Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 04:15 AM JST

PDB ID	:	6KAD / pdb_00006kad
EMDB ID	:	EMD-9956
Title	:	Cryo-EM structure of the C2S2M2L2-type PSII-LHCII supercomplex from Chlamydomonas reihardtii
Authors	:	Sheng, X.; Watanabe, A.; Li, A.J.; Kim, E.; Song, C.; Murata, K.; Song, D.F.; Minagawa, J.; Liu, Z.F.
Deposited on	:	2019-06-21
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

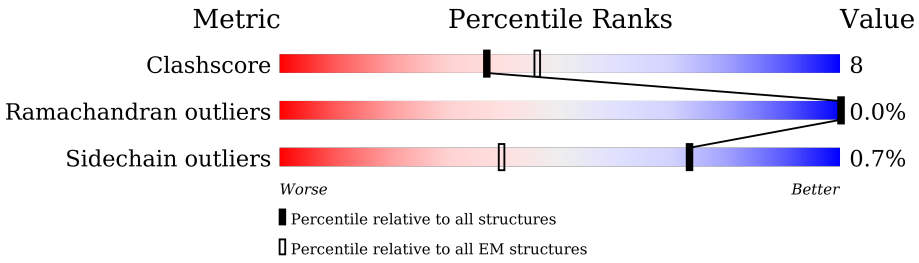
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

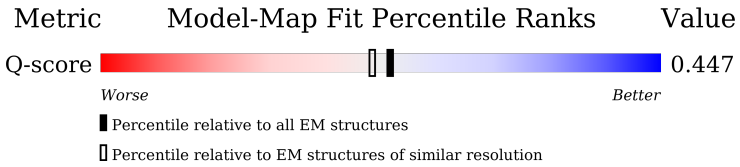
1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	0	256	8% 63% 21% 16%
1	1	256	76% 9% 15%
1	6	256	11% 62% 23% 16%
1	7	256	74% 11% 15%

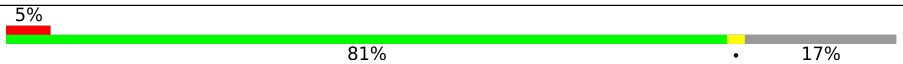
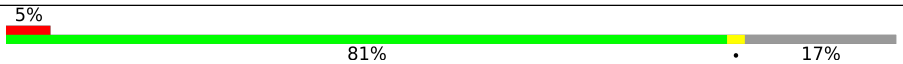
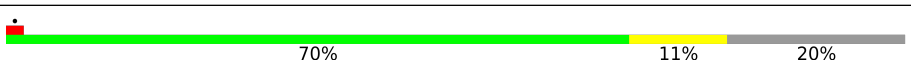
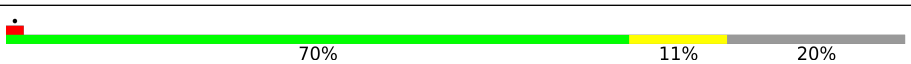
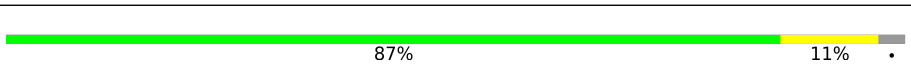
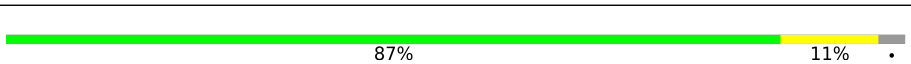
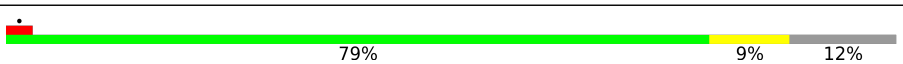
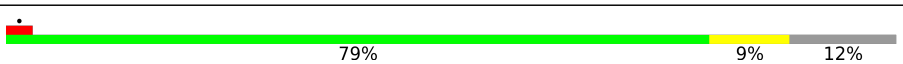
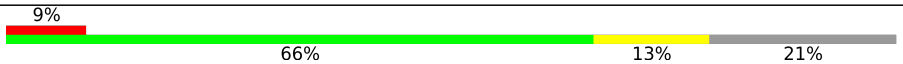
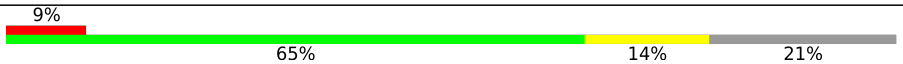
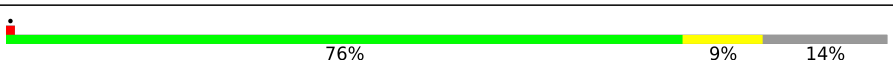
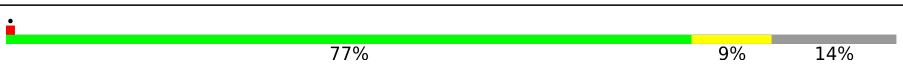
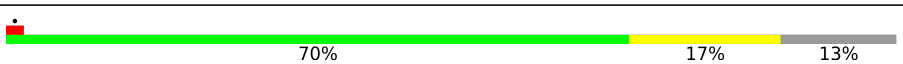
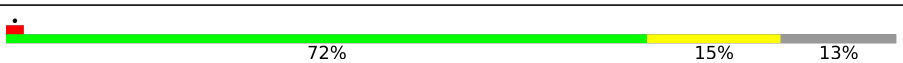
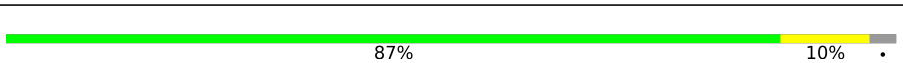
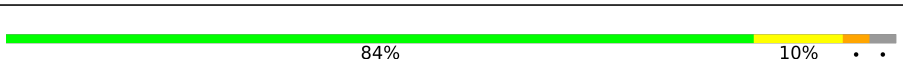
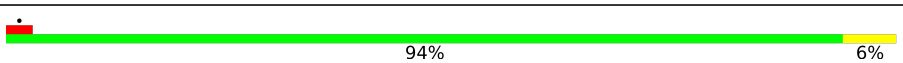
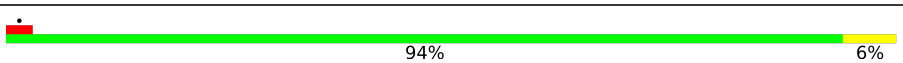
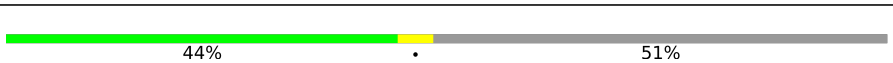
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Mol	Chain	Length	Quality of chain
1	Y	256	79% 8% 14%
1	y	256	78% 9% 14%
2	2	257	19% 70% 15% 15%
2	3	257	12% 68% 17% 15%
2	5	257	48% 69% 15% 16%
2	8	257	11% 68% 17% 15%
2	9	257	19% 68% 16% 15%
2	N	257	72% 12% 15%
2	n	257	71% 14% 15%
2	p	257	49% 71% 13% 16%
3	4	249	27% 68% 19% 13%
3	G	249	80% 8% 12%
3	g	249	76% 12% 12%
3	q	249	30% 77% 10% 13%
4	A	352	83% 12% 5%
4	a	352	83% 12% 5%
5	B	508	85% 11%
5	b	508	85% 11%
6	C	461	84% 13%
6	c	461	85% 13%
7	D	352	85% 13%
7	d	352	85% 13%
8	E	82	78% 15% 7%
8	e	82	79% 13% 7%
9	F	44	52% 16% 30%

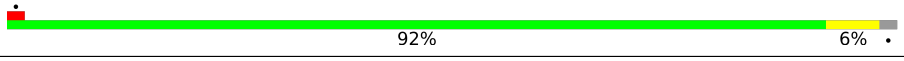
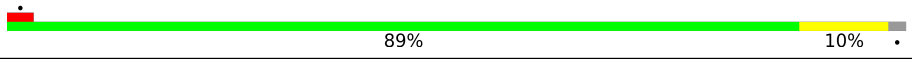
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Mol	Chain	Length	Quality of chain
9	f	44	
10	H	88	
10	h	88	
11	I	37	
11	i	37	
12	J	42	
12	j	42	
13	K	46	
13	k	46	
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	291	
16	o	291	
17	R	280	
17	r	280	
18	S	289	
18	s	289	
19	T	31	
19	t	31	
20	V	33	
20	v	33	
21	W	115	
21	w	115	

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Mol	Chain	Length	Quality of chain
22	X	101	
22	x	101	
23	Z	62	
23	z	62	

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
38	BCT	D	401	-	-	X	-
38	BCT	d	401	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 105342 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	6	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
1	0	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	7	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	3	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	5	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
2	8	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	9	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	p	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
3	q	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		
4	a	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		
5	b	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		
6	c	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		
7	d	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	76	Total 619	C 404	N 102	O 113	0	0
8	e	76	Total 619	C 404	N 102	O 113	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total 251	C 171	N 42	O 37	S 1	0	0
9	f	31	Total 251	C 171	N 42	O 37	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	68	Total 519	C 347	N 77	O 93	S 2	0	0
10	h	68	Total 519	C 347	N 77	O 93	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total 283	C 193	N 43	O 45	S 2	0	0
11	i	35	Total 283	C 193	N 43	O 45	S 2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total 255	C 174	N 39	O 42	0	0
12	j	35	Total 255	C 174	N 39	O 42	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	K	37	Total 297	C 209	N 43	O 45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	k	37	Total 297	C 209	N 43	O 45	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total 306	C 205	N 50	O 51	0	0
14	l	37	Total 306	C 205	N 50	O 51	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	30	Total 230	C 158	N 32	O 40	0	0
15	m	30	Total 230	C 158	N 32	O 40	0	0

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	230	Total 1742	C 1109	N 278	O 351	S 4	0	0
16	o	230	Total 1742	C 1109	N 278	O 351	S 4	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	240	Total 1826	C 1156	N 313	O 352	S 5	0	0
17	r	240	Total 1826	C 1156	N 313	O 352	S 5	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	252	Total 1907	C 1232	N 312	O 359	S 4	0	0
18	s	252	Total 1907	C 1232	N 312	O 359	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
19	t	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	33	Total	C	N	O	S	0	0
			232	152	38	41	1		
20	v	33	Total	C	N	O	S	0	0
			232	152	38	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		
21	w	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

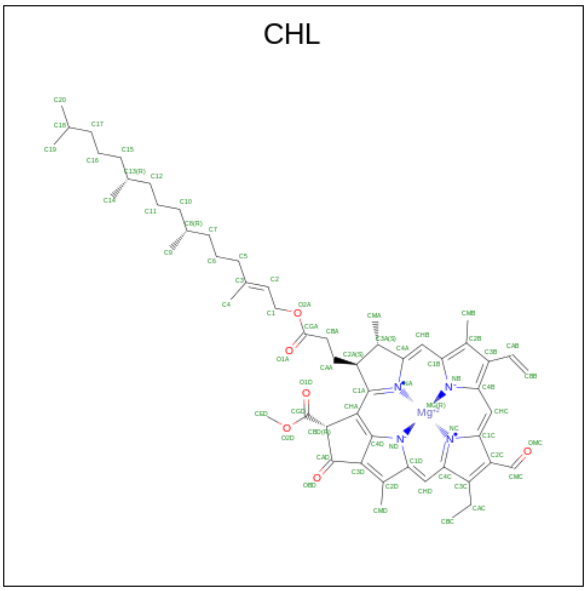
- Molecule 22 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	34	Total	C	N	O	0	0
			233	153	37	43		
22	x	34	Total	C	N	O	0	0
			233	153	37	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
23	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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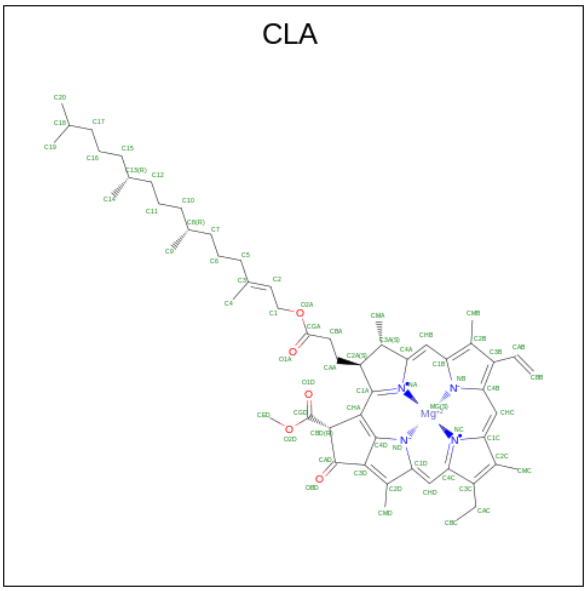
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	0	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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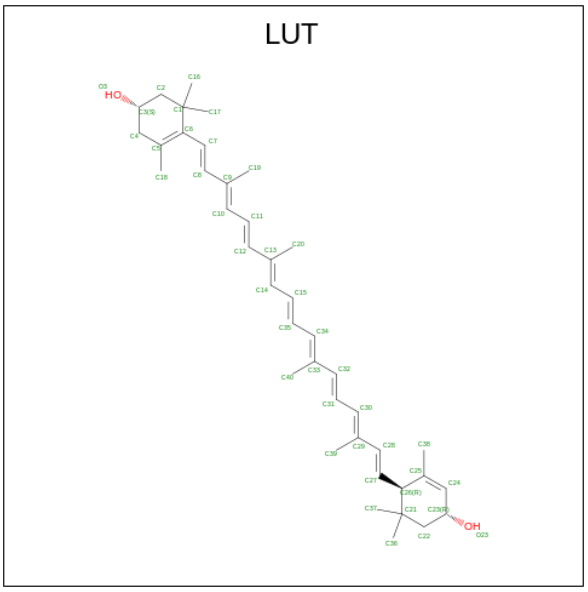
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	

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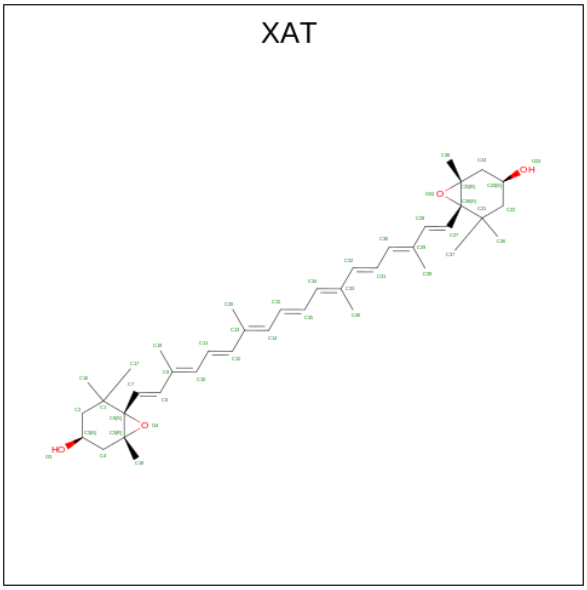
Mol	Chain	Residues	Atoms			AltConf
26	N	1	Total	C	O	0
			42	40	2	
26	N	1	Total	C	O	0
			42	40	2	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	
26	Y	1	Total	C	O	0
			42	40	2	
26	Y	1	Total	C	O	0
			42	40	2	
26	0	1	Total	C	O	0
			42	40	2	
26	0	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	8	1	Total	C	O	0
			42	40	2	
26	8	1	Total	C	O	0
			42	40	2	
26	9	1	Total	C	O	0
			42	40	2	
26	9	1	Total	C	O	0
			42	40	2	
26	p	1	Total	C	O	0
			42	40	2	
26	p	1	Total	C	O	0
			42	40	2	
26	q	1	Total	C	O	0
			42	40	2	
26	q	1	Total	C	O	0
			42	40	2	
26	g	1	Total	C	O	0
			42	40	2	
26	g	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
26	n	1	Total C O 42 40 2	0
26	n	1	Total C O 42 40 2	0
26	s	1	Total C O 42 40 2	0
26	s	1	Total C O 42 40 2	0
26	y	1	Total C O 42 40 2	0
26	y	1	Total C O 42 40 2	0
26	r	1	Total C O 42 40 2	0

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



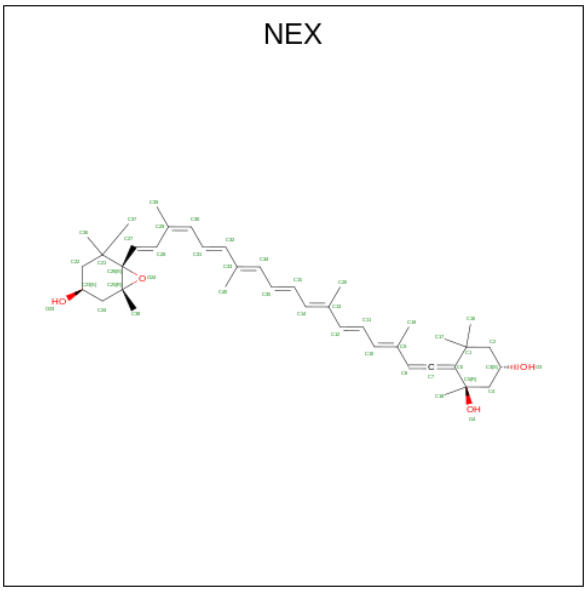
Mol	Chain	Residues	Atoms	AltConf
27	1	1	Total C O 44 40 4	0
27	2	1	Total C O 44 40 4	0
27	3	1	Total C O 44 40 4	0
27	4	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	0	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	9	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	q	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	
27	y	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



