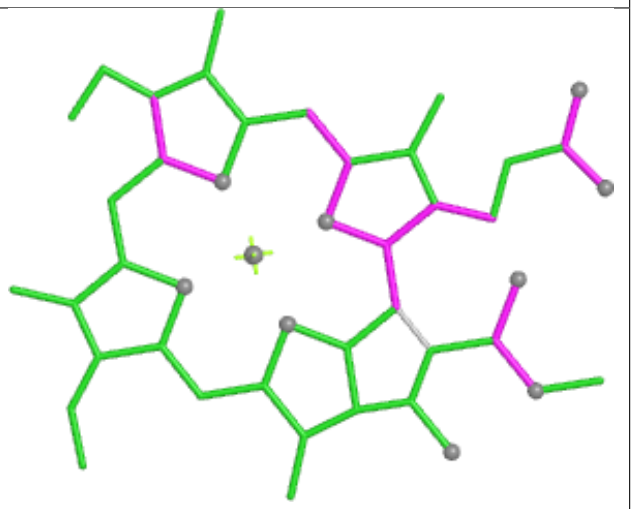

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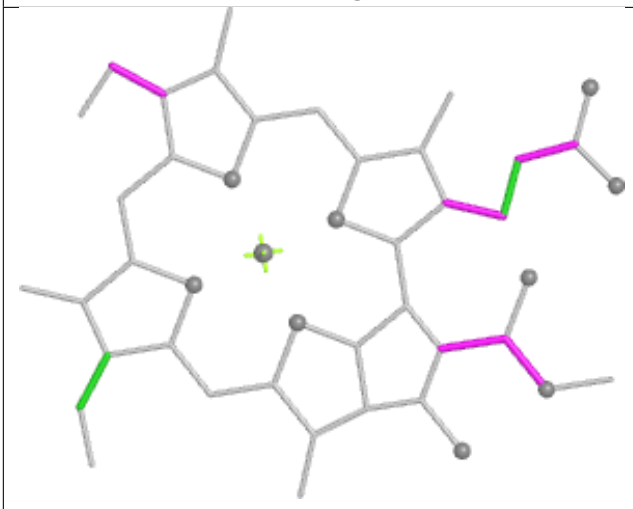

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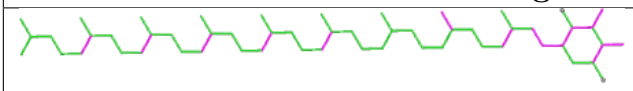

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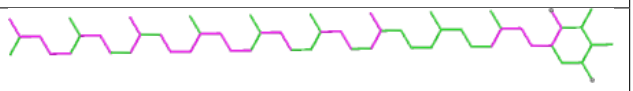

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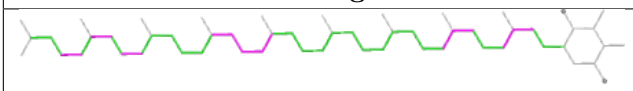

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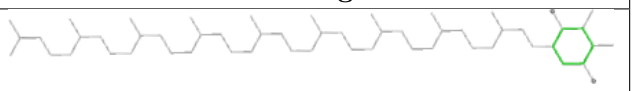

Rings

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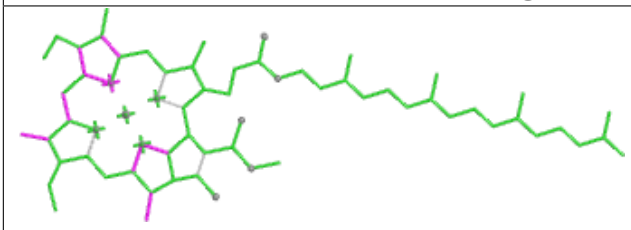

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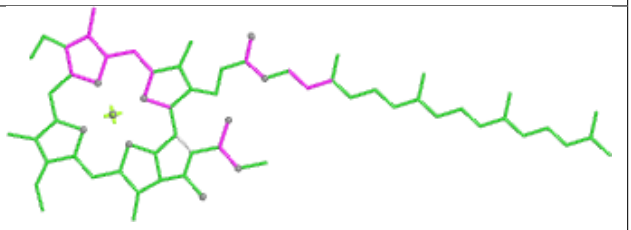

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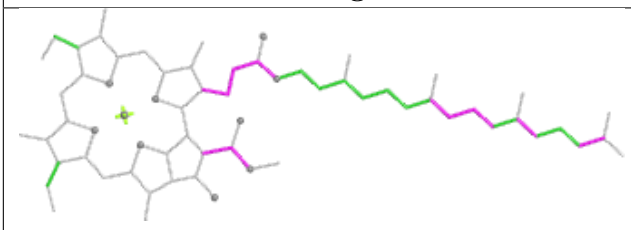

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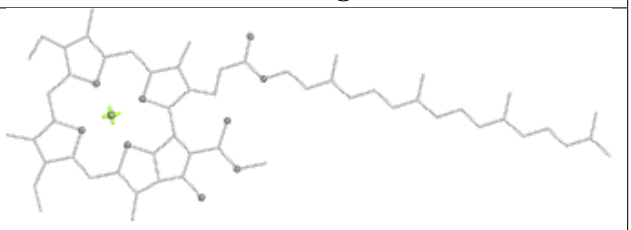

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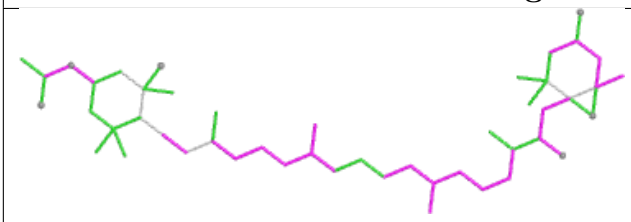

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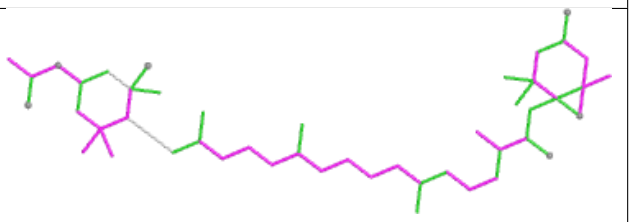

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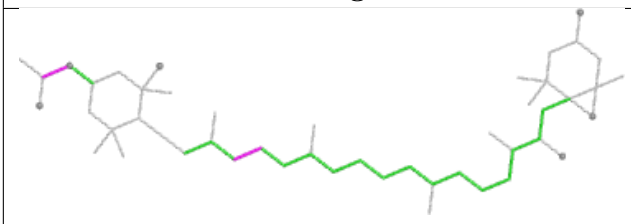

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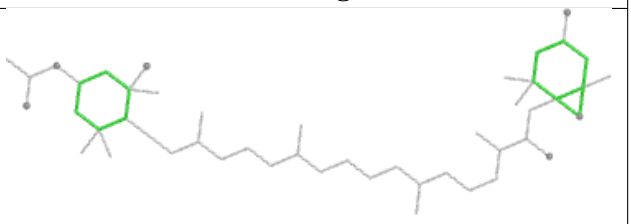

Rings

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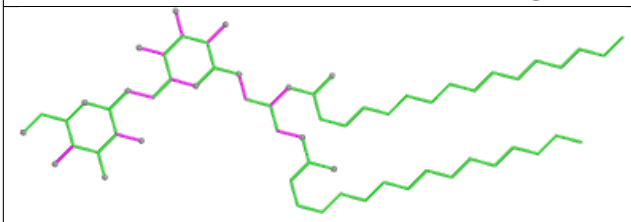

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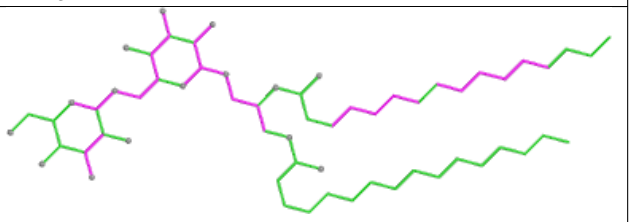

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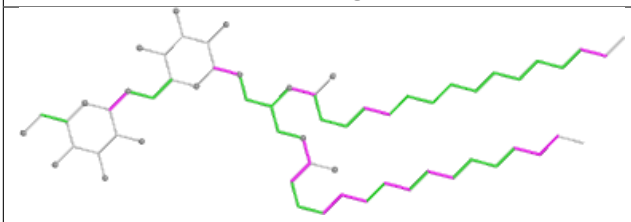

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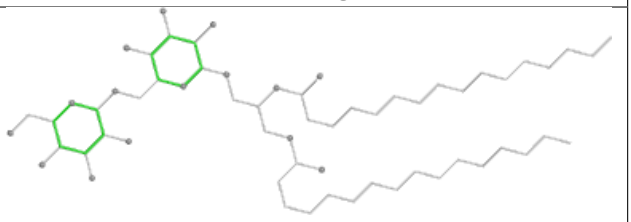
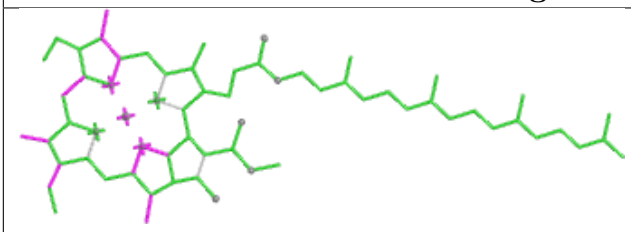


Rings

Ligand CLA c 503



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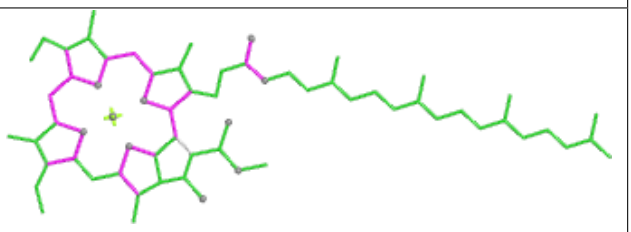

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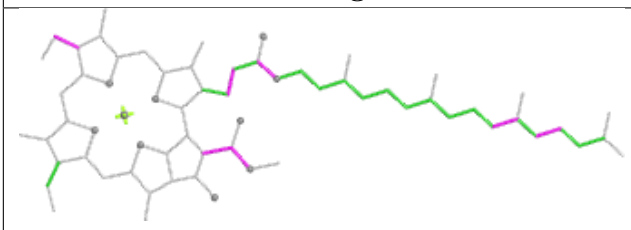

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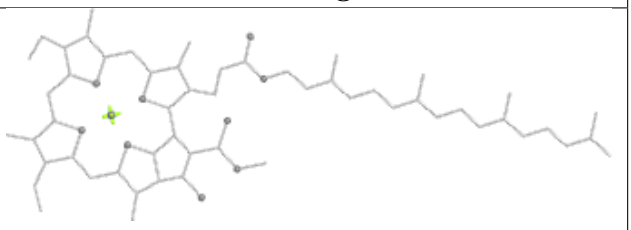
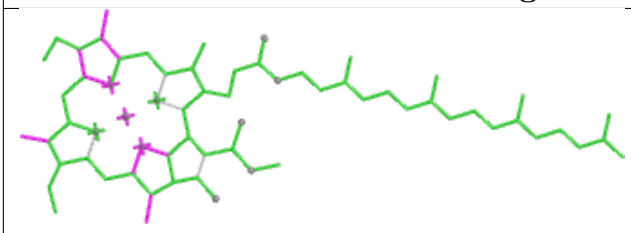


Rings

Ligand CLA 12 303



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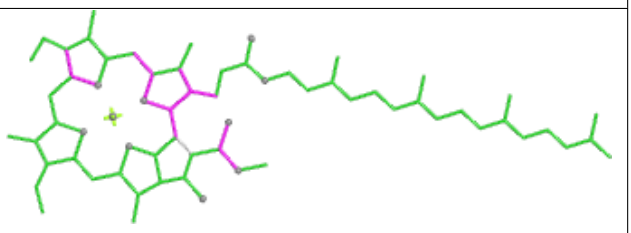

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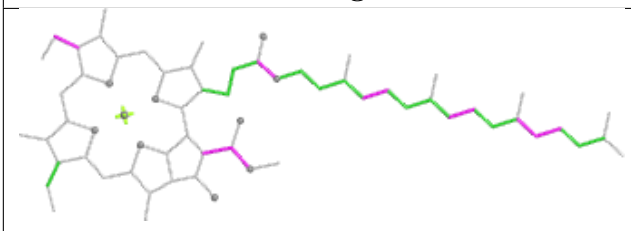

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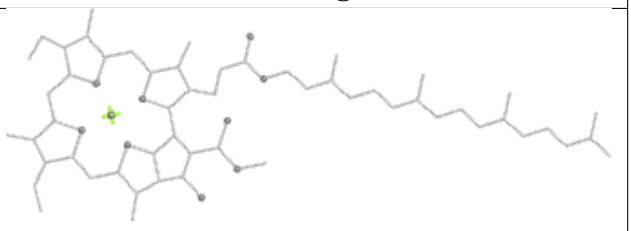
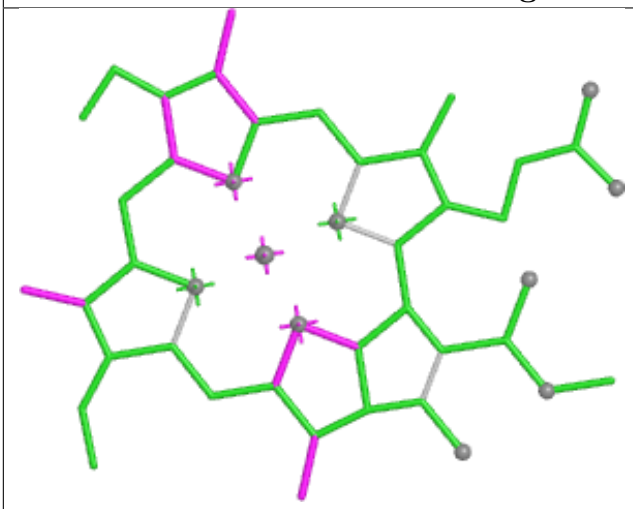