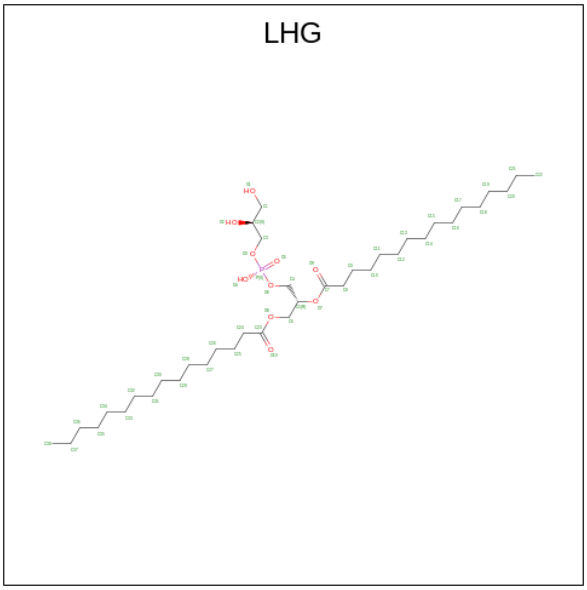
Mol	Chain	Residues	Atoms	AltConf
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	4	1	Total C O 44 40 4	0
28	5	1	Total C O 44 40 4	0
28	6	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	R	1	Total C O 44 40 4	0
28	S	1	Total C O 44 40 4	0
28	Y	1	Total C O 44 40 4	0
28	0	1	Total C O 44 40 4	0
28	7	1	Total C O 44 40 4	0
28	8	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
28	9	1	Total C O 44 40 4	0
28	p	1	Total C O 44 40 4	0
28	q	1	Total C O 44 40 4	0
28	g	1	Total C O 44 40 4	0
28	n	1	Total C O 44 40 4	0
28	s	1	Total C O 44 40 4	0
28	y	1	Total C O 44 40 4	0
28	r	1	Total C O 44 40 4	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O P 49 38 10 1	0
29	2	1	Total C O P 49 38 10 1	0
29	3	1	Total C O P 49 38 10 1	0

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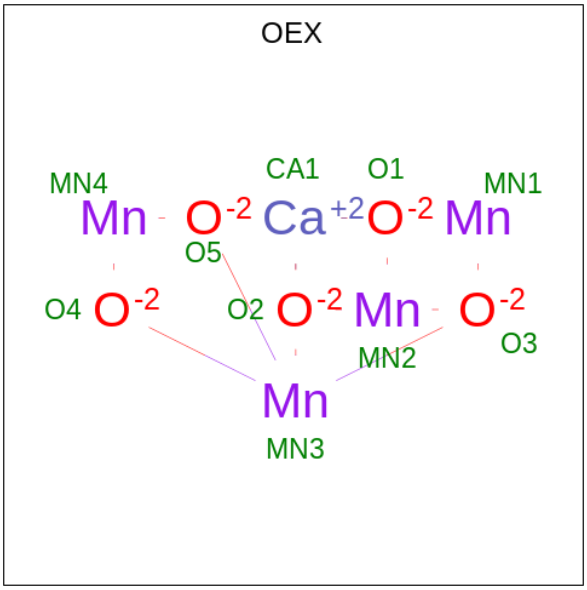
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	6	1	Total	C	O	P	0
			49	38	10	1	
29	C	1	Total	C	O	P	0
			47	36	10	1	
29	D	1	Total	C	O	P	0
			44	33	10	1	
29	D	1	Total	C	O	P	0
			49	38	10	1	
29	D	1	Total	C	O	P	0
			39	28	10	1	
29	G	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	N	1	Total	C	O	P	0
			49	38	10	1	
29	R	1	Total	C	O	P	0
			38	27	10	1	
29	S	1	Total	C	O	P	0
			45	34	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	0	1	Total	C	O	P	0
			49	38	10	1	
29	7	1	Total	C	O	P	0
			49	38	10	1	
29	8	1	Total	C	O	P	0
			49	38	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	p	1	Total	C	O	P	0
			49	38	10	1	
29	q	1	Total	C	O	P	0
			49	38	10	1	
29	c	1	Total	C	O	P	0
			47	36	10	1	
29	d	1	Total	C	O	P	0
			44	33	10	1	

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Mol	Chain	Residues	Atoms				AltConf
29	d	1	Total	C	O	P	0
			49	38	10	1	
29	d	1	Total	C	O	P	0
			39	28	10	1	
29	g	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	
29	n	1	Total	C	O	P	0
			49	38	10	1	
29	s	1	Total	C	O	P	0
			45	34	10	1	
29	y	1	Total	C	O	P	0
			49	38	10	1	
29	r	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

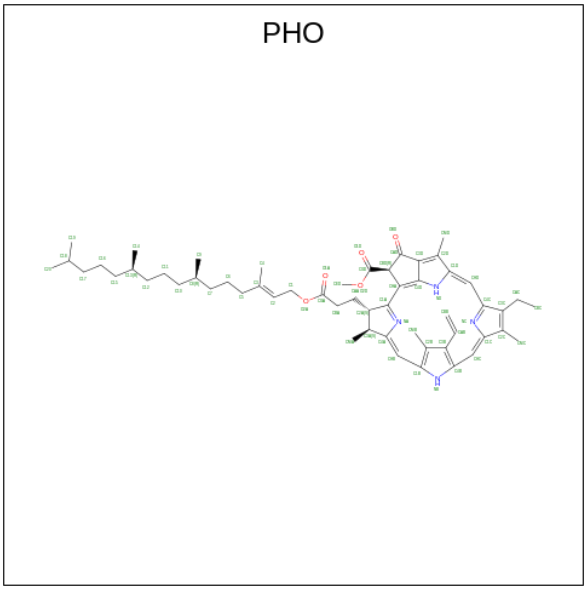
- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

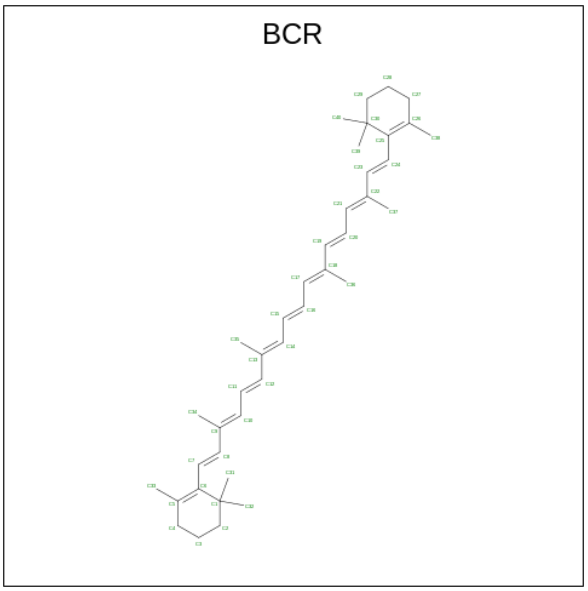
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Cl 1 1	0
32	a	1	Total Cl 1 1	0

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



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

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



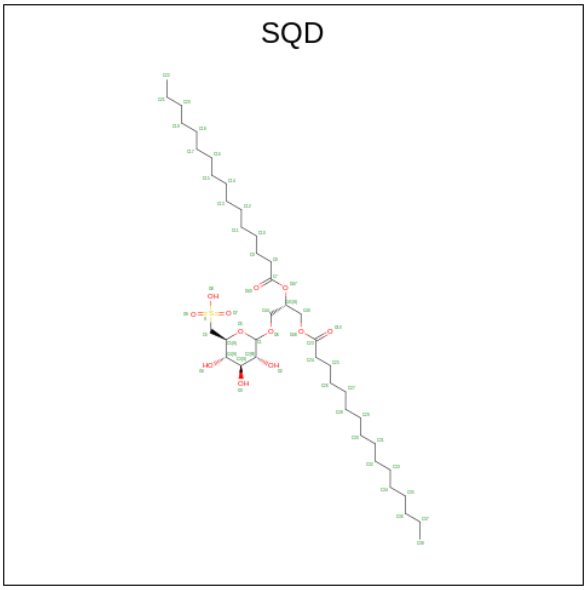
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	D	1	Total C 40 40	0
34	H	1	Total C 40 40	0
34	a	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	d	1	Total C 40 40	0
34	h	1	Total C 40 40	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



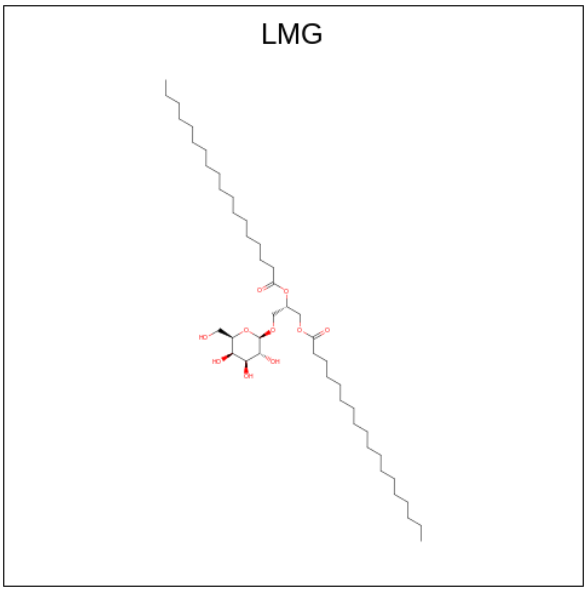
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C O S 51 38 12 1	0
35	B	1	Total C O S 54 41 12 1	0
35	B	1	Total C O S 50 37 12 1	0
35	D	1	Total C O S 52 39 12 1	0
35	a	1	Total C O S 51 38 12 1	0

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Mol	Chain	Residues	Atoms	AltConf
35	b	1	Total C O S 54 41 12 1	0
35	b	1	Total C O S 50 37 12 1	0
35	d	1	Total C O S 52 39 12 1	0

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



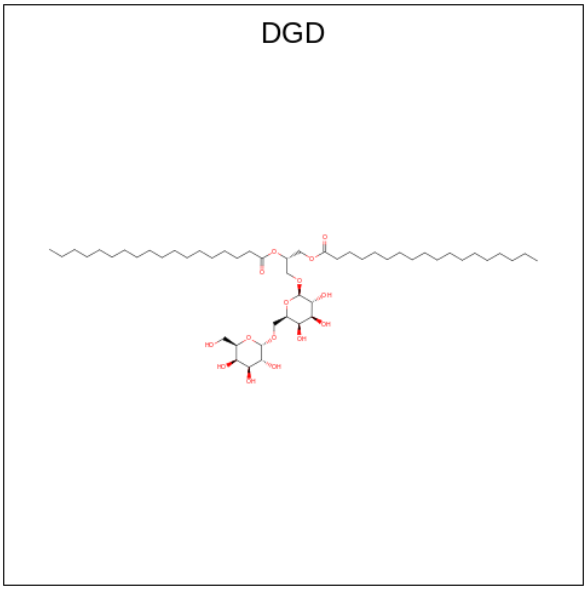
Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C O 48 38 10	0
36	B	1	Total C O 51 41 10	0
36	C	1	Total C O 51 41 10	0
36	D	1	Total C O 46 36 10	0
36	D	1	Total C O 46 36 10	0
36	H	1	Total C O 48 38 10	0
36	S	1	Total C O 52 42 10	0
36	a	1	Total C O 48 38 10	0

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Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total 51	C 41	O 10	0
36	c	1	Total 51	C 41	O 10	0
36	d	1	Total 46	C 36	O 10	0
36	d	1	Total 46	C 36	O 10	0
36	h	1	Total 48	C 38	O 10	0
36	s	1	Total 52	C 42	O 10	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



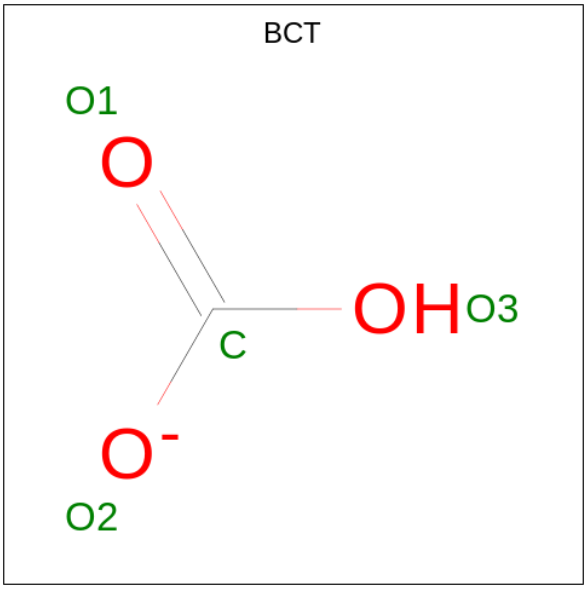
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total 55	C 40	O 15	0
37	C	1	Total 62	C 47	O 15	0
37	C	1	Total 59	C 44	O 15	0
37	C	1	Total 66	C 51	O 15	0
37	C	1	Total 66	C 51	O 15	0

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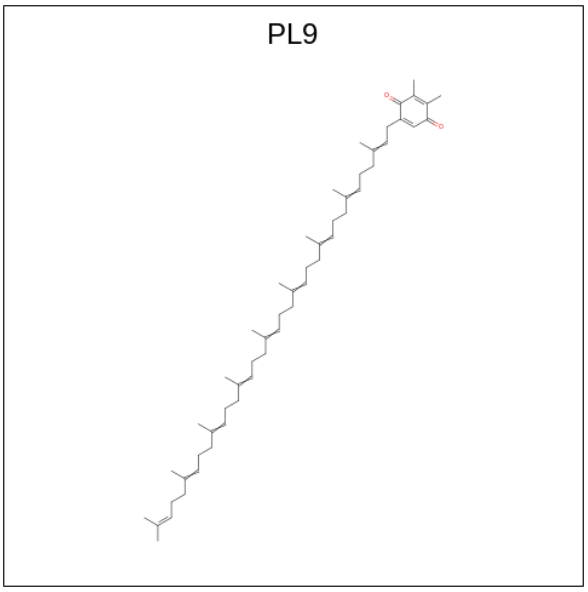
Mol	Chain	Residues	Atoms	AltConf
37	c	1	Total C O 55 40 15	0
37	c	1	Total C O 62 47 15	0
37	c	1	Total C O 59 44 15	0
37	c	1	Total C O 66 51 15	0
37	c	1	Total C O 66 51 15	0

- Molecule 38 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



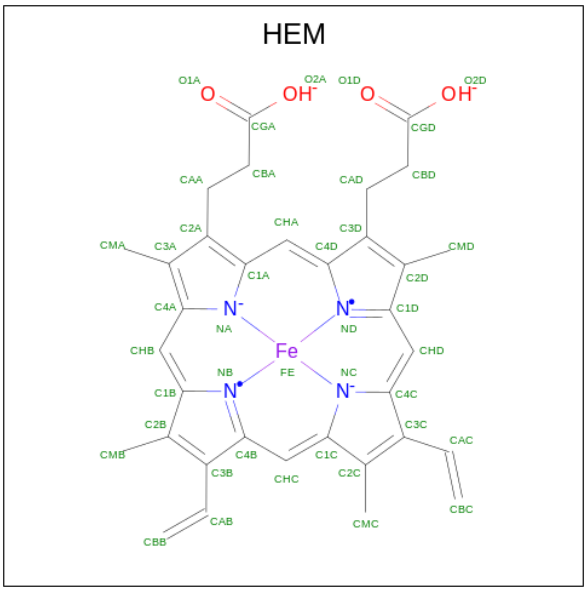
Mol	Chain	Residues	Atoms	AltConf
38	D	1	Total C O 4 1 3	0
38	d	1	Total C O 4 1 3	0

- Molecule 39 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
39	D	1	Total C O 55 53 2	0
39	d	1	Total C O 55 53 2	0

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	AltConf
40	F	1	Total C Fe N O 43 34 1 4 4	0

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Mol	Chain	Residues	Atoms					AltConf
40	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

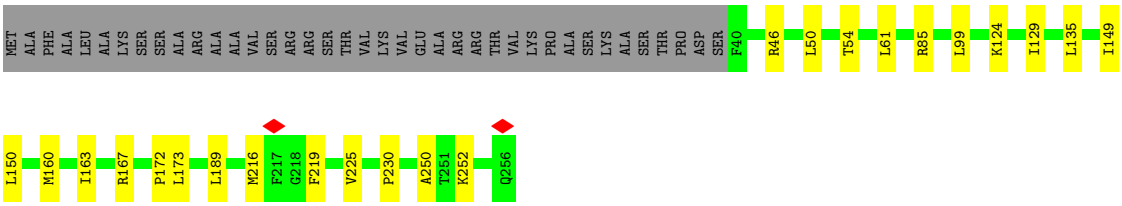
3 Residue-property plots (i)