Rings

Ligand CLA 17 310



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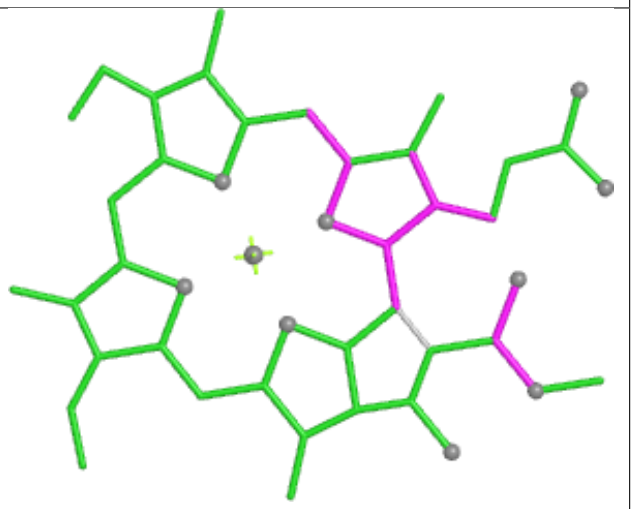
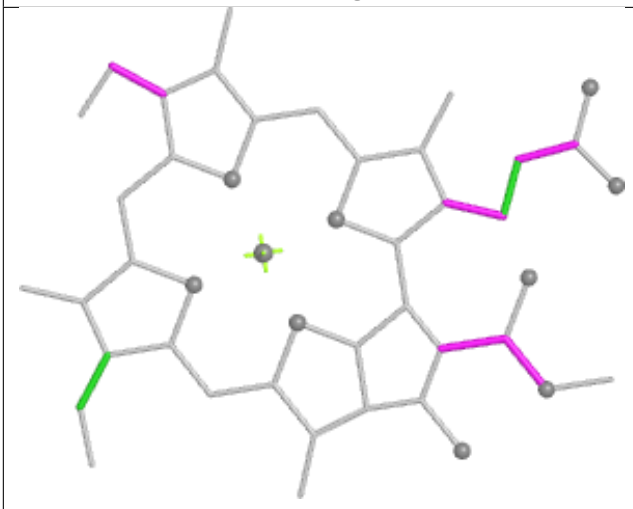


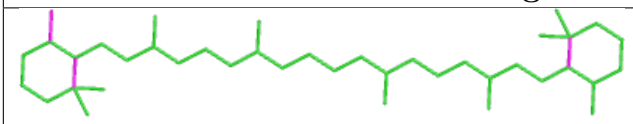
Bond angles



Torsions

Rings

Ligand BCR B 624



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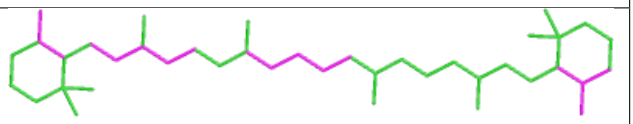

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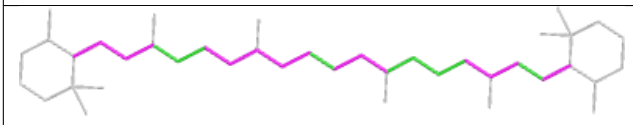

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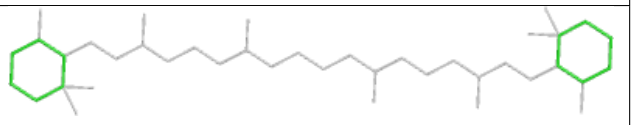
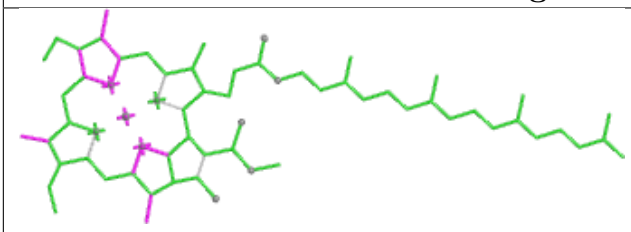


Rings

Ligand CLA c 514



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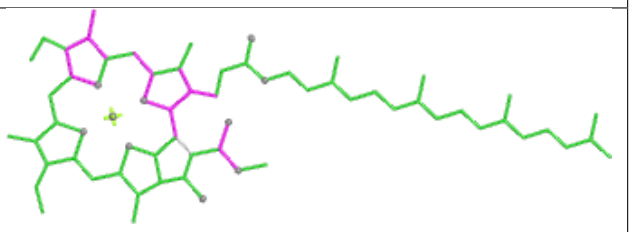
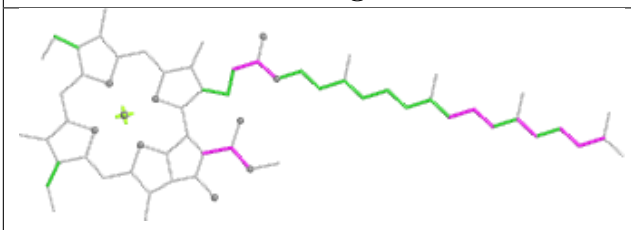
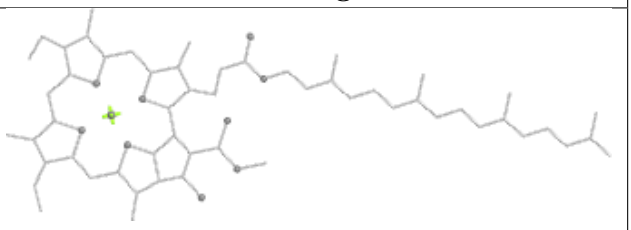


Bond angles

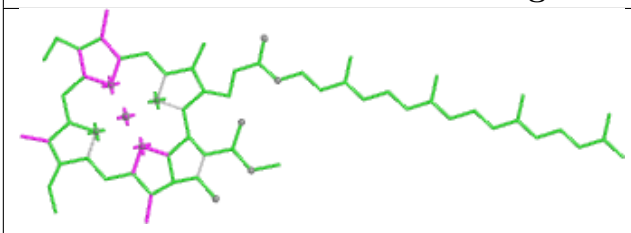


Torsions

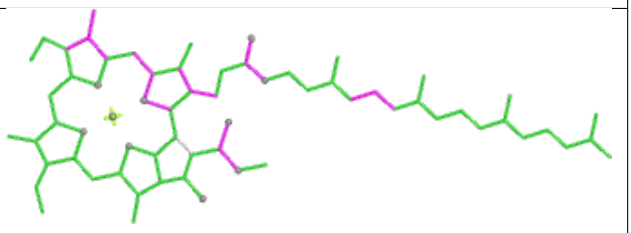


Rings

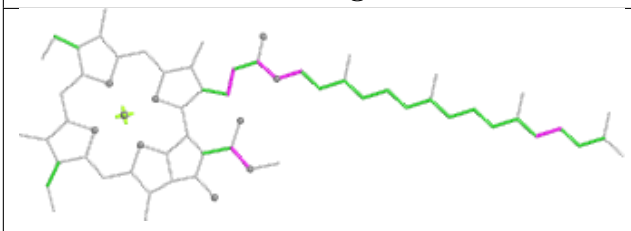
Ligand CLA a 402



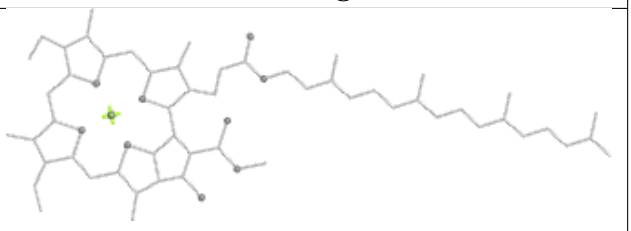
Bond lengths



Bond angles

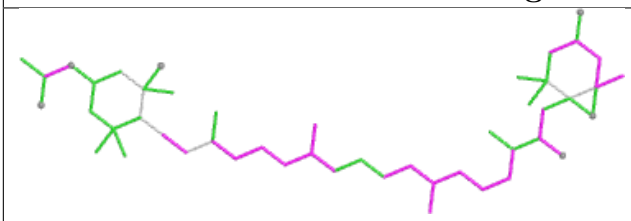


Torsions

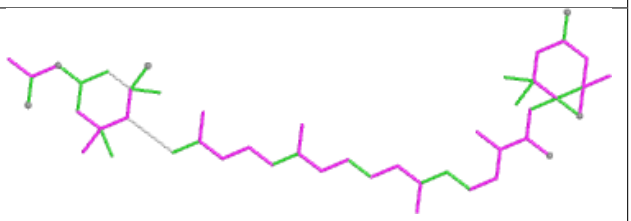


Rings

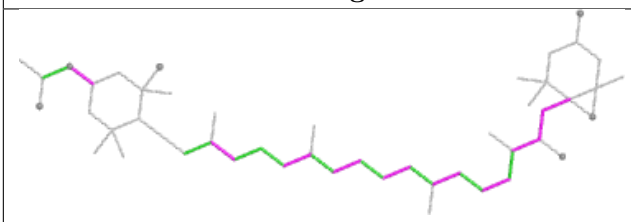
Ligand A86 19 311



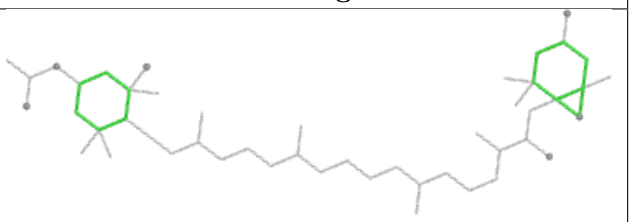
Bond lengths



Bond angles

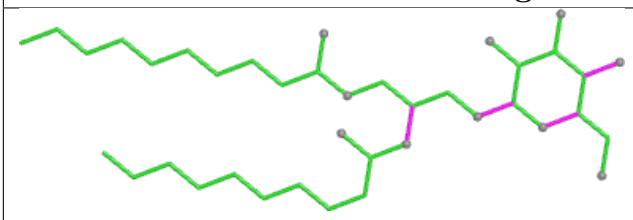


Torsions

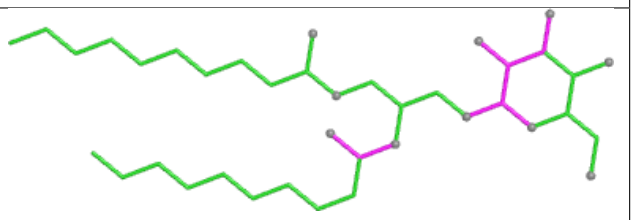


Rings

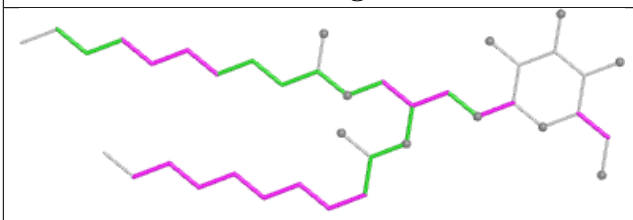
Ligand LMG 12 301



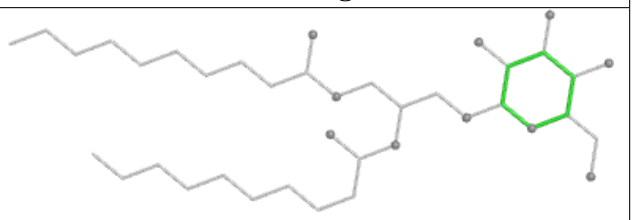
Bond lengths



Bond angles

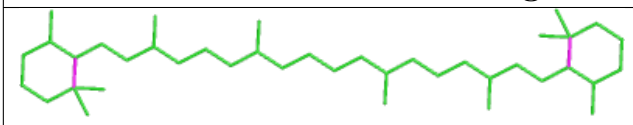


Torsions

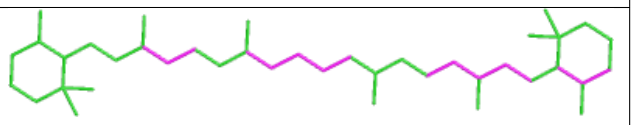


Rings

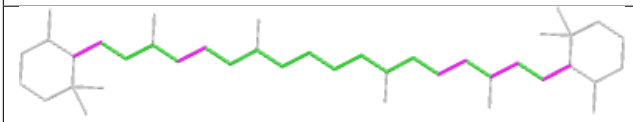
Ligand BCR C 518



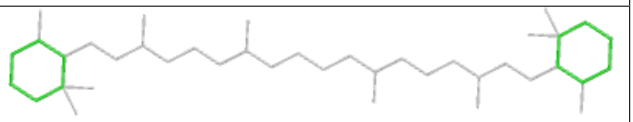
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

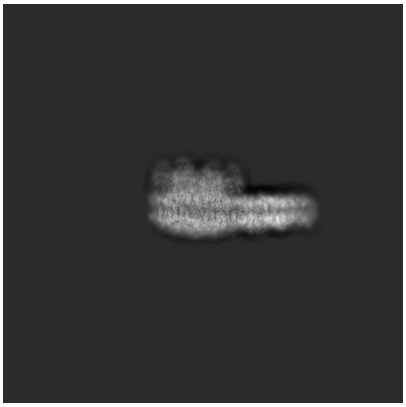
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9776. These allow visual inspection of the internal detail of the map and identification of artifacts.

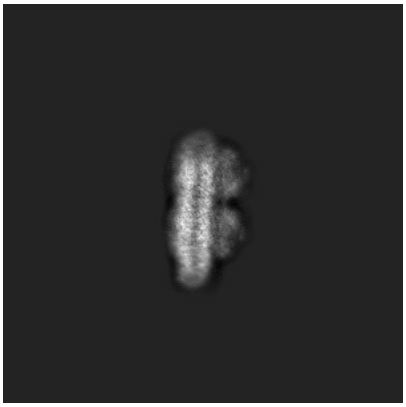
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

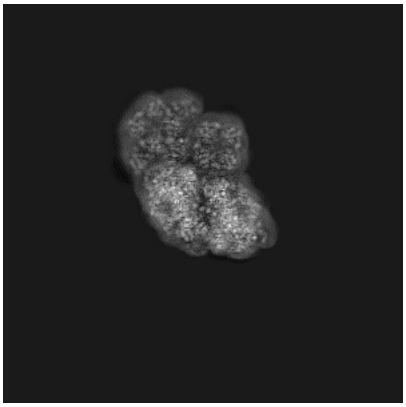
6.1.1 Primary map



X



Y



Z

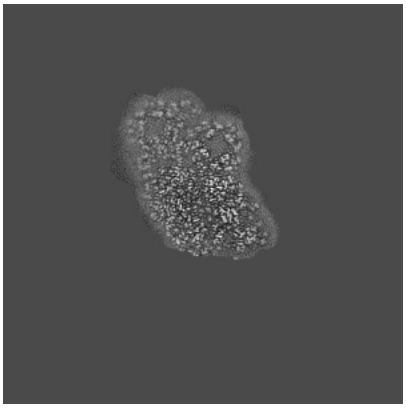
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 256