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: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

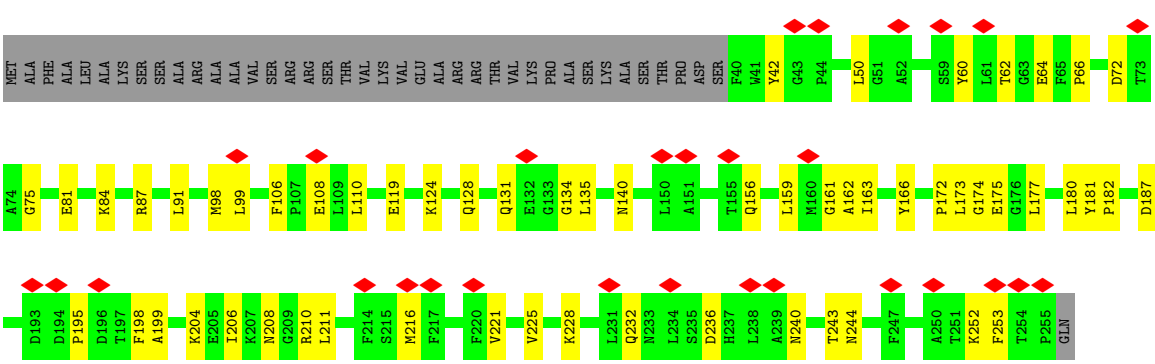




• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

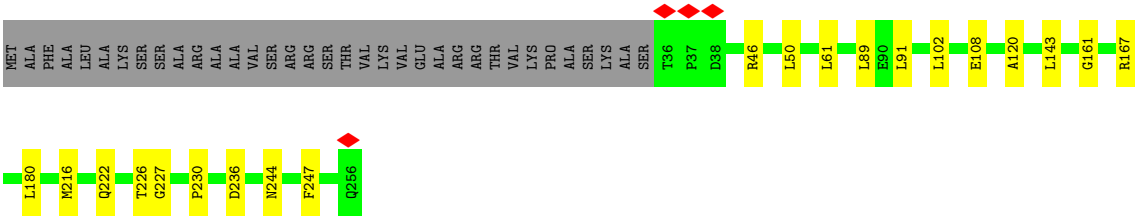




• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain Y:

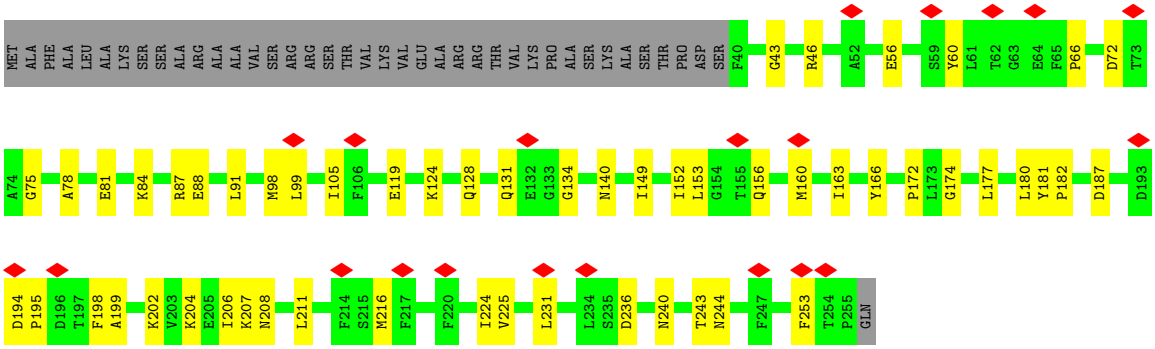




• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 0:

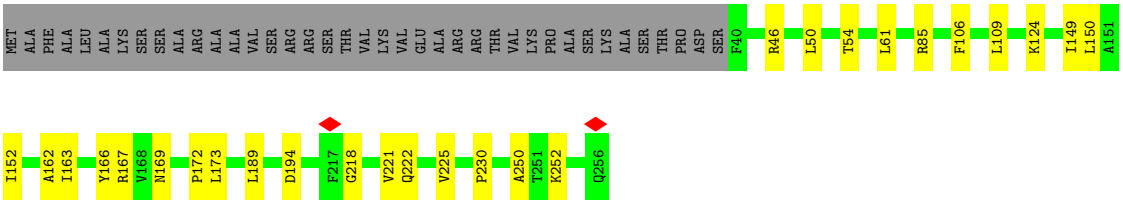




• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

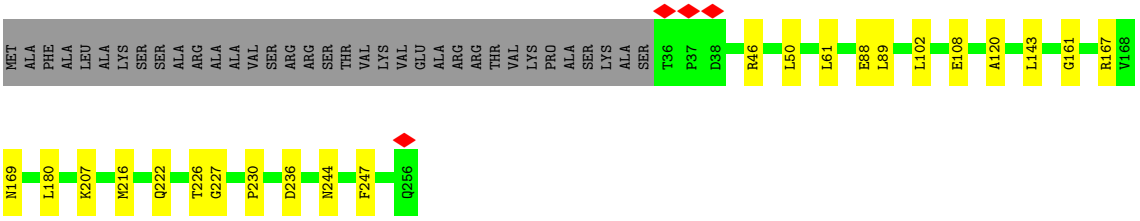




• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain y:

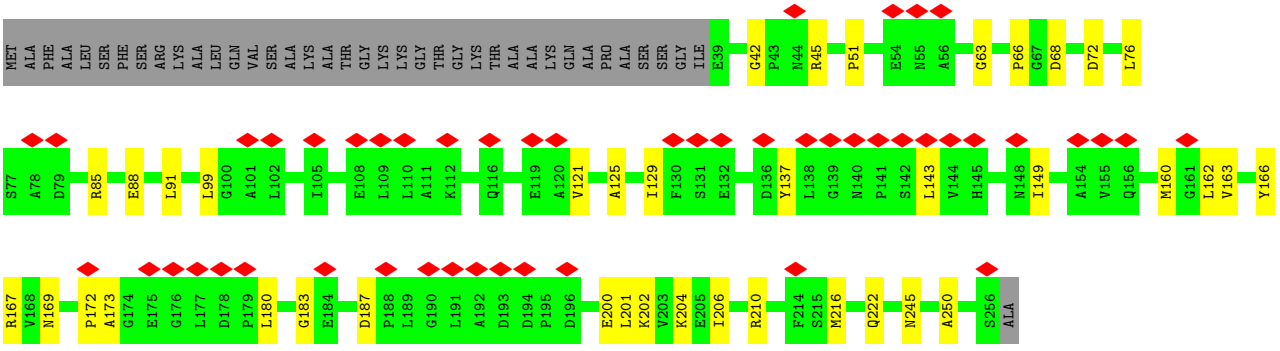




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

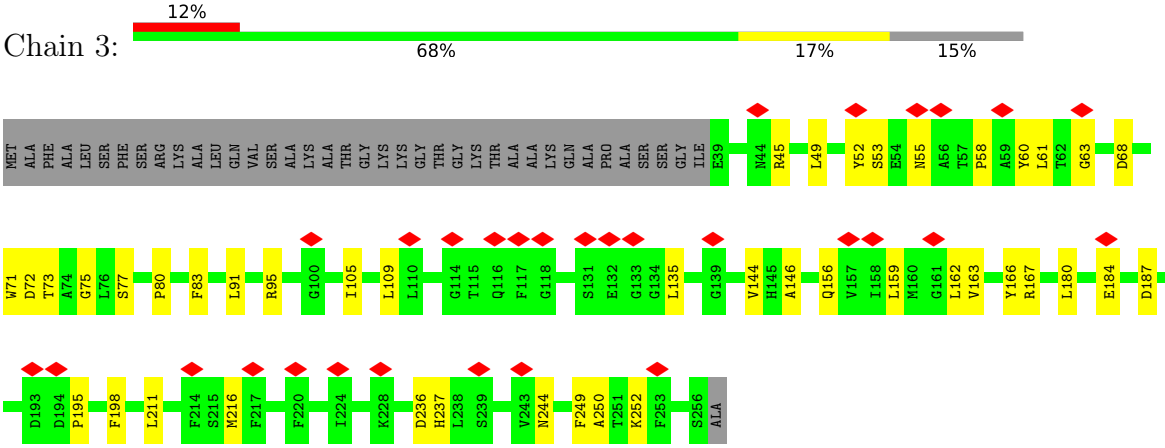
Chain 2:





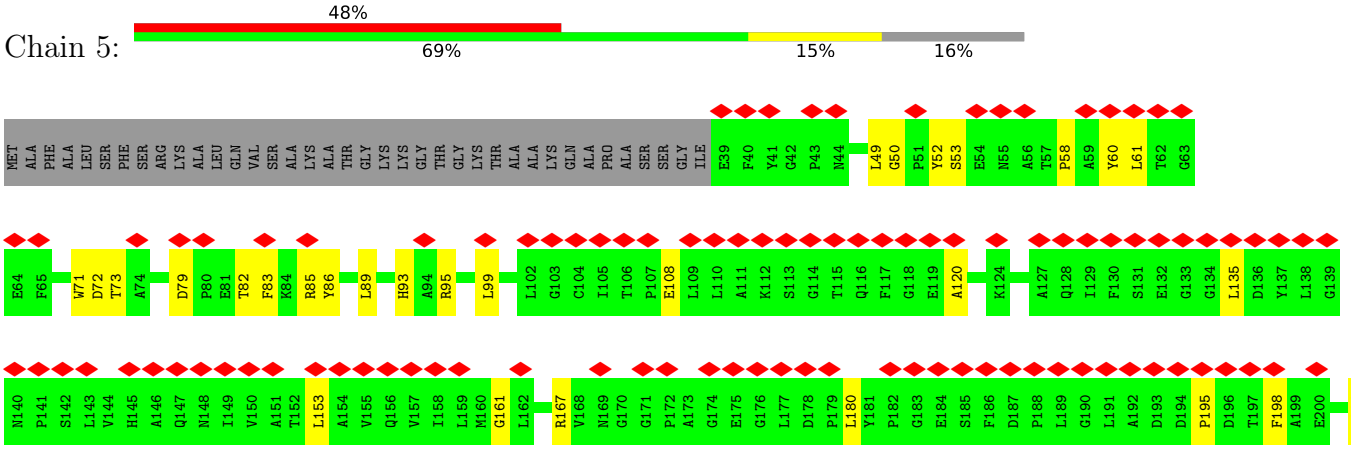
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



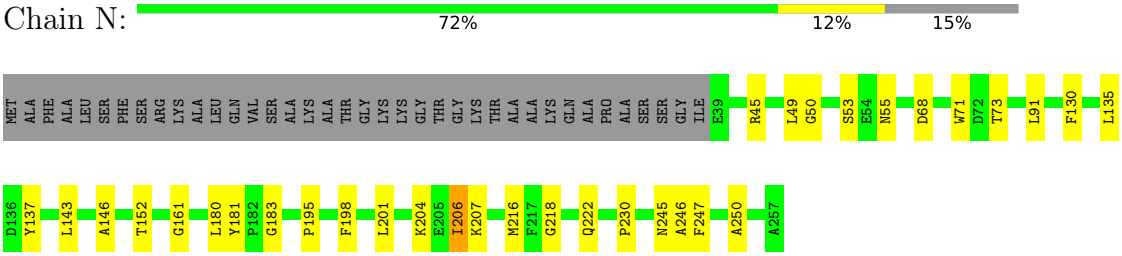
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



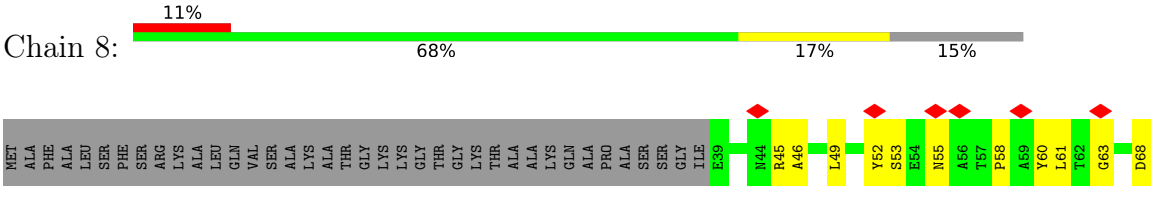
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

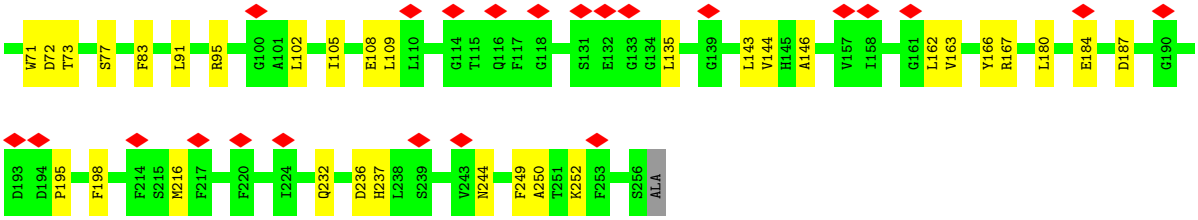
Chain N:



• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

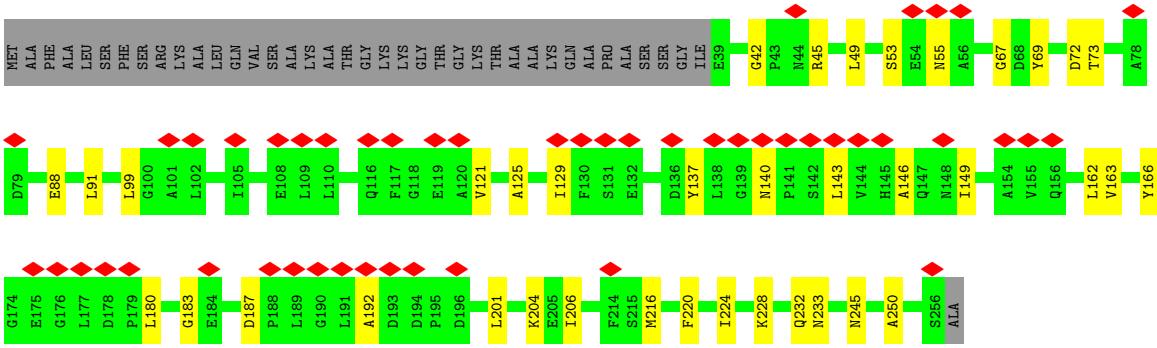
Chain 8:





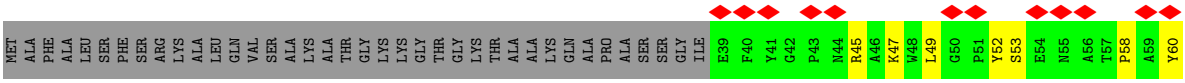
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