Y Index: 256



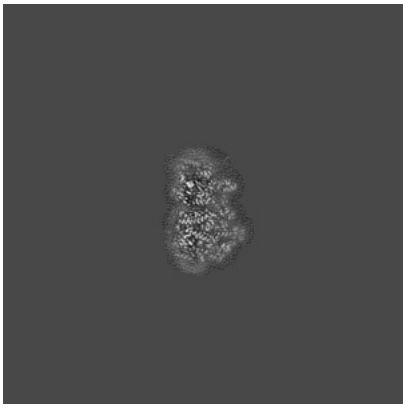
Z Index: 256

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

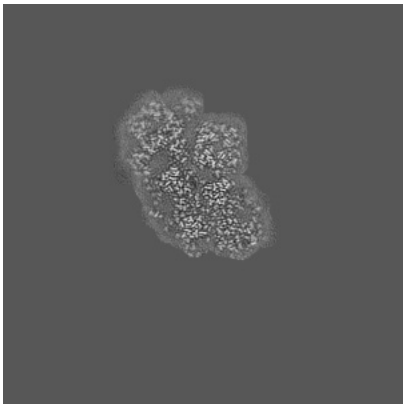
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 283



Y Index: 274

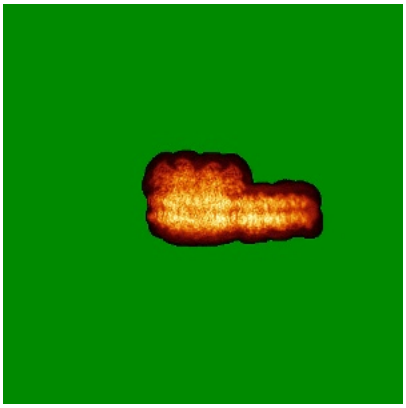


Z Index: 237

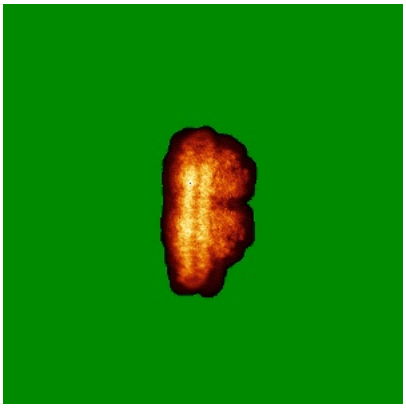
The images above show the largest variance slices of the map in three orthogonal directions.

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

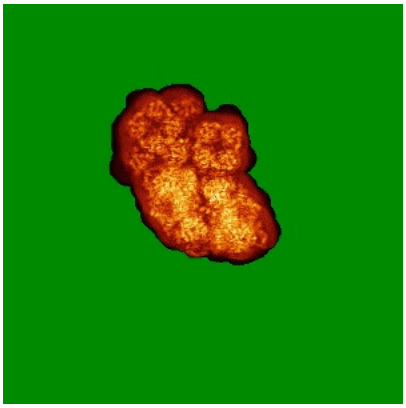
6.4.1 Primary map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

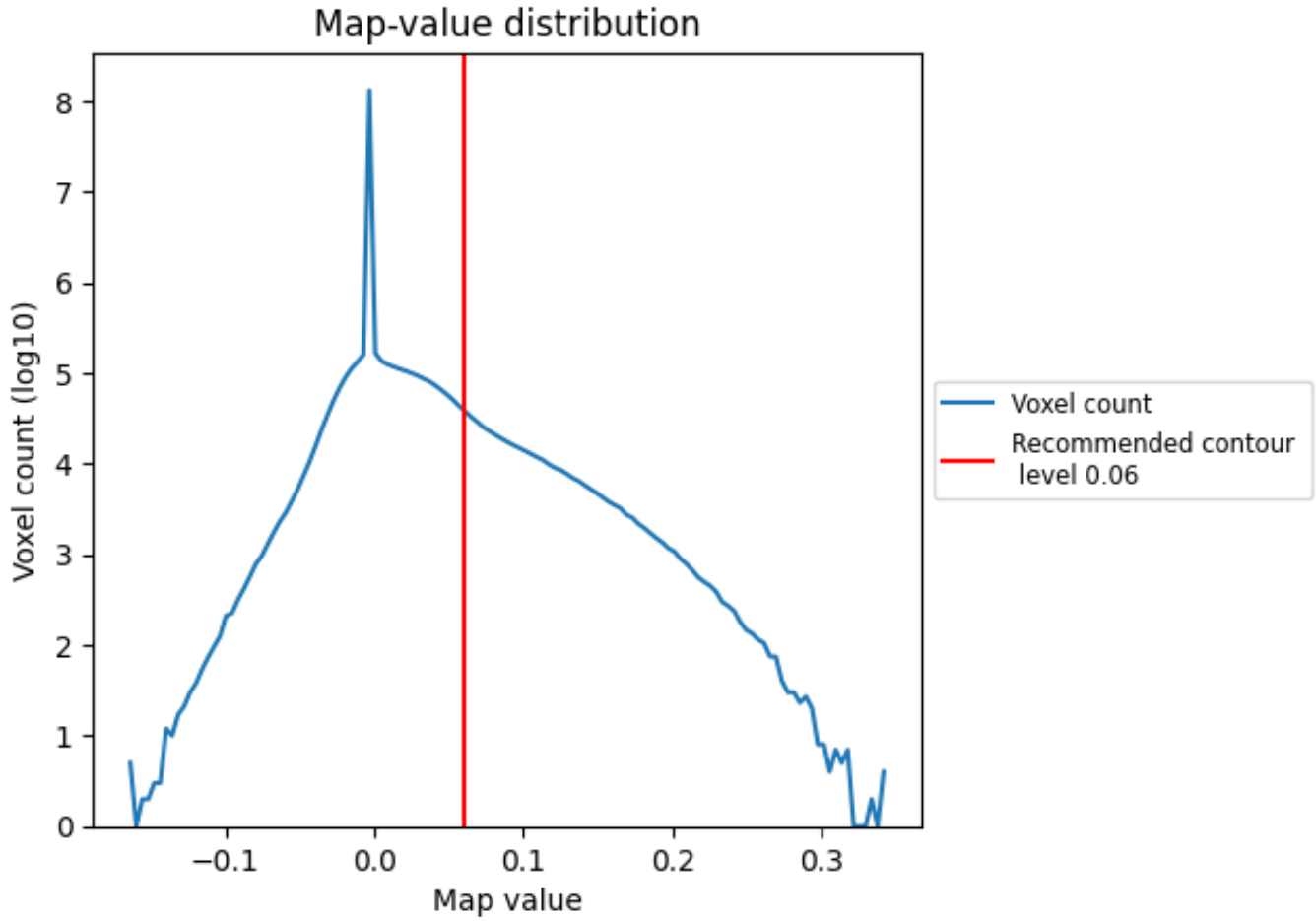
6.6 Mask visualisation (i)