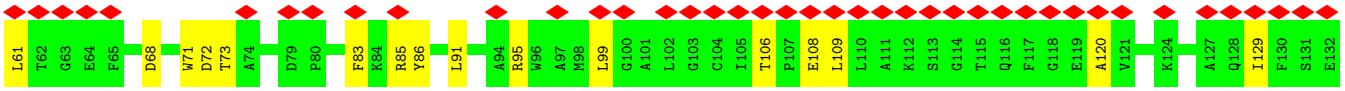


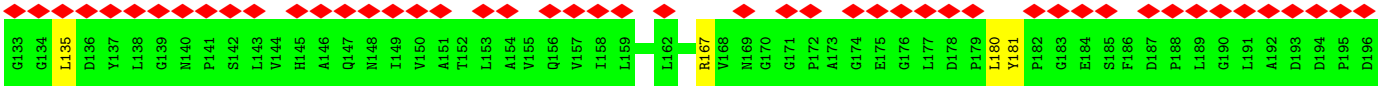


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

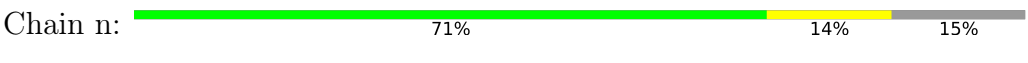


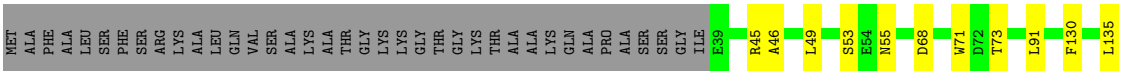






• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

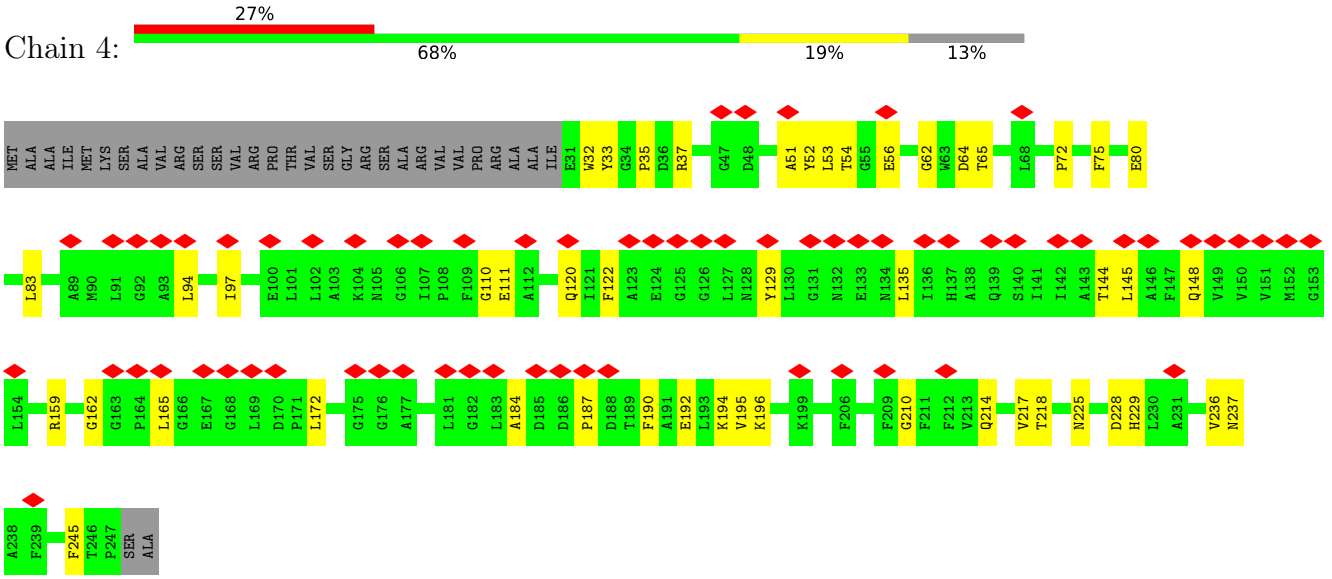






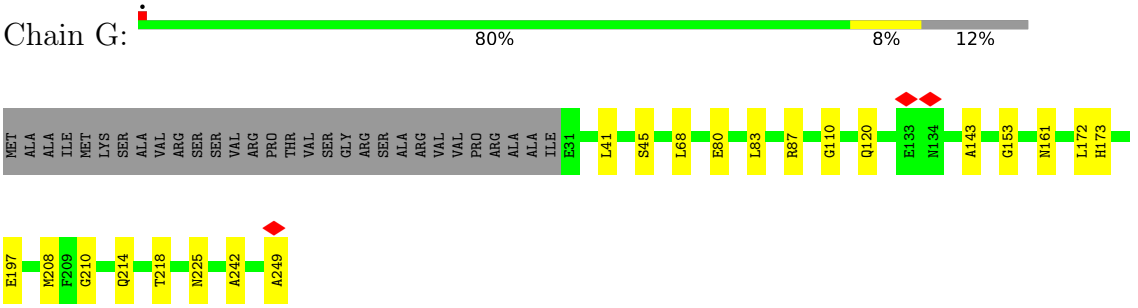
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



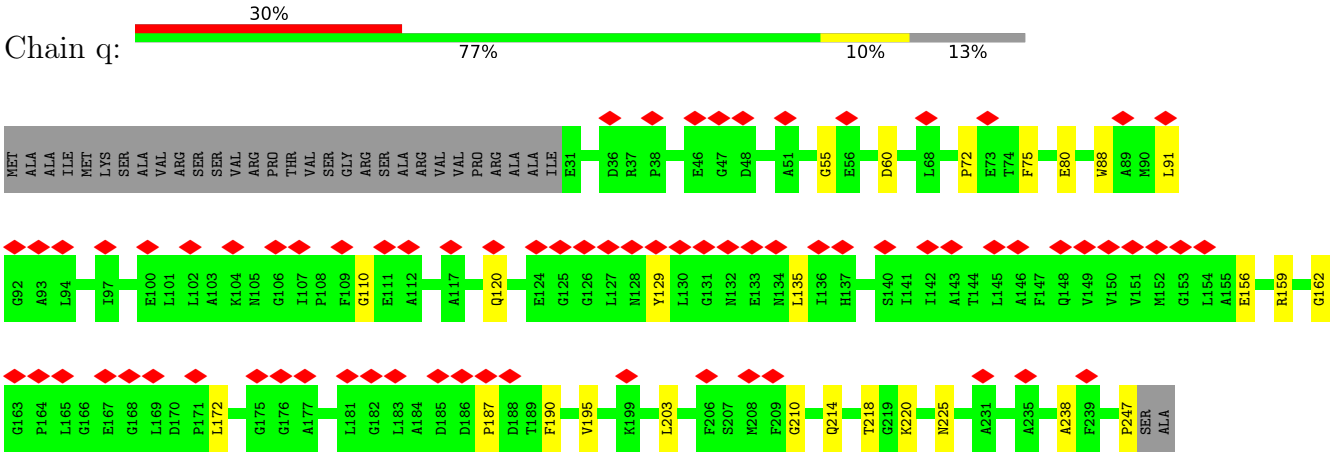
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain G:



• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

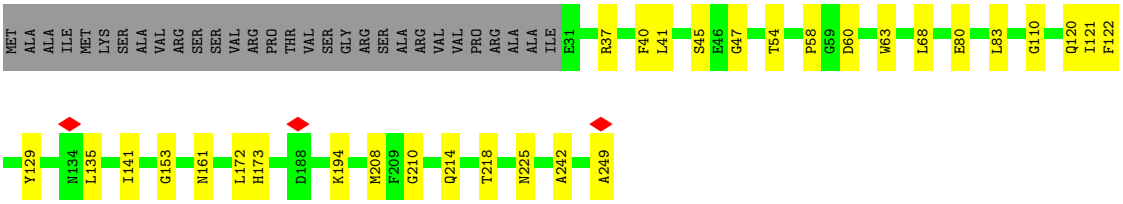
Chain q:



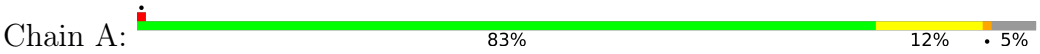
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

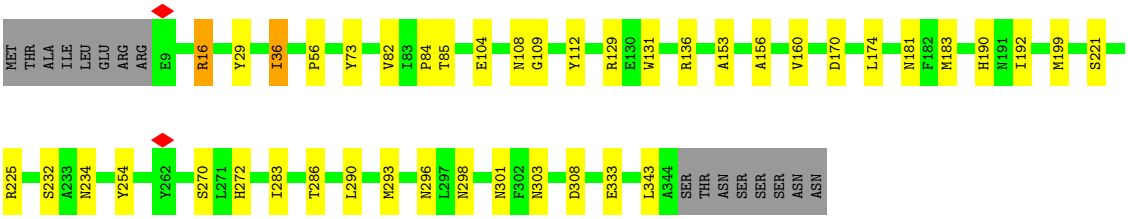
Chain g:



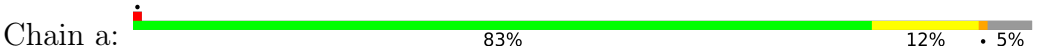


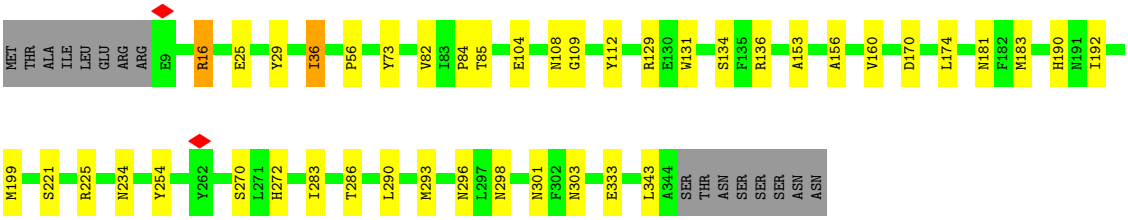
• Molecule 4: Photosystem II protein D1



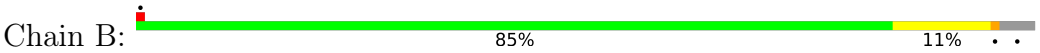


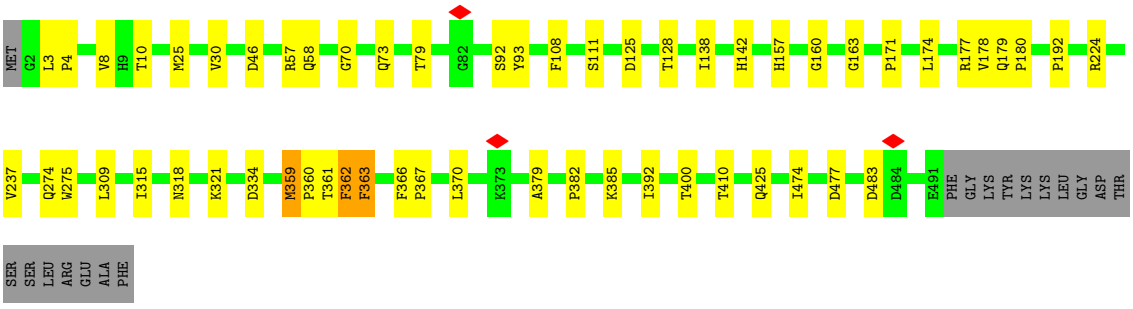
• Molecule 4: Photosystem II protein D1



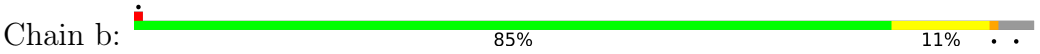


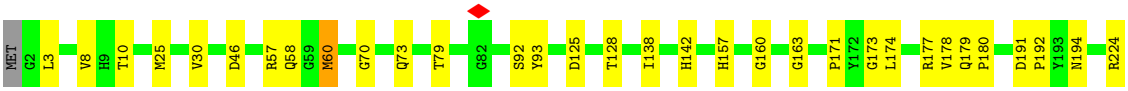
• Molecule 5: Photosystem II CP47 reaction center protein

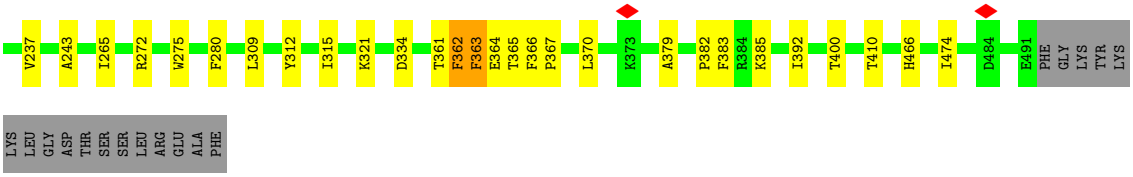




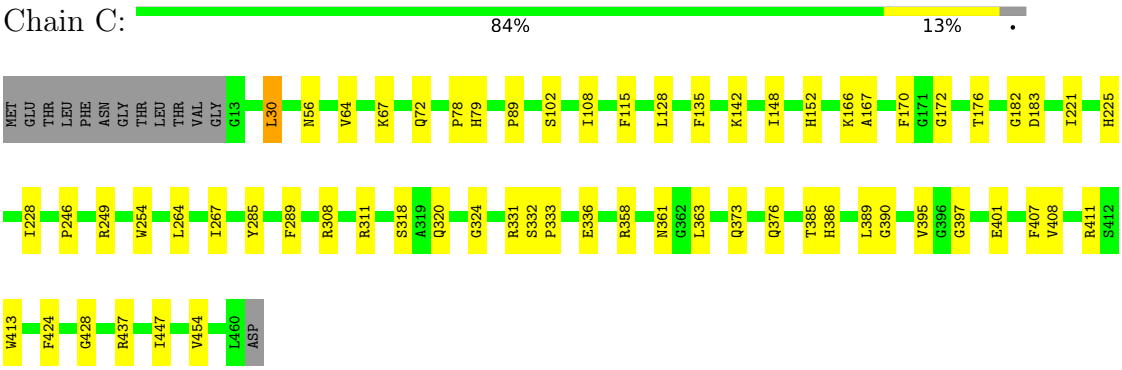
• Molecule 5: Photosystem II CP47 reaction center protein



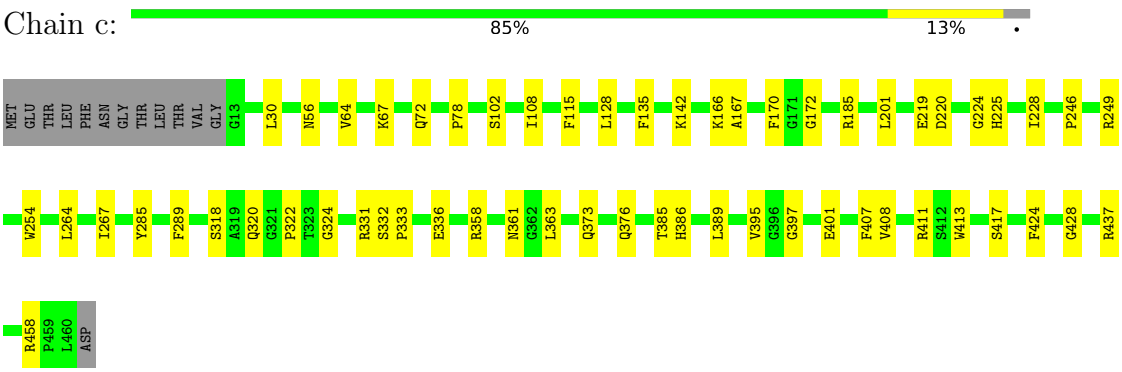




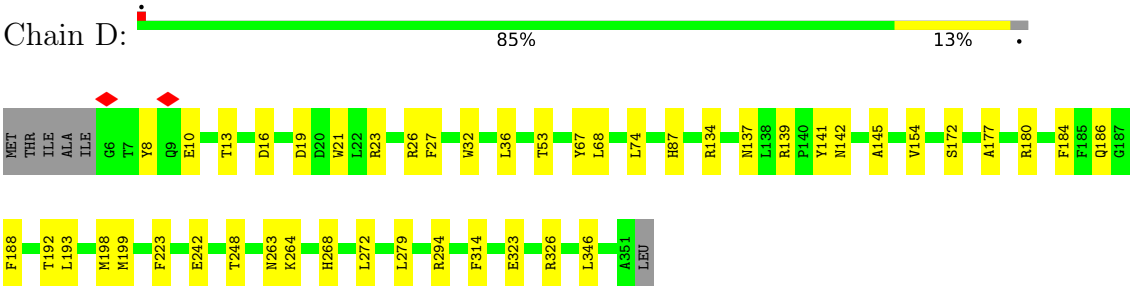
• Molecule 6: Photosystem II CP43 reaction center protein



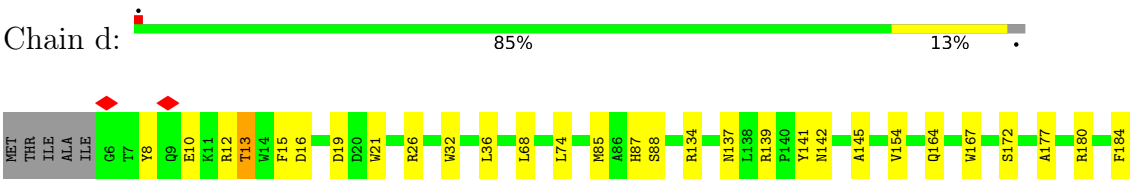
• Molecule 6: Photosystem II CP43 reaction center protein

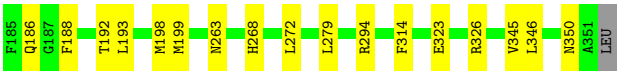


• Molecule 7: Photosystem II D2 protein



• Molecule 7: Photosystem II D2 protein





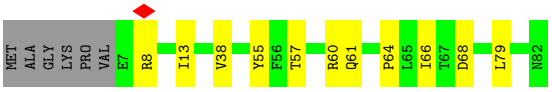
• Molecule 8: Cytochrome b559 subunit alpha





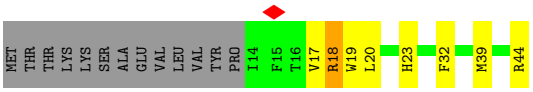
• Molecule 8: Cytochrome b559 subunit alpha





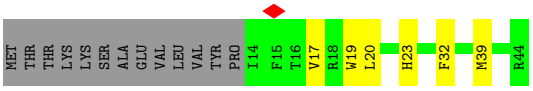
• Molecule 9: Cytochrome b559 subunit beta





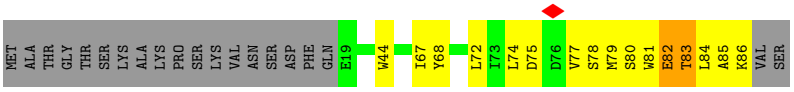
• Molecule 9: Cytochrome b559 subunit beta





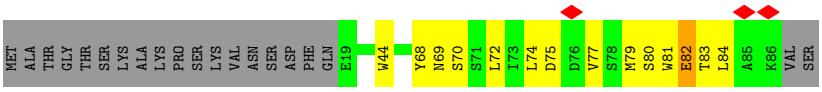
• Molecule 10: Photosystem II reaction center protein H