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

7 Map analysis

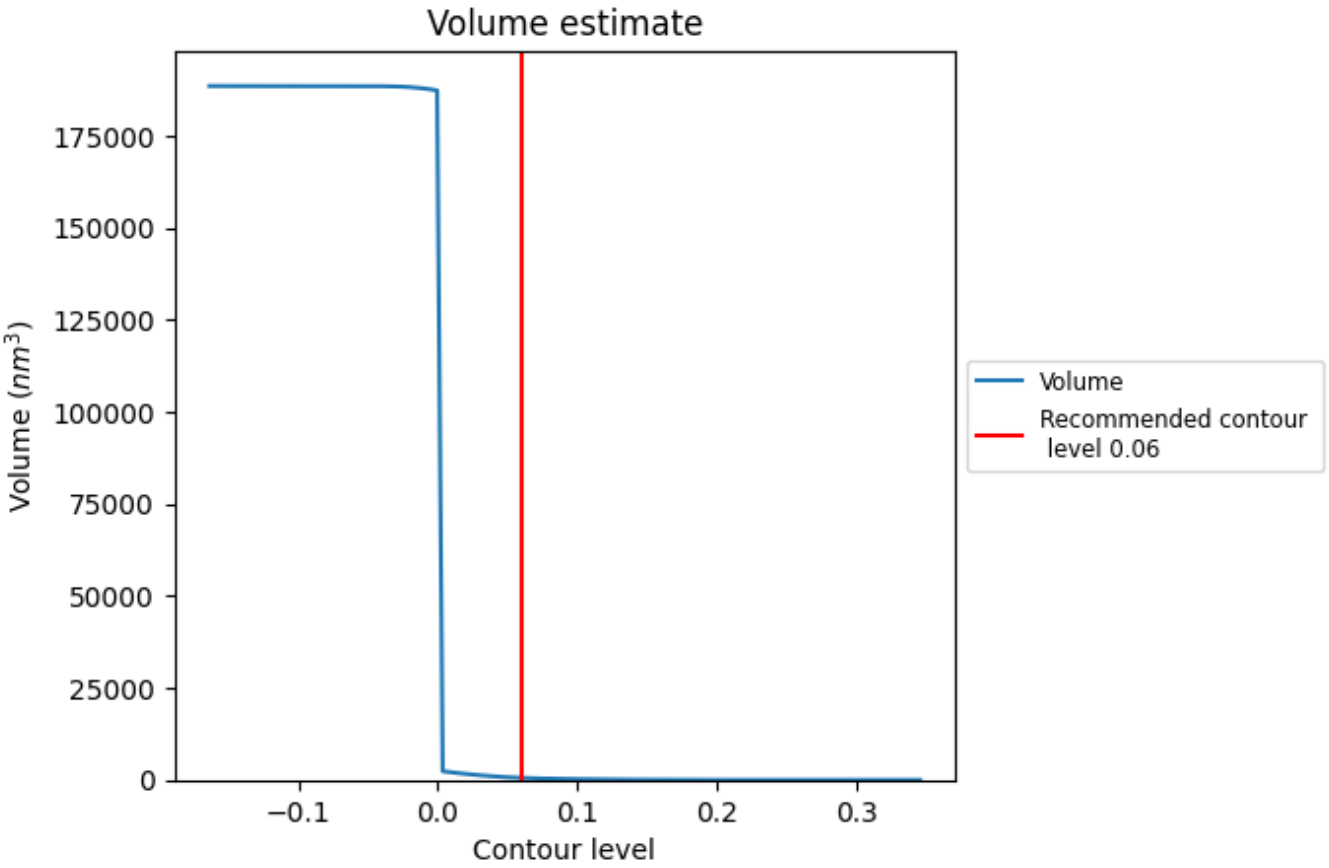
This section contains the results of statistical analysis of the map.

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.

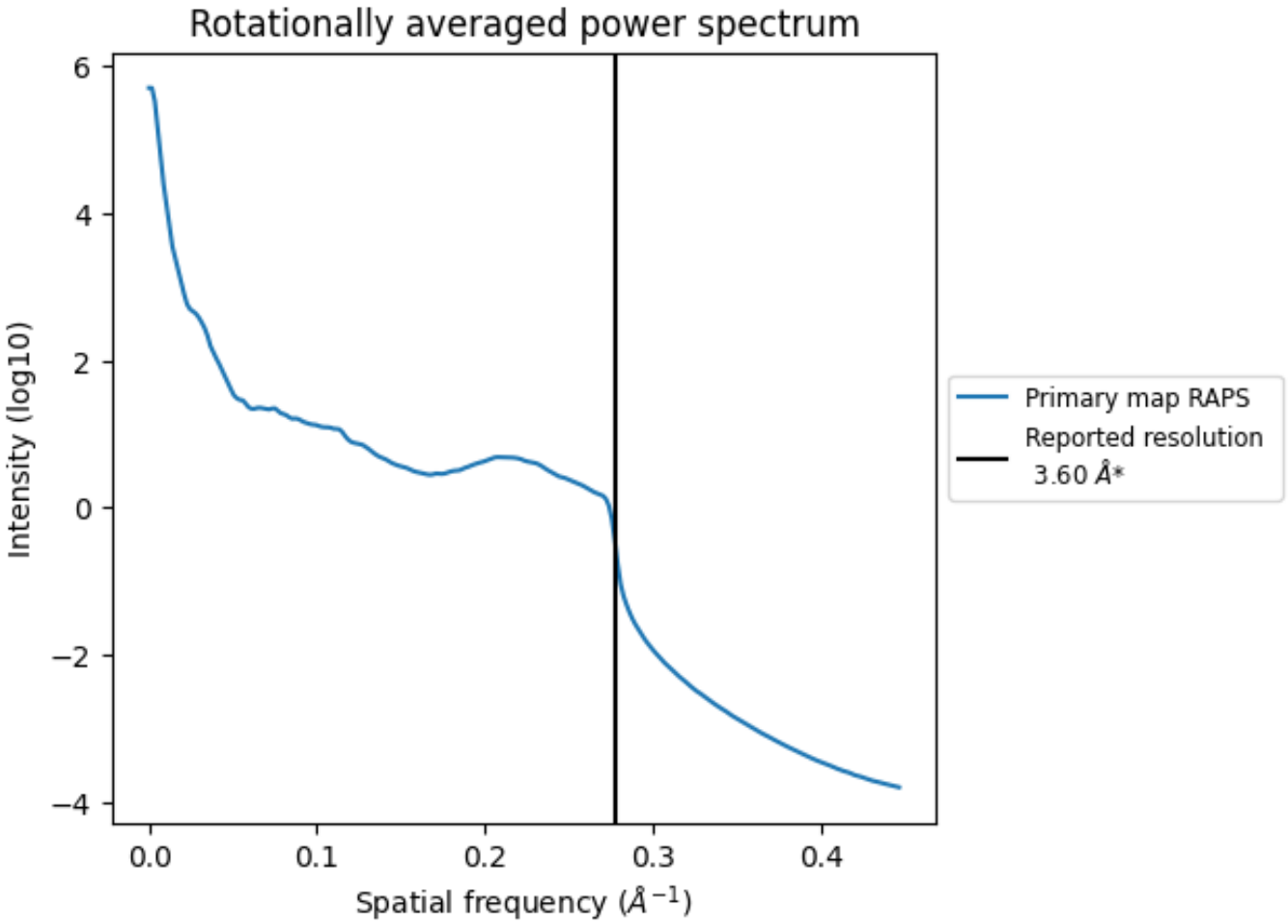
7.2 Volume estimate



The volume at the recommended contour level is 558 nm^3; this corresponds to an approximate mass of 504 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)