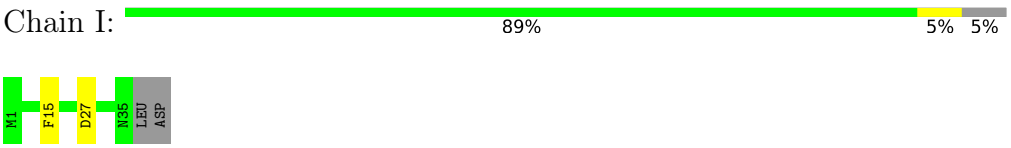
• Molecule 10: Photosystem II reaction center protein H





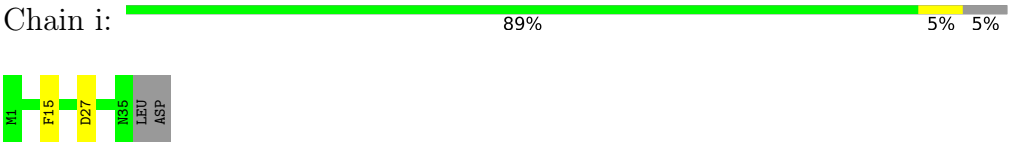
• Molecule 11: Photosystem II reaction center protein I

Chain I:



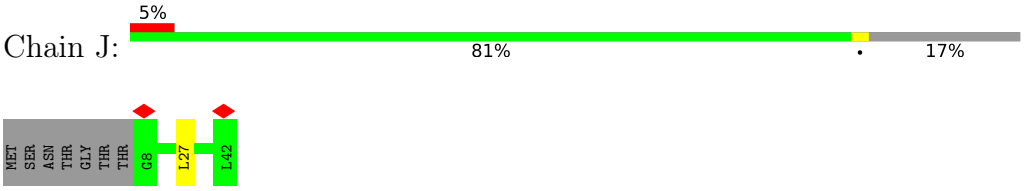
• Molecule 11: Photosystem II reaction center protein I

Chain i:



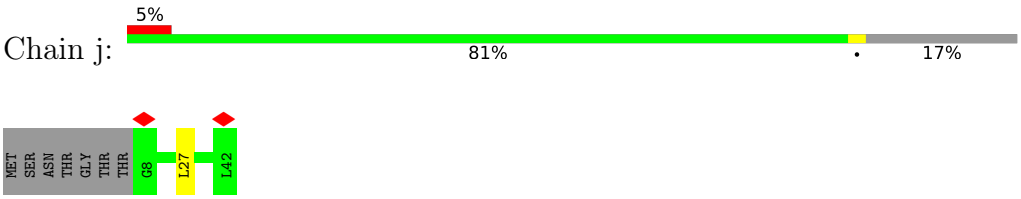
• Molecule 12: Photosystem II reaction center protein J

Chain J:



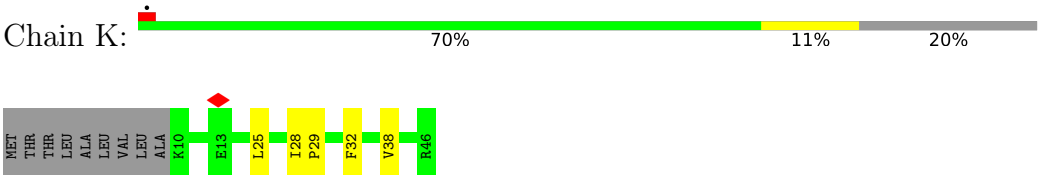
• Molecule 12: Photosystem II reaction center protein J

Chain j:



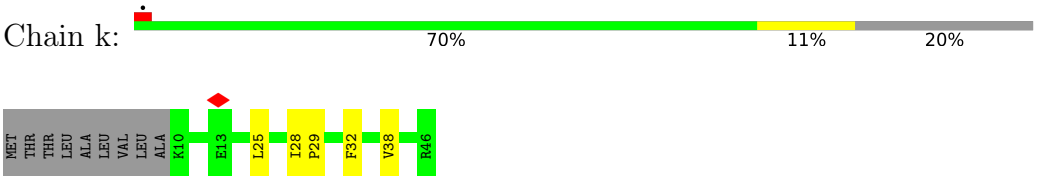
• Molecule 13: Photosystem II reaction center protein K

Chain K:



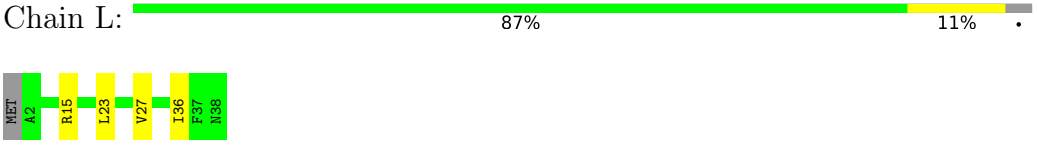
• Molecule 13: Photosystem II reaction center protein K

Chain k:



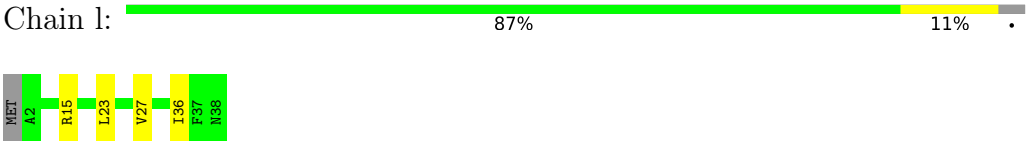
• Molecule 14: Photosystem II reaction center protein L

Chain L:



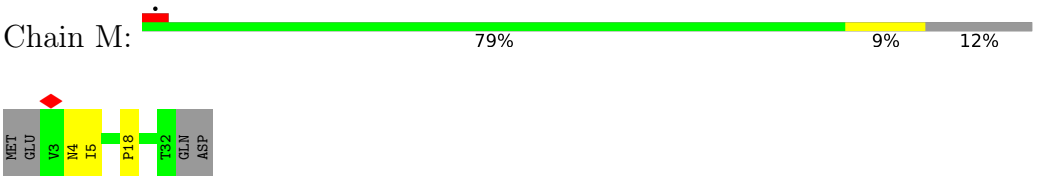
• Molecule 14: Photosystem II reaction center protein L

Chain l:



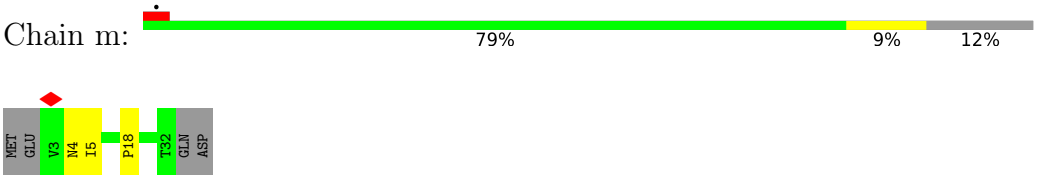
• Molecule 15: Photosystem II reaction center protein M

Chain M:



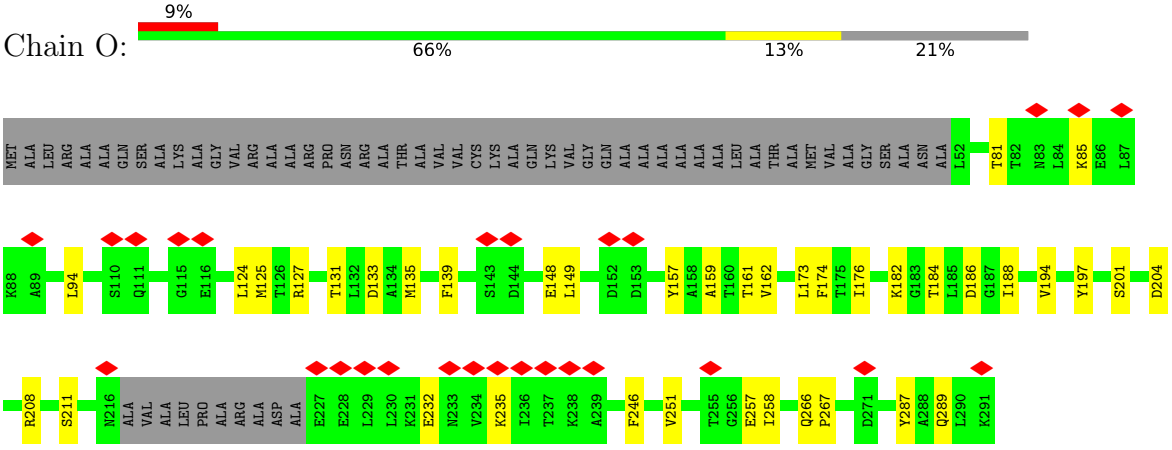
• Molecule 15: Photosystem II reaction center protein M

Chain m:



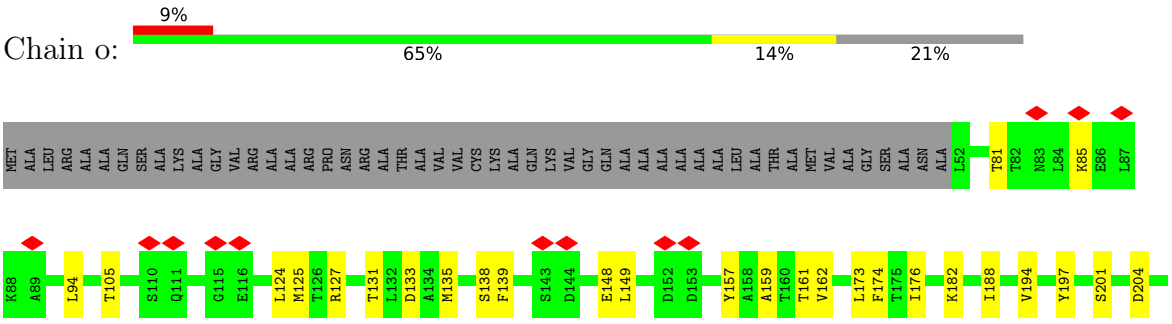
• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

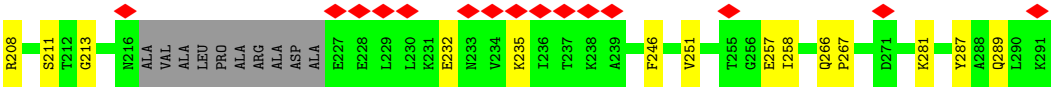
Chain O:



• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:

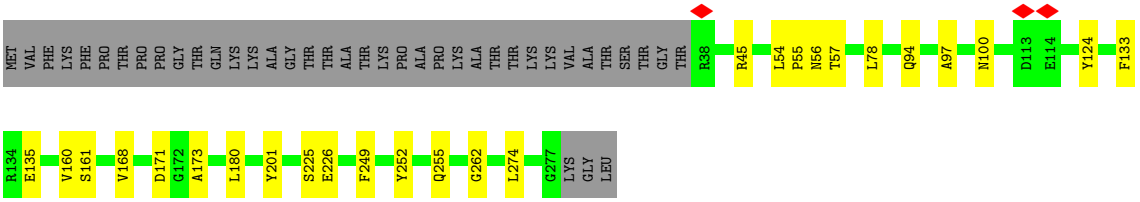




• Molecule 17: Chlorophyll a-b binding protein CP29

Chain R:

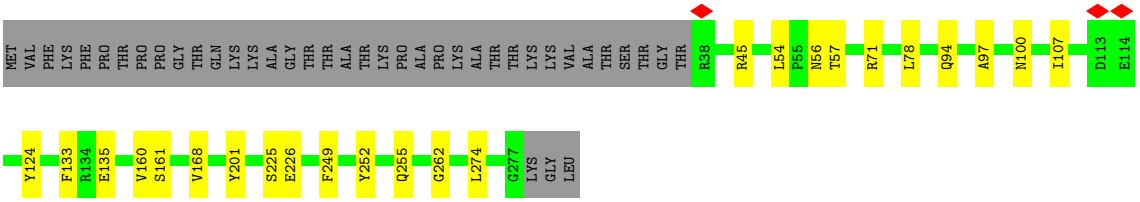




• Molecule 17: Chlorophyll a-b binding protein CP29

Chain r:

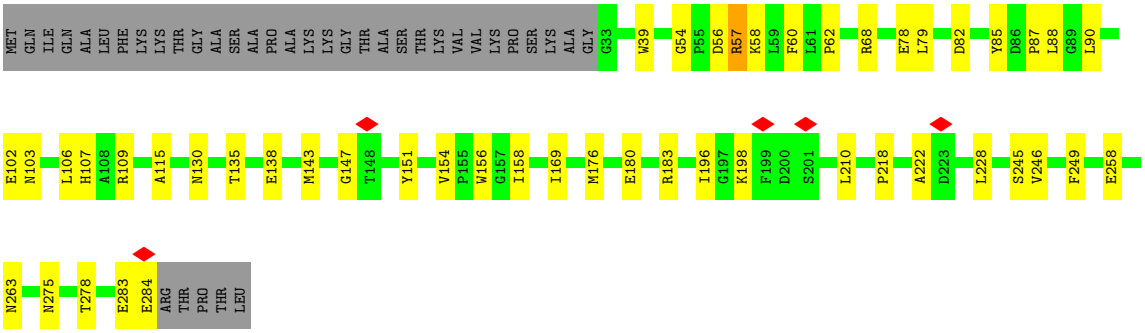




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain S:

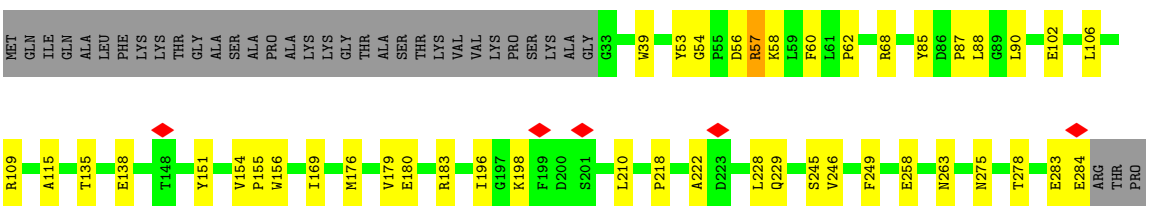




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain s:



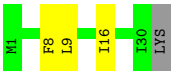




• Molecule 19: Photosystem II reaction center protein T

Chain T:

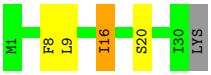




• Molecule 19: Photosystem II reaction center protein T

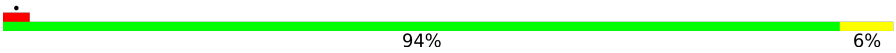
Chain t:





• Molecule 20: Photosystem II reaction center protein Ycf12

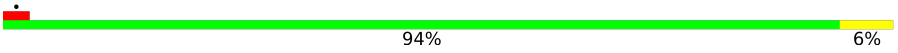
Chain V:





• Molecule 20: Photosystem II reaction center protein Ycf12

Chain v:



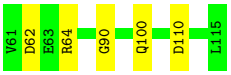


• Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W:





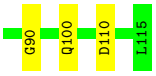


• Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain w:

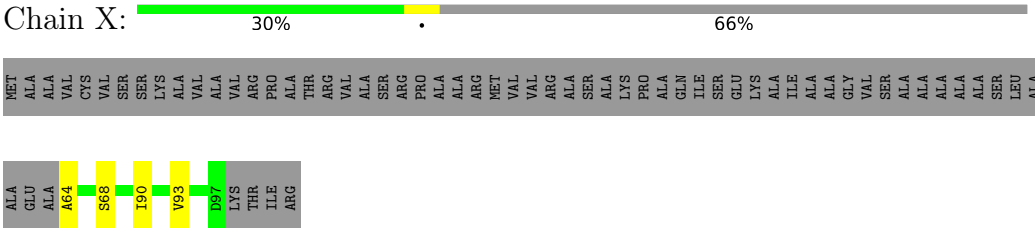






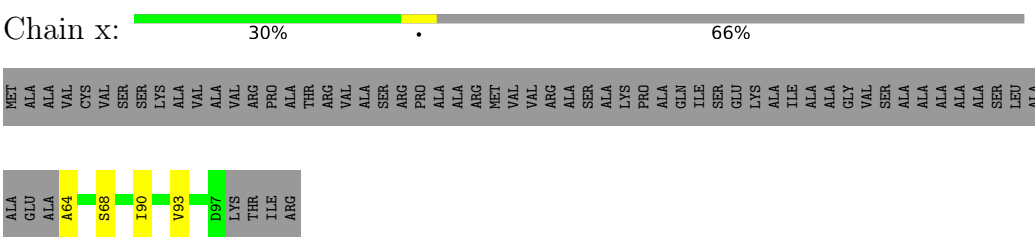
• Molecule 22: 4.1 kDa photosystem II subunit

Chain X:



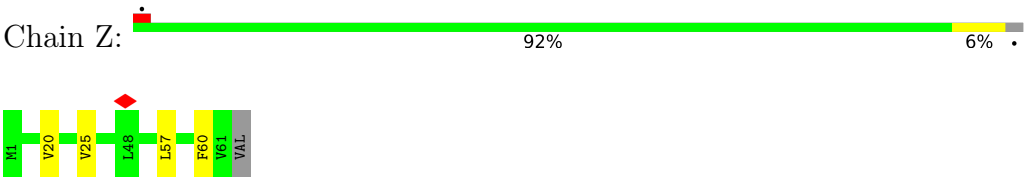
• Molecule 22: 4.1 kDa photosystem II subunit

Chain x:



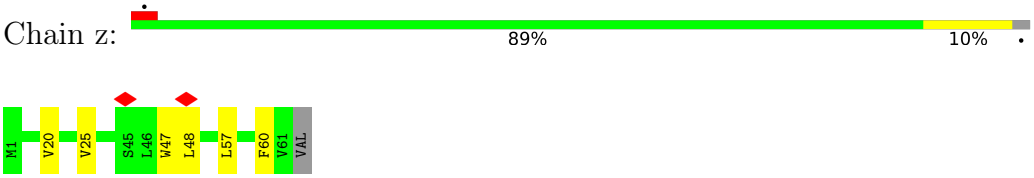
• Molecule 23: Photosystem II reaction center protein Z

Chain Z:



• Molecule 23: Photosystem II reaction center protein Z

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	118423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.31	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0	0.22	0/1708	0.51	1/2322 (0.0%)
1	1	0.28	0/1717	0.54	0/2334
1	6	0.23	0/1708	0.51	0/2322
1	7	0.27	0/1717	0.53	0/2334
1	Y	0.41	0/1746	0.52	0/2375
1	y	0.40	0/1746	0.52	0/2375
2	2	0.22	0/1715	0.49	0/2334
2	3	0.19	0/1715	0.49	0/2334
2	5	0.19	0/1709	0.50	0/2326
2	8	0.19	0/1715	0.48	0/2334
2	9	0.23	0/1715	0.52	0/2334
2	N	0.32	0/1720	0.53	0/2341
2	n	0.32	0/1720	0.54	0/2341
2	p	0.17	0/1709	0.46	0/2326
3	4	0.20	0/1706	0.49	0/2322
3	G	0.31	0/1717	0.54	0/2337
3	g	0.31	0/1717	0.53	0/2337
3	q	0.20	0/1706	0.50	0/2322
4	A	0.49	2/2718 (0.1%)	0.62	1/3706 (0.0%)
4	a	0.49	2/2718 (0.1%)	0.62	1/3706 (0.0%)
5	B	0.41	0/3964	0.54	0/5397
5	b	0.41	0/3964	0.55	2/5397 (0.0%)
6	C	0.40	0/3611	0.52	0/4920
6	c	0.39	0/3611	0.52	0/4920
7	D	0.47	0/2850	0.62	0/3887
7	d	0.47	0/2850	0.61	0/3887
8	E	0.28	0/637	0.54	0/869
8	e	0.28	0/637	0.54	0/869
9	F	0.44	0/258	0.71	0/349
9	f	0.44	0/258	0.72	0/349
10	H	0.48	0/530	0.64	0/725

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
10	h	0.47	0/530	0.64	0/725
11	I	0.45	0/291	0.56	0/394
11	i	0.45	0/291	0.56	0/394
12	J	0.29	0/261	0.47	0/356
12	j	0.28	0/261	0.48	0/356
13	K	0.38	0/309	0.74	0/425
13	k	0.38	0/309	0.74	0/425
14	L	0.45	0/314	0.59	0/427
14	l	0.45	0/314	0.59	0/427
15	M	0.43	0/234	0.54	0/321
15	m	0.42	0/234	0.55	0/321
16	O	0.24	0/1771	0.50	0/2386
16	o	0.24	0/1771	0.51	0/2386
17	R	0.33	0/1866	0.59	0/2529
17	r	0.33	0/1866	0.59	0/2529
18	S	0.34	0/1961	0.55	0/2670
18	s	0.35	0/1961	0.56	0/2670
19	T	0.38	0/254	0.58	0/343
19	t	0.39	0/254	0.59	0/343
20	V	0.22	0/232	0.48	0/317
20	v	0.21	0/232	0.47	0/317
21	W	0.35	0/445	0.55	0/603
21	w	0.35	0/445	0.54	0/603
22	X	0.29	0/235	0.48	0/319
22	x	0.29	0/235	0.49	0/319
23	Z	0.24	0/469	0.52	0/644
23	z	0.24	0/469	0.55	0/644
All	All	0.35	4/77326 (0.0%)	0.55	5/105224 (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
2	N	0	1
2	n	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	333	GLU	C-N	-7.66	1.23	1.33
4	a	333	GLU	C-N	-7.36	1.23	1.33
4	a	170	ASP	C-N	6.70	1.42	1.33
4	A	170	ASP	C-N	6.70	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	333	GLU	O-C-N	7.21	132.18	122.59
4	a	333	GLU	O-C-N	7.12	132.07	122.59
5	b	362	PHE	N-CA-C	5.90	117.80	111.36
5	b	60	MET	CG-SD-CE	-5.11	89.66	100.90
1	0	56	GLU	N-CA-C	5.04	120.96	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	183	GLY	Peptide
2	n	183	GLY	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	0	1656	0	1598	41	0
1	1	1665	0	1606	19	0
1	6	1656	0	1598	43	0
1	7	1665	0	1606	19	0
1	Y	1693	0	1629	18	0
1	y	1693	0	1629	19	0
2	2	1667	0	1606	31	0
2	3	1667	0	1606	35	0
2	5	1661	0	1601	28	0
2	8	1667	0	1606	34	0
2	9	1667	0	1606	33	0
2	N	1672	0	1611	26	0
2	n	1672	0	1611	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	p	1661	0	1601	25	0
3	4	1656	0	1596	31	0
3	G	1667	0	1606	17	0
3	g	1667	0	1606	22	0
3	q	1656	0	1596	19	0
4	A	2636	0	2533	33	0
4	a	2636	0	2533	34	0
5	B	3836	0	3709	67	0
5	b	3836	0	3709	49	0
6	C	3490	0	3368	45	0
6	c	3490	0	3368	40	0
7	D	2755	0	2633	41	0
7	d	2755	0	2633	49	0
8	E	619	0	605	6	0
8	e	619	0	605	5	0
9	F	251	0	263	12	0
9	f	251	0	263	10	0
10	H	519	0	549	31	0
10	h	519	0	549	15	0
11	I	283	0	293	2	0
11	i	283	0	293	2	0
12	J	255	0	269	1	0
12	j	255	0	269	1	0
13	K	297	0	308	4	0
13	k	297	0	308	4	0
14	L	306	0	315	5	0
14	l	306	0	315	5	0
15	M	230	0	252	3	0
15	m	230	0	252	3	0
16	O	1742	0	1743	25	0
16	o	1742	0	1743	27	0
17	R	1826	0	1777	27	0
17	r	1826	0	1777	26	0
18	S	1907	0	1847	56	0
18	s	1907	0	1847	63	0
19	T	247	0	260	1	0
19	t	247	0	260	2	0
20	V	232	0	268	3	0
20	v	232	0	268	3	0
21	W	434	0	411	4	0
21	w	434	0	411	3	0
22	X	233	0	253	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	x	233	0	253	3	0
23	Z	458	0	490	3	0
23	z	458	0	490	4	0
24	0	360	0	348	5	0
24	1	360	0	348	13	0
24	2	324	0	278	6	0
24	3	360	0	348	7	0
24	4	324	0	278	4	0
24	5	360	0	348	6	0
24	6	360	0	348	12	0
24	7	360	0	348	10	0
24	8	360	0	348	8	0
24	9	324	0	278	6	0
24	G	324	0	278	10	0
24	N	360	0	348	14	0
24	R	183	0	174	5	0
24	S	182	0	125	10	0
24	Y	360	0	348	15	0
24	g	324	0	278	10	0
24	n	360	0	348	11	0
24	p	360	0	348	5	0
24	q	324	0	278	4	0
24	r	183	0	174	5	0
24	s	182	0	125	8	0
24	y	360	0	348	19	0
25	0	509	0	552	10	0
25	1	509	0	552	7	0
25	2	446	0	432	7	0
25	3	468	0	471	8	0
25	4	446	0	432	6	0
25	5	468	0	471	9	0
25	6	509	0	552	8	0
25	7	509	0	552	5	0
25	8	468	0	471	5	0
25	9	446	0	432	12	0
25	A	239	0	242	5	0
25	B	1040	0	1152	28	0
25	C	845	0	936	21	0
25	D	130	0	144	7	0
25	G	446	0	432	9	0
25	N	468	0	471	8	0
25	R	563	0	529	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	471	0	363	19	0
25	Y	509	0	552	19	0
25	a	239	0	242	5	0
25	b	1040	0	1152	27	0
25	c	845	0	936	15	0
25	d	130	0	144	5	0
25	g	446	0	432	10	0
25	n	468	0	471	5	0
25	p	468	0	471	8	0
25	q	446	0	432	9	0
25	r	563	0	529	11	0
25	s	471	0	363	23	0
25	y	509	0	552	20	0
26	0	84	0	112	6	0
26	1	84	0	112	4	0
26	2	84	0	112	5	0
26	3	84	0	112	7	0
26	4	84	0	112	0	0
26	5	84	0	112	1	0
26	6	84	0	112	5	0
26	7	84	0	112	6	0
26	8	84	0	112	9	0
26	9	84	0	112	5	0
26	G	84	0	112	9	0
26	N	84	0	112	5	0
26	R	42	0	56	4	0
26	S	84	0	112	6	0
26	Y	84	0	112	8	0
26	g	84	0	112	5	0
26	n	84	0	112	6	0
26	p	84	0	112	2	0
26	q	84	0	112	1	0
26	r	42	0	56	2	0
26	s	84	0	112	6	0
26	y	84	0	112	8	0
27	0	44	0	56	0	0
27	1	44	0	56	5	0
27	2	44	0	56	1	0
27	3	44	0	56	2	0
27	4	44	0	56	0	0
27	5	44	0	56	0	0
27	6	44	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	7	44	0	56	4	0
27	8	44	0	56	1	0
27	9	44	0	56	2	0
27	G	44	0	56	6	0
27	N	44	0	56	5	0
27	R	44	0	56	4	0
27	Y	44	0	56	5	0
27	g	44	0	56	6	0
27	n	44	0	56	5	0
27	p	44	0	56	0	0
27	q	44	0	56	0	0
27	r	44	0	56	4	0
27	y	44	0	56	3	0
28	0	44	0	56	1	0
28	1	44	0	56	3	0
28	2	44	0	56	0	0
28	3	44	0	56	1	0
28	4	44	0	56	0	0
28	5	44	0	56	0	0
28	6	44	0	56	3	0
28	7	44	0	56	2	0
28	8	44	0	56	1	0
28	9	44	0	56	0	0
28	G	44	0	56	0	0
28	N	44	0	56	4	0
28	R	44	0	56	1	0
28	S	44	0	56	3	0
28	Y	44	0	56	3	0
28	g	44	0	56	0	0
28	n	44	0	56	3	0
28	p	44	0	56	0	0
28	q	44	0	56	0	0
28	r	44	0	56	2	0
28	s	44	0	56	3	0
28	y	44	0	56	2	0
29	0	49	0	74	2	0
29	1	49	0	74	2	0
29	2	49	0	74	0	0
29	3	49	0	74	0	0
29	4	49	0	74	1	0
29	5	49	0	74	0	0
29	6	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	7	49	0	74	2	0
29	8	49	0	74	0	0
29	9	49	0	74	0	0
29	C	47	0	67	5	0
29	D	132	0	183	5	0
29	G	49	0	74	6	0
29	L	49	0	74	5	0
29	N	49	0	74	3	0
29	R	38	0	46	1	0
29	S	45	0	63	5	0
29	Y	49	0	74	3	0
29	c	47	0	67	2	0
29	d	132	0	183	6	0
29	g	49	0	74	6	0
29	l	49	0	74	5	0
29	n	49	0	74	3	0
29	p	49	0	74	0	0
29	q	49	0	74	0	0
29	r	38	0	46	1	0
29	s	45	0	63	10	0
29	y	49	0	74	4	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	128	0	148	4	0
33	a	128	0	148	3	0
34	A	40	0	56	3	0
34	B	120	0	168	10	0
34	C	160	0	224	10	0
34	D	40	0	56	4	0
34	H	40	0	56	1	0
34	a	40	0	56	2	0
34	b	120	0	168	6	0
34	c	160	0	224	12	0
34	d	40	0	56	5	0
34	h	40	0	56	2	0
35	A	51	0	69	4	0
35	B	104	0	142	2	0
35	D	52	0	71	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	a	51	0	69	3	0
35	b	104	0	142	2	0
35	d	52	0	71	2	0
36	A	48	0	66	2	0
36	B	51	0	72	4	0
36	C	51	0	72	0	0
36	D	92	0	124	0	0
36	H	48	0	66	3	0
36	S	52	0	77	2	0
36	a	48	0	66	2	0
36	b	51	0	72	3	0
36	c	51	0	72	0	0
36	d	92	0	124	0	0
36	h	48	0	66	2	0
36	s	52	0	77	1	0
37	C	308	0	418	10	0
37	c	308	0	418	12	0
38	D	4	0	0	2	0
38	d	4	0	0	2	0
39	D	55	0	80	3	0
39	d	55	0	80	3	0
40	F	43	0	30	0	0
40	f	43	0	30	0	0
All	All	105342	0	106006	1526	0