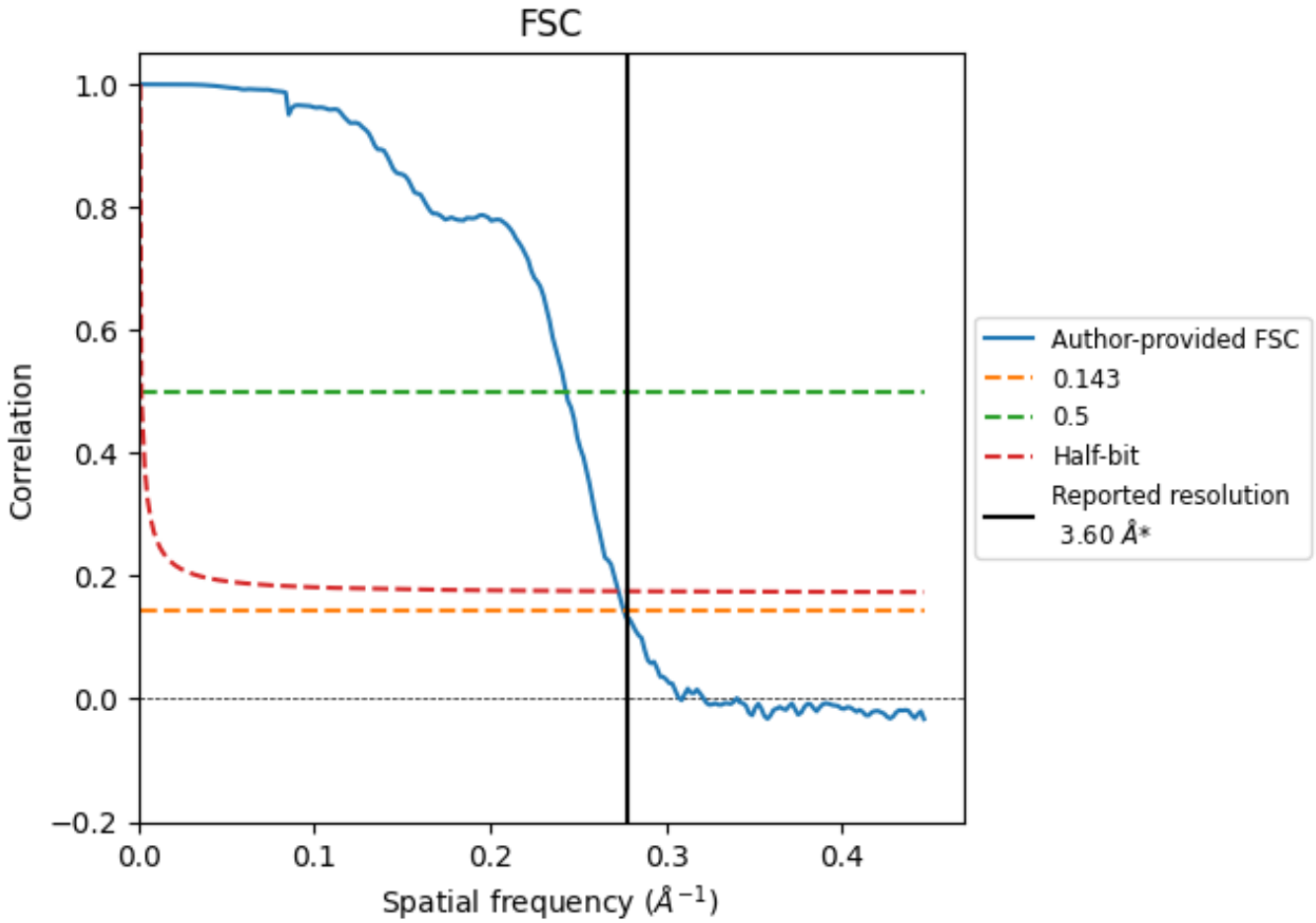


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

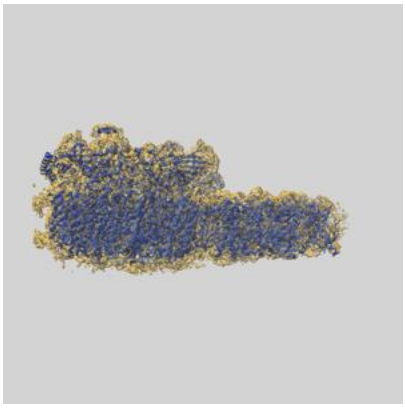
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	4.12	3.67
Unmasked-calculated*	-	-	-

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

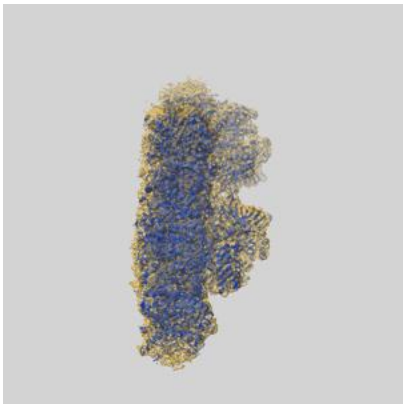
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9776 and PDB model 6J3Z. Per-residue inclusion information can be found in section 3 on page 34.

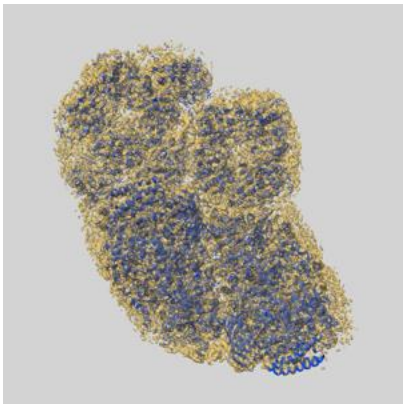
9.1 Map-model overlay



X



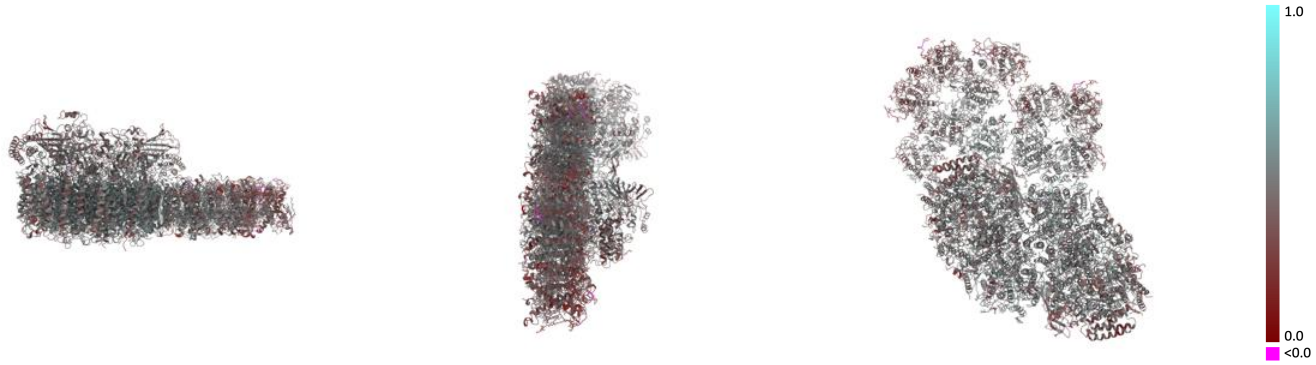
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