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

All (1526) 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)
5:B:171:PRO:CD	10:H:85:ALA:HB2	1.58	1.33
5:B:171:PRO:HD3	10:H:85:ALA:CB	1.56	1.32
18:s:58:LYS:HE3	29:s:2630:LHG:O2	1.29	1.23
5:b:366:PHE:HD1	5:b:367:PRO:HD2	1.07	1.19
5:B:171:PRO:CD	10:H:85:ALA:CB	2.19	1.15
5:B:318:ASN:ND2	5:B:361:THR:HG21	1.59	1.15
5:B:171:PRO:CG	10:H:85:ALA:CB	2.25	1.15
5:B:366:PHE:HD1	5:B:367:PRO:HD2	1.08	1.14
5:B:171:PRO:CG	10:H:85:ALA:HB3	1.78	1.13
5:b:366:PHE:CD1	5:b:367:PRO:HD2	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:171:PRO:HG3	10:H:85:ALA:HB3	1.31	1.09
18:S:58:LYS:HE3	29:S:2630:LHG:O2	1.53	1.08
5:B:171:PRO:HG3	10:H:85:ALA:CB	1.86	1.05
18:s:54:GLY:O	18:s:57:ARG:NH2	1.93	1.01
5:B:366:PHE:CD1	5:B:367:PRO:HD2	1.93	1.01
2:3:71:TRP:CD1	2:3:73:THR:HG23	1.96	1.01
17:R:54:LEU:HD12	17:R:57:THR:HG21	1.41	1.00
2:8:71:TRP:CD1	2:8:73:THR:HG23	1.96	0.99
17:r:54:LEU:HD12	17:r:57:THR:HG21	1.45	0.98
5:B:171:PRO:HD3	10:H:85:ALA:HB2	0.95	0.94
7:d:13:THR:HG21	10:h:44:TRP:NE1	1.84	0.92
2:3:71:TRP:HD1	2:3:73:THR:HG23	1.34	0.92
17:R:54:LEU:HD12	17:R:57:THR:CG2	1.98	0.92
2:8:71:TRP:HD1	2:8:73:THR:HG23	1.29	0.91
18:s:156:TRP:CH2	25:s:605:CLA:HMC3	2.06	0.91
18:s:57:ARG:HG2	18:s:57:ARG:HH21	1.36	0.90
2:N:71:TRP:CD1	2:N:73:THR:HG23	2.08	0.88
7:D:19:ASP:OD1	7:D:32:TRP:NE1	2.05	0.88
9:f:19:TRP:NE1	9:f:23:HIS:CE1	2.43	0.87
18:S:54:GLY:O	18:S:57:ARG:HD3	1.74	0.87
5:B:366:PHE:HD1	5:B:367:PRO:CD	1.89	0.85
18:s:58:LYS:CE	29:s:2630:LHG:O2	2.20	0.85
7:d:19:ASP:OD1	7:d:32:TRP:NE1	2.09	0.85
9:f:19:TRP:CD1	9:f:23:HIS:CE1	2.65	0.84
18:s:58:LYS:HE3	29:s:2630:LHG:C2	2.08	0.83
18:s:151:TYR:HD2	25:s:604:CLA:O1A	1.61	0.83
2:n:71:TRP:CD1	2:n:73:THR:HG23	2.14	0.82
5:B:318:ASN:HD21	5:B:361:THR:HG21	1.42	0.81
5:B:274:GLN:HE21	10:H:81:TRP:NE1	1.77	0.81
18:S:57:ARG:NH1	18:S:82:ASP:O	2.14	0.80
9:f:19:TRP:HE1	9:f:23:HIS:CE1	1.99	0.80
18:s:58:LYS:HE3	29:s:2630:LHG:H02	1.44	0.79
5:B:171:PRO:CG	10:H:85:ALA:HB2	2.00	0.78
18:s:151:TYR:CD2	25:s:604:CLA:CGA	2.66	0.78
7:d:13:THR:HG21	10:h:44:TRP:HE1	1.49	0.77
17:r:54:LEU:HD12	17:r:57:THR:CG2	2.13	0.77
5:B:171:PRO:HD3	10:H:85:ALA:HB1	1.65	0.76
17:R:54:LEU:CD1	17:R:57:THR:HG21	2.16	0.76
9:F:19:TRP:NE1	9:F:23:HIS:CE1	2.54	0.75
25:1:604:CLA:HBB1	28:1:1623:NEX:H27	1.69	0.74
10:h:80:SER:OG	10:h:82:GLU:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:174:PHE:HA	16:O:266:GLN:HE22	1.53	0.74
2:n:152:THR:HG22	24:n:605:CHL:HAC1	1.70	0.73
5:B:318:ASN:ND2	5:B:361:THR:CG2	2.46	0.73
18:s:151:TYR:CE2	25:s:604:CLA:H11	2.24	0.73
9:F:19:TRP:HE1	9:F:23:HIS:CE1	2.06	0.72
7:d:13:THR:CG2	10:h:44:TRP:HE1	2.01	0.72
16:o:174:PHE:HA	16:o:266:GLN:HE22	1.52	0.72
9:f:19:TRP:CD1	9:f:23:HIS:ND1	2.57	0.72
2:N:152:THR:HG22	24:N:605:CHL:HAC1	1.72	0.71
18:s:151:TYR:CE2	25:s:604:CLA:CGA	2.72	0.70
2:5:49:LEU:HB2	2:5:53:SER:HB3	1.72	0.70
18:S:156:TRP:CH2	25:S:605:CLA:HMC3	2.25	0.70
25:9:602:CLA:H52	26:9:1621:LUT:H28	1.73	0.70
18:s:151:TYR:CD2	25:s:604:CLA:O1A	2.43	0.70
17:R:54:LEU:CD1	17:R:57:THR:CG2	2.70	0.70
18:S:151:TYR:HD2	25:S:604:CLA:O1A	1.75	0.69
1:7:163:ILE:HD11	28:7:1623:NEX:H15	1.72	0.69
5:B:318:ASN:HD22	5:B:361:THR:HG21	1.54	0.69
18:S:57:ARG:HG3	18:S:57:ARG:HH11	1.58	0.69
18:s:57:ARG:NH2	18:s:57:ARG:HG2	2.09	0.68
2:N:161:GLY:HA2	24:N:609:CHL:HAB	1.74	0.68
18:S:151:TYR:CD2	25:S:604:CLA:CGA	2.77	0.67
18:S:151:TYR:CE2	25:S:604:CLA:H11	2.29	0.67
9:f:19:TRP:NE1	9:f:23:HIS:ND1	2.43	0.67
10:H:80:SER:H	10:H:83:THR:CG2	2.08	0.66
4:a:16:ARG:HG3	4:a:16:ARG:HH11	1.61	0.66
18:S:154:VAL:CG2	25:S:605:CLA:C4D	2.73	0.66
39:d:405:PL9:H122	29:d:409:LHG:HC92	1.78	0.66
7:D:268:HIS:CE1	38:D:401:BCT:O3	2.48	0.65
2:8:46:ALA:HB1	24:8:601:CHL:HBC1	1.77	0.65
2:3:49:LEU:HB2	2:3:53:SER:HB3	1.76	0.65
2:3:71:TRP:CD1	2:3:73:THR:CG2	2.77	0.65
39:D:405:PL9:H122	29:D:409:LHG:HC92	1.78	0.65
10:H:80:SER:H	10:H:83:THR:HG23	1.61	0.65
1:6:66:PRO:HB2	1:6:206:ILE:HD12	1.77	0.65
25:N:603:CLA:HBB1	24:N:609:CHL:H161	1.76	0.65
7:d:199:MET:HG2	39:d:405:PL9:H321	1.79	0.65
17:R:201:TYR:HD2	24:R:608:CHL:HBB1	1.62	0.65
5:b:171:PRO:HB3	10:h:81:TRP:O	1.96	0.65
7:d:268:HIS:CE1	38:d:401:BCT:O3	2.49	0.65
1:0:66:PRO:HB2	1:0:206:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:r:201:TYR:HD2	24:r:608:CHL:HBB1	1.62	0.64
25:2:602:CLA:H52	26:2:1621:LUT:H28	1.79	0.64
18:S:58:LYS:CE	29:S:2630:LHG:O2	2.40	0.64
18:s:283:GLU:HG2	18:s:284:GLU:HG3	1.80	0.64
2:8:71:TRP:CD1	2:8:73:THR:CG2	2.77	0.64
25:b:616:CLA:H2	25:b:617:CLA:HBB2	1.79	0.64
7:D:199:MET:HG2	39:D:405:PL9:H321	1.79	0.64
18:S:283:GLU:HG2	18:S:284:GLU:HG3	1.79	0.64
5:b:382:PRO:HD2	5:b:385:LYS:HZ3	1.63	0.63
18:s:154:VAL:CG2	25:s:605:CLA:C4D	2.76	0.63
1:6:174:GLY:HA2	17:R:56:ASN:HD22	1.63	0.63
9:F:19:TRP:CD1	9:F:23:HIS:CE1	2.87	0.63
18:S:246:VAL:HG11	26:S:1621:LUT:H12	1.81	0.63
25:B:616:CLA:H2	25:B:617:CLA:HBB2	1.79	0.63
2:8:49:LEU:HB2	2:8:53:SER:HB3	1.80	0.63
5:B:382:PRO:HD2	5:B:385:LYS:HZ3	1.64	0.63
3:G:208:MET:HE2	26:G:1621:LUT:H10	1.81	0.63
35:a:412:SQD:HO3	35:a:412:SQD:HO8	1.46	0.63
2:n:226:THR:HG21	2:n:233:ASN:HD21	1.62	0.63
2:5:58:PRO:HD2	2:5:61:LEU:HD12	1.81	0.62
4:a:16:ARG:HG3	4:a:16:ARG:NH1	2.13	0.62
3:q:159:ARG:HA	24:q:608:CHL:HHD	1.81	0.62
6:c:67:LYS:HB2	6:c:72:GLN:HE21	1.64	0.62
1:6:124:LYS:HA	24:6:607:CHL:HED2	1.82	0.62
7:d:13:THR:HG21	10:h:44:TRP:CD1	2.34	0.62
1:1:99:LEU:HD13	25:1:604:CLA:HBB2	1.82	0.62
29:d:408:LHG:HC91	29:l:101:LHG:HC81	1.81	0.62
10:H:80:SER:OG	10:H:82:GLU:OE1	2.15	0.61
2:p:49:LEU:HB2	2:p:53:SER:HB3	1.80	0.61
6:c:78:PRO:HB3	6:c:289:PHE:HB3	1.82	0.61
3:g:153:GLY:HA2	24:g:609:CHL:HAB	1.82	0.61
2:5:153:LEU:HD21	24:5:607:CHL:HAC2	1.83	0.61
5:b:366:PHE:CD1	5:b:367:PRO:CD	2.73	0.61
7:d:186:GLN:HB2	25:d:402:CLA:HBC1	1.82	0.61
2:5:228:LYS:HD3	2:5:232:GLN:HG3	1.82	0.61
29:D:408:LHG:HC91	29:L:101:LHG:HC81	1.80	0.61
5:b:73:GLN:HG2	5:b:79:THR:HG22	1.83	0.61
25:n:603:CLA:HBB1	24:n:609:CHL:H161	1.81	0.61
18:s:154:VAL:HG23	25:s:605:CLA:C4D	2.30	0.61
18:s:218:PRO:HD2	26:s:1620:LUT:H23	1.82	0.61
18:s:246:VAL:HG11	26:s:1621:LUT:H12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:78:PRO:HB3	6:C:289:PHE:HB3	1.83	0.61
7:d:134:ARG:HH21	7:d:137:ASN:HD22	1.48	0.61
3:g:208:MET:HE2	26:g:1621:LUT:H10	1.82	0.61
18:s:222:ALA:HA	18:s:228:LEU:HD11	1.82	0.61
25:0:602:CLA:H52	26:0:1621:LUT:H28	1.81	0.61
6:C:67:LYS:HB2	6:C:72:GLN:HE21	1.64	0.61
1:7:124:LYS:HA	24:7:607:CHL:HED2	1.82	0.61
7:D:27:PHE:CD2	9:F:18:ARG:HD3	2.36	0.61
1:0:172:PRO:HB2	17:r:54:LEU:HD13	1.82	0.61
3:q:80:GLU:HG2	3:q:172:LEU:HD21	1.82	0.61
7:D:13:THR:HG21	10:H:44:TRP:HE1	1.65	0.61
2:p:58:PRO:HD2	2:p:61:LEU:HD12	1.81	0.61
6:c:246:PRO:HG3	6:c:249:ARG:HH21	1.66	0.61
5:B:73:GLN:HG2	5:B:79:THR:HG22	1.82	0.60
1:0:152:ILE:HG22	24:0:605:CHL:HAC1	1.81	0.60
5:B:70:GLY:HA2	5:B:178:VAL:HG21	1.83	0.60
7:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.82	0.60
6:c:185:ARG:NH2	6:c:219:GLU:OE2	2.34	0.60
35:A:412:SQD:HO3	35:A:412:SQD:HO8	1.49	0.60
25:6:602:CLA:H52	26:6:1621:LUT:H28	1.82	0.60
6:c:358:ARG:HA	6:c:363:LEU:HA	1.83	0.60
10:h:80:SER:OG	10:h:82:GLU:CG	2.48	0.60
25:1:602:CLA:HBA1	26:1:1621:LUT:H382	1.83	0.60
2:8:52:TYR:HA	2:9:169:ASN:HD22	1.66	0.60
25:b:605:CLA:HBB1	25:b:614:CLA:HBC2	1.84	0.60
3:4:110:GLY:O	3:4:120:GLN:NE2	2.35	0.60
4:a:56:PRO:HA	4:a:73:TYR:HE2	1.66	0.60
7:D:134:ARG:HH21	7:D:137:ASN:HD22	1.48	0.60
4:A:56:PRO:HA	4:A:73:TYR:HE2	1.66	0.60
6:C:246:PRO:HG3	6:C:249:ARG:HH21	1.66	0.60
18:S:218:PRO:HD2	26:S:1620:LUT:H23	1.83	0.60
5:b:362:PHE:CE2	7:d:184:PHE:CZ	2.89	0.60
1:1:124:LYS:HA	24:1:607:CHL:HED2	1.84	0.60
1:Y:91:LEU:HD23	1:Y:180:LEU:HD22	1.84	0.59
2:8:135:LEU:HB3	2:8:146:ALA:HB3	1.83	0.59
2:5:108:GLU:HA	2:5:120:ALA:HB1	1.84	0.59
25:B:605:CLA:HBB1	25:B:614:CLA:HBC2	1.84	0.59
25:B:608:CLA:H2	36:B:622:LMG:H161	1.85	0.59
1:0:240:ASN:ND2	1:0:243:THR:OG1	2.36	0.59
37:c:523:DGD:HAH1	25:y:611:CLA:HBB2	1.84	0.59
18:s:151:TYR:HD2	25:s:604:CLA:CGA	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:156:TRP:HE1	25:s:605:CLA:HBB1	1.67	0.59
4:A:290:LEU:HA	4:A:293:MET:HB2	1.84	0.59
5:B:315:ILE:HD11	5:B:361:THR:CG2	2.33	0.59
3:G:153:GLY:HA2	24:G:609:CHL:HAB	1.82	0.59
2:5:233:ASN:ND2	25:5:613:CLA:O1D	2.36	0.58
1:0:172:PRO:CB	17:r:54:LEU:HD13	2.32	0.58
2:8:167:ARG:NH2	24:8:609:CHL:HMA3	2.17	0.58
18:s:58:LYS:HD2	24:s:601:CHL:HBC1	1.84	0.58
2:3:71:TRP:HD1	2:3:73:THR:CG2	2.12	0.58
1:0:149:ILE:HD12	1:0:152:ILE:HD11	1.86	0.58
25:7:602:CLA:HBA1	26:7:1621:LUT:H382	1.84	0.58
5:b:70:GLY:HA2	5:b:178:VAL:HG21	1.84	0.58
2:3:91:LEU:HD13	2:3:180:LEU:HD22	1.85	0.58
25:A:407:CLA:HAB	25:D:402:CLA:H51	1.85	0.58
2:2:99:LEU:HB3	25:2:604:CLA:HBB2	1.85	0.58
1:6:240:ASN:ND2	1:6:243:THR:OG1	2.36	0.58
25:Y:603:CLA:H91	24:Y:609:CHL:H142	1.84	0.58
1:0:199:ALA:HA	1:0:202:LYS:HD3	1.86	0.58
2:5:218:GLY:O	2:5:222:GLN:NE2	2.37	0.58
2:8:91:LEU:HD13	2:8:180:LEU:HD22	1.86	0.58
4:a:290:LEU:HA	4:a:293:MET:HB2	1.84	0.58
18:s:39:TRP:HE1	36:s:2631:LMG:HC3	1.69	0.58
2:3:216:MET:HE2	26:3:1621:LUT:H10	1.86	0.58
24:N:606:CHL:HBA2	28:N:1623:NEX:H403	1.86	0.58
5:b:362:PHE:HE2	7:d:184:PHE:HE2	1.51	0.58
2:3:135:LEU:HB3	2:3:146:ALA:HB3	1.84	0.57
8:E:8:ARG:HB3	8:E:13:ILE:HD11	1.86	0.57
2:5:99:LEU:HB3	25:5:604:CLA:HBB2	1.84	0.57
2:n:49:LEU:HB2	2:n:53:SER:HB3	1.86	0.57
17:R:160:VAL:HG11	17:R:168:VAL:HG21	1.86	0.57
6:c:320:GLN:HE21	6:c:324:GLY:HA2	1.69	0.57
9:F:19:TRP:NE1	9:F:23:HIS:ND1	2.53	0.57
2:N:195:PRO:HA	2:N:198:PHE:HB3	1.85	0.57
5:b:362:PHE:HE2	7:d:184:PHE:CE2	2.23	0.57
18:S:151:TYR:CD2	25:S:604:CLA:O1A	2.56	0.57
2:2:169:ASN:HD22	2:3:52:TYR:HA	1.70	0.57
3:4:72:PRO:HA	3:4:75:PHE:HB3	1.86	0.57
6:C:320:GLN:HE21	6:C:324:GLY:HA2	1.69	0.57
37:C:523:DGD:HAH1	25:Y:611:CLA:HBB2	1.84	0.57
18:S:58:LYS:CG	24:S:601:CHL:HBC1	2.35	0.57
5:b:362:PHE:CE2	7:d:184:PHE:CE2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:167:ARG:NH2	24:5:609:CHL:O1D	2.37	0.57
25:b:608:CLA:H2	36:b:622:LMG:H161	1.85	0.57
18:s:151:TYR:CE2	25:s:604:CLA:C1	2.86	0.57
18:s:169:ILE:HG12	24:s:607:CHL:HBC1	1.87	0.57
24:g:601:CHL:HMA3	29:g:2630:LHG:H121	1.86	0.56
7:D:26:ARG:HH11	9:F:17:VAL:HG21	1.70	0.56
17:r:160:VAL:HG11	17:r:168:VAL:HG21	1.86	0.56
17:r:161:SER:HB2	17:r:262:GLY:HA3	1.88	0.56