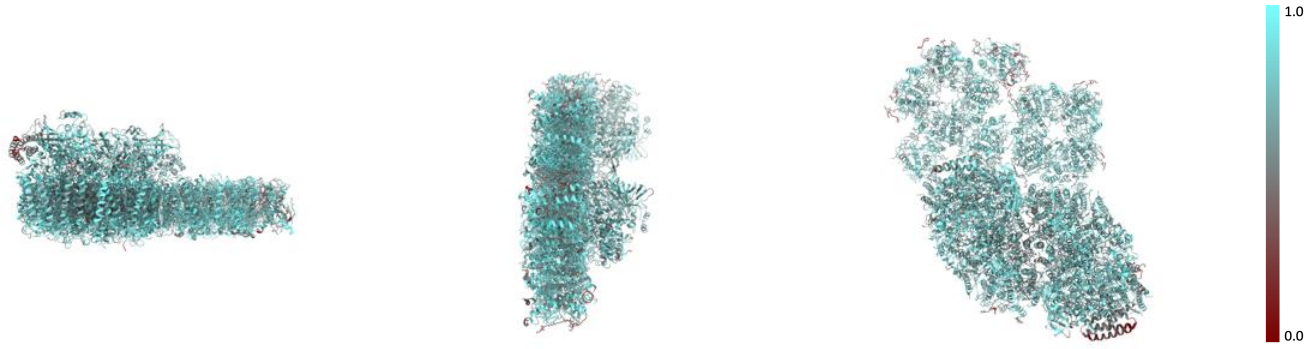
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

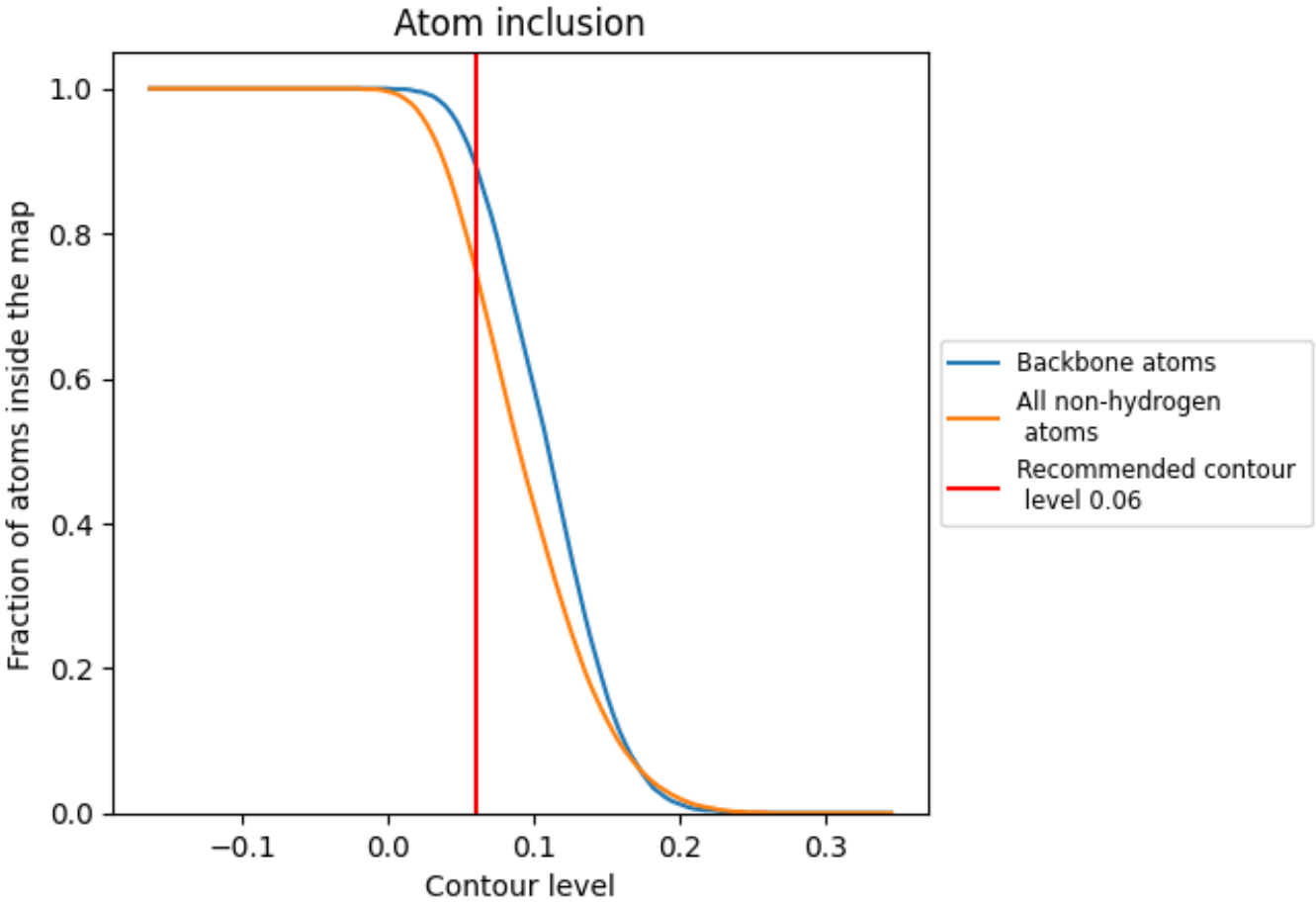
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.4440
0	0.8060	0.4800
1	0.7990	0.4560
11	0.8000	0.4590
12	0.7620	0.4290
13	0.7400	0.3620
14	0.7470	0.3900
15	0.6860	0.3320
16	0.7630	0.4130
17	0.7650	0.4300
18	0.7030	0.3440
19	0.8770	0.4910
2	0.9200	0.4440
20	0.7920	0.4140
21	0.6320	0.3220
5	0.8450	0.5000
6	0.9070	0.4900
7	0.7800	0.4160
A	0.7910	0.4950
B	0.7670	0.4850
C	0.7830	0.4850
D	0.7590	0.4850
E	0.7750	0.4020
F	0.7120	0.4340
H	0.7690	0.4620
I	0.7770	0.4740
J	0.7010	0.4580
K	0.7800	0.4690
L	0.6670	0.4870
M	0.6230	0.4450
O	0.7260	0.4240
Q	0.6860	0.3850
T	0.7180	0.4600
U	0.7340	0.4100
V	0.7720	0.4250

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
W	0.6360	0.4260
X	0.6760	0.3880
Y	0.6370	0.4140
Z	0.7210	0.4190
a	0.7940	0.4950
b	0.7950	0.4960
c	0.7700	0.4750
d	0.7600	0.4960
e	0.7800	0.4230
f	0.7420	0.4250
h	0.7720	0.4750
i	0.7870	0.4590
j	0.7040	0.4360
k	0.7500	0.4510
l	0.6620	0.4800
m	0.6540	0.4620
o	0.6960	0.4120
q	0.4380	0.3550
t	0.7060	0.4560
u	0.7360	0.4070
v	0.7780	0.4320
w	0.5870	0.3920
x	0.6910	0.3720
y	0.5980	0.3680
z	0.7000	0.3950