18:S:169:ILE:HG12	24:S:607:CHL:HBC1	1.87	0.56
5:b:363:PHE:N	5:b:363:PHE:CD1	2.73	0.56
7:D:323:GLU:OE1	7:D:326:ARG:NH2	2.39	0.56
9:F:19:TRP:CD1	9:F:23:HIS:ND1	2.73	0.56
18:S:39:TRP:HE1	36:S:2631:LMG:HC3	1.70	0.56
25:C:513:CLA:H121	29:C:2630:LHG:H131	1.87	0.56
29:C:2630:LHG:H241	24:S:601:CHL:HMC	1.88	0.56
2:3:236:ASP:O	2:3:244:ASN:ND2	2.39	0.56
2:5:71:TRP:CD1	2:5:73:THR:HG23	2.41	0.56
24:G:601:CHL:HMA3	29:G:2630:LHG:H121	1.87	0.56
2:N:49:LEU:HB2	2:N:53:SER:HB3	1.87	0.56
1:Y:108:GLU:HA	1:Y:120:ALA:HB1	1.88	0.56
2:8:71:TRP:HD1	2:8:73:THR:CG2	2.09	0.56
2:n:216:MET:HE2	26:n:1621:LUT:H10	1.88	0.56
24:n:606:CHL:HBA2	28:n:1623:NEX:H403	1.87	0.56
17:R:161:SER:HB2	17:R:262:GLY:HA3	1.88	0.56
2:8:236:ASP:O	2:8:244:ASN:ND2	2.39	0.56
7:d:88:SER:O	7:d:167:TRP:NE1	2.39	0.56
18:S:222:ALA:HA	18:S:228:LEU:HD11	1.86	0.56
2:2:172:PRO:HB2	24:2:608:CHL:HBB2	1.88	0.56
2:3:211:LEU:HD11	25:3:611:CLA:HAC2	1.87	0.56
2:5:95:ARG:NH1	24:5:608:CHL:OBD	2.37	0.56
25:A:405:CLA:H122	33:A:408:PHO:H3A	1.88	0.56
5:B:318:ASN:HD22	5:B:361:THR:CG2	2.14	0.56
18:S:151:TYR:HD2	25:S:604:CLA:CGA	2.18	0.56
1:y:108:GLU:HA	1:y:120:ALA:HB1	1.88	0.56
25:2:603:CLA:H2A	25:2:603:CLA:HED2	1.87	0.56
2:p:167:ARG:NH2	24:p:609:CHL:O1D	2.39	0.56
5:b:363:PHE:HD1	5:b:363:PHE:H	1.52	0.56
25:c:501:CLA:H171	25:c:507:CLA:H102	1.87	0.56
37:c:523:DGD:HA21	25:y:611:CLA:H42	1.87	0.56
2:3:167:ARG:NH2	24:3:609:CHL:HMA3	2.21	0.55
2:3:195:PRO:HA	2:3:198:PHE:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:607:CHL:HAA2	27:N:1622:XAT:H41	1.88	0.55
1:Y:46:ARG:NH2	1:Y:61:LEU:O	2.39	0.55
1:0:204:LYS:HD3	25:0:612:CLA:HAA2	1.87	0.55
2:8:195:PRO:HA	2:8:198:PHE:HB3	1.87	0.55
2:p:108:GLU:HA	2:p:120:ALA:HB1	1.88	0.55
29:c:2630:LHG:H241	24:s:601:CHL:HMC	1.88	0.55
2:n:135:LEU:HB3	2:n:146:ALA:HB3	1.88	0.55
25:3:602:CLA:H52	26:3:1621:LUT:H28	1.87	0.55
5:B:366:PHE:O	5:B:425:GLN:NE2	2.30	0.55
25:0:602:CLA:HBA1	26:0:1621:LUT:H382	1.88	0.55
1:6:204:LYS:O	1:6:208:ASN:ND2	2.36	0.55
25:8:602:CLA:HBA1	26:8:1621:LUT:H382	1.89	0.55
25:a:405:CLA:H122	33:a:408:PHO:H3A	1.88	0.55
25:y:603:CLA:H91	24:y:609:CHL:H142	1.88	0.55
24:y:608:CHL:HHC	24:y:608:CHL:HBB1	1.88	0.55
4:A:16:ARG:HH21	4:A:16:ARG:HG3	1.71	0.55
25:C:501:CLA:H171	25:C:507:CLA:H102	1.89	0.55
7:D:13:THR:HG21	10:H:44:TRP:NE1	2.20	0.55
2:9:149:ILE:HD11	24:9:607:CHL:HAC1	1.87	0.55
25:q:603:CLA:H2A	25:q:603:CLA:HED2	1.87	0.55
1:1:167:ARG:NH2	24:1:609:CHL:O1D	2.40	0.55
7:D:242:GLU:OE1	7:D:264:LYS:NZ	2.37	0.55
2:8:184:GLU:HA	2:8:187:ASP:HB3	1.87	0.55
2:p:198:PHE:HB2	25:p:610:CLA:HMA2	1.89	0.55
1:6:236:ASP:O	1:6:244:ASN:ND2	2.40	0.55
10:H:78:SER:OG	10:H:83:THR:HG22	2.06	0.55
27:7:1622:XAT:H22	2:9:250:ALA:HA	1.89	0.55
25:8:602:CLA:H52	26:8:1621:LUT:H28	1.89	0.55
37:C:523:DGD:HA21	25:Y:611:CLA:H42	1.87	0.55
1:7:50:LEU:O	24:7:601:CHL:HBB1	2.06	0.55
3:q:187:PRO:HA	3:q:190:PHE:HB3	1.88	0.55
4:a:131:TRP:HZ2	6:c:437:ARG:HG2	1.72	0.55
7:d:323:GLU:OE1	7:d:326:ARG:NH2	2.39	0.55
1:y:46:ARG:NH2	1:y:61:LEU:O	2.39	0.55
1:6:187:ASP:OD2	17:R:45:ARG:NH2	2.40	0.55
5:B:25:MET:HE3	34:B:618:BCR:H23C	1.89	0.55
5:b:25:MET:HE3	34:b:618:BCR:H23C	1.89	0.55
3:g:47:GLY:HA3	1:y:169:ASN:HB3	1.89	0.55
2:n:45:ARG:NH1	2:n:68:ASP:O	2.40	0.55
5:B:174:LEU:HD21	5:B:309:LEU:HB2	1.89	0.54
15:M:5:ILE:HG23	15:m:5:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:105:ILE:HG23	2:8:109:LEU:HD13	1.90	0.54
25:g:603:CLA:H72	25:n:602:CLA:H102	1.89	0.54
6:C:89:PRO:HA	6:C:183:ASP:HB3	1.87	0.54
1:0:187:ASP:OD2	17:r:45:ARG:NH2	2.40	0.54
3:g:83:LEU:HD23	3:g:172:LEU:HD22	1.89	0.54
5:B:10:THR:OG1	17:R:94:GLN:NE2	2.41	0.54
2:8:58:PRO:HD2	2:8:61:LEU:HD12	1.90	0.54
4:A:16:ARG:HG3	4:A:16:ARG:NH2	2.22	0.54
16:O:251:VAL:HA	16:O:258:ILE:HG22	1.89	0.54
34:c:516:BCR:HC41	13:k:25:LEU:HD21	1.89	0.54
3:g:161:ASN:OD1	2:n:55:ASN:ND2	2.39	0.54
18:s:57:ARG:HH21	18:s:57:ARG:CG	2.14	0.54
18:s:156:TRP:CH2	25:s:605:CLA:CMC	2.85	0.54
5:B:360:PRO:CG	5:B:363:PHE:HE1	2.20	0.54
1:0:204:LYS:O	1:0:208:ASN:ND2	2.38	0.54
25:b:609:CLA:H162	25:d:403:CLA:HBA1	1.90	0.54
6:c:361:ASN:ND2	16:o:133:ASP:OD2	2.40	0.54
16:o:251:VAL:HA	16:o:258:ILE:HG22	1.89	0.54
5:B:360:PRO:HG2	5:B:363:PHE:HE1	1.72	0.54
6:C:361:ASN:ND2	16:O:133:ASP:OD2	2.41	0.54
3:G:83:LEU:HD23	3:G:172:LEU:HD22	1.89	0.54
7:d:87:HIS:O	10:h:69:ASN:ND2	2.31	0.54
24:g:609:CHL:HMB3	24:n:601:CHL:HHB	1.89	0.54
18:s:151:TYR:CD2	25:s:604:CLA:C1	2.90	0.54
27:1:1622:XAT:H22	2:2:250:ALA:HA	1.89	0.54
14:L:36:ILE:O	15:M:4:ASN:ND2	2.41	0.54
2:3:184:GLU:HA	2:3:187:ASP:HB3	1.88	0.54
6:C:166:LYS:HA	6:C:170:PHE:HB2	1.89	0.54
5:b:191:ASP:HB3	5:b:194:ASN:HB2	1.90	0.54
7:d:68:LEU:HD13	9:f:39:MET:HE2	1.89	0.54
25:3:602:CLA:HBA1	26:3:1621:LUT:H382	1.89	0.54
4:A:131:TRP:HZ2	6:C:437:ARG:HG2	1.72	0.54
6:C:385:THR:HG1	6:C:386:HIS:HD1	1.54	0.54
3:q:72:PRO:HA	3:q:75:PHE:HB3	1.89	0.54
2:n:130:PHE:HZ	1:y:247:PHE:HB3	1.73	0.54
3:G:161:ASN:OD1	2:N:55:ASN:ND2	2.41	0.54
25:a:407:CLA:HAB	25:d:402:CLA:H51	1.90	0.54
1:1:50:LEU:O	24:1:601:CHL:HBB1	2.08	0.53
25:6:602:CLA:HBA1	26:6:1621:LUT:H382	1.88	0.53
6:c:285:TYR:O	6:c:411:ARG:NH2	2.41	0.53
18:s:58:LYS:HE2	29:s:2630:LHG:HC31	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:o:204:ASP:OD1	16:o:208:ARG:N	2.38	0.53
2:5:195:PRO:HA	2:5:198:PHE:HB3	1.89	0.53
1:0:181:TYR:HB3	25:0:610:CLA:HED2	1.90	0.53
3:q:218:THR:HG21	3:q:220:LYS:HZ3	1.73	0.53
5:b:10:THR:OG1	17:r:94:GLN:NE2	2.40	0.53
20:v:26:LEU:HD21	23:z:25:VAL:HA	1.90	0.53
4:A:301:ASN:HB3	6:C:395:VAL:HG21	1.90	0.53
5:B:171:PRO:HG2	10:H:85:ALA:HB3	1.81	0.53
7:D:68:LEU:HD13	9:F:39:MET:HE2	1.89	0.53
20:V:26:LEU:HD21	23:Z:25:VAL:HA	1.89	0.53
14:l:36:ILE:O	15:m:4:ASN:ND2	2.41	0.53
25:B:605:CLA:H92	25:B:605:CLA:H41	1.90	0.53
25:B:609:CLA:H162	25:D:403:CLA:HBA1	1.91	0.53
18:S:151:TYR:CE2	25:S:604:CLA:CGA	2.92	0.53
25:9:603:CLA:H2A	25:9:603:CLA:HED2	1.88	0.53
2:p:45:ARG:NH1	2:p:68:ASP:O	2.42	0.53
1:6:135:LEU:HD21	24:6:606:CHL:HMD3	1.90	0.53
4:A:29:TYR:O	4:A:129:ARG:NH2	2.39	0.53
29:G:2630:LHG:H211	27:Y:1622:XAT:H10	1.90	0.53
29:L:101:LHG:H241	29:L:101:LHG:H102	1.91	0.53
24:S:606:CHL:HBA2	28:S:1623:NEX:H403	1.90	0.53
7:d:12:ARG:CB	7:d:12:ARG:HH11	2.21	0.53
18:s:58:LYS:CE	29:s:2630:LHG:C2	2.85	0.53
1:6:156:GLN:HE22	24:6:607:CHL:HMC	1.73	0.53
2:p:95:ARG:NH1	24:p:608:CHL:OBD	2.36	0.53
5:b:57:ARG:NH2	5:b:334:ASP:OD1	2.41	0.53
27:g:1622:XAT:H193	2:n:246:ALA:HB3	1.91	0.53
18:s:176:MET:HE1	24:s:606:CHL:HMA1	1.90	0.53
2:3:95:ARG:NH1	24:3:608:CHL:OBD	2.39	0.53
1:6:181:TYR:HB3	25:6:610:CLA:HED2	1.91	0.53
17:R:201:TYR:CD2	24:R:608:CHL:HBB1	2.42	0.53
6:C:285:TYR:O	6:C:411:ARG:NH2	2.42	0.53
7:D:180:ARG:O	7:D:184:PHE:N	2.42	0.53
25:G:603:CLA:H72	25:N:602:CLA:H102	1.90	0.53
2:8:102:LEU:HA	2:8:105:ILE:HD12	1.89	0.53
29:l:101:LHG:H241	29:l:101:LHG:H102	1.91	0.53
34:C:516:BCR:HC41	13:K:25:LEU:HD21	1.89	0.53
1:7:225:VAL:O	1:7:252:LYS:NZ	2.42	0.53
2:8:237:HIS:ND1	2:8:244:ASN:O	2.42	0.53
6:c:166:LYS:HA	6:c:170:PHE:HB2	1.90	0.53
7:d:26:ARG:HH11	9:f:17:VAL:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:g:601:CHL:HED3	29:g:2630:LHG:H142	1.91	0.53
29:g:2630:LHG:H211	27:y:1622:XAT:H10	1.91	0.53
24:n:607:CHL:HAA2	27:n:1622:XAT:H41	1.90	0.53
24:s:606:CHL:HBA2	28:s:1623:NEX:H403	1.91	0.53
5:B:379:ALA:HB1	5:B:392:ILE:HG22	1.91	0.52
5:B:400:THR:HG22	5:B:410:THR:HG22	1.91	0.52
6:C:135:PHE:CE2	25:C:513:CLA:H3A	2.44	0.52
18:S:176:MET:HE1	24:S:606:CHL:HMA1	1.90	0.52
3:q:110:GLY:O	3:q:120:GLN:NE2	2.42	0.52
3:g:121:ILE:HG21	3:g:141:ILE:HD12	1.92	0.52
17:r:201:TYR:CD2	24:r:608:CHL:HBB1	2.42	0.52
16:o:188:ILE:HB	16:o:246:PHE:HB2	1.90	0.52
1:6:140:ASN:HD21	17:R:274:LEU:HA	1.75	0.52
1:6:161:GLY:HA2	24:6:609:CHL:HAB	1.91	0.52
2:N:91:LEU:HD23	2:N:180:LEU:HD22	1.91	0.52
16:O:208:ARG:HD2	16:O:232:GLU:HB3	1.92	0.52
3:q:55:GLY:HA2	3:q:60:ASP:HB3	1.91	0.52
4:a:192:ILE:HG13	4:a:293:MET:HE1	1.91	0.52
2:n:161:GLY:HA2	24:n:609:CHL:HAB	1.89	0.52
4:A:104:GLU:O	4:A:108:ASN:ND2	2.42	0.52
24:G:601:CHL:HED3	29:G:2630:LHG:H142	1.90	0.52
2:8:95:ARG:NH1	24:8:608:CHL:OBD	2.39	0.52
2:p:71:TRP:CD1	2:p:73:THR:HG23	2.44	0.52
5:b:174:LEU:HD21	5:b:309:LEU:HB2	1.91	0.52
25:b:605:CLA:H41	25:b:605:CLA:H92	1.90	0.52
6:c:135:PHE:CE2	25:c:513:CLA:H3A	2.44	0.52
1:6:204:LYS:HD3	25:6:612:CLA:HAA2	1.91	0.52
1:7:167:ARG:NH2	24:7:609:CHL:O1D	2.41	0.52
18:s:56:ASP:HA	18:s:68:ARG:HH12	1.74	0.52
18:s:58:LYS:CE	29:s:2630:LHG:HC31	2.40	0.52
16:o:208:ARG:HD2	16:o:232:GLU:HB3	1.91	0.52
3:4:159:ARG:HH21	24:4:609:CHL:HMA3	1.75	0.52
4:A:296:ASN:HB3	6:C:389:LEU:HA	1.91	0.52
2:N:130:PHE:HZ	1:Y:247:PHE:HB3	1.74	0.52
1:0:207:LYS:NZ	29:0:2630:LHG:O4	2.40	0.52
6:c:220:ASP:O	6:c:224:GLY:N	2.43	0.52
10:h:70:SER:OG	10:h:79:MET:SD	2.65	0.52
2:2:129:ILE:HG21	2:2:149:ILE:HD12	1.90	0.52
1:6:62:THR:OG1	1:6:64:GLU:OE1	2.26	0.52
2:N:216:MET:HE2	26:N:1621:LUT:H10	1.91	0.52
17:R:133:PHE:HB3	25:R:602:CLA:HHB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:57:ARG:NH1	18:S:57:ARG:HG3	2.22	0.52
1:1:129:ILE:HG21	1:1:149:ILE:HD13	1.90	0.52
1:1:250:ALA:HA	27:3:1622:XAT:H22	1.91	0.52
2:2:149:ILE:HD11	24:2:607:CHL:HAC1	1.92	0.52
2:2:206:ILE:O	2:2:210:ARG:N	2.36	0.52
25:C:508:CLA:HBC3	25:C:510:CLA:H71	1.91	0.52
2:N:71:TRP:CD1	2:N:73:THR:CG2	2.89	0.52
16:O:188:ILE:HB	16:O:246:PHE:HB2	1.91	0.52
4:a:104:GLU:O	4:a:108:ASN:ND2	2.43	0.52
2:2:160:MET:HE1	24:2:606:CHL:HHB	1.92	0.52
25:2:604:CLA:HMB2	24:2:606:CHL:HBB1	1.92	0.52
24:G:609:CHL:HMB3	24:N:601:CHL:HHB	1.91	0.52
18:S:154:VAL:HG23	25:S:605:CLA:C4D	2.38	0.52
6:c:385:THR:HG1	6:c:386:HIS:HD1	1.55	0.52
1:1:46:ARG:NH2	1:1:61:LEU:O	2.43	0.52
1:6:216:MET:HE2	26:6:1621:LUT:H10	1.92	0.52
5:B:57:ARG:NH2	5:B:334:ASP:OD1	2.41	0.52
5:B:360:PRO:HG2	5:B:363:PHE:CE1	2.45	0.52
34:C:516:BCR:H10C	20:V:15:VAL:HG13	1.91	0.52
2:8:250:ALA:HA	27:9:1622:XAT:H22	1.91	0.52
2:p:129:ILE:HD11	2:p:135:LEU:HD12	1.91	0.52
34:c:516:BCR:H10C	20:v:15:VAL:HG13	1.91	0.52
16:o:232:GLU:HA	16:o:235:LYS:HE2	1.92	0.52
2:5:229:GLY:O	2:5:233:ASN:N	2.41	0.52
1:6:81:GLU:OE2	1:6:84:LYS:NZ	2.44	0.52
1:6:172:PRO:HG2	24:6:608:CHL:HBB2	1.92	0.52
4:a:272:HIS:CE1	38:d:401:BCT:O2	2.63	0.52
1:y:236:ASP:O	1:y:244:ASN:ND2	2.43	0.52
3:4:83:LEU:HD23	3:4:172:LEU:HD12	1.92	0.51
16:O:232:GLU:HA	16:O:235:LYS:HE2	1.92	0.51
1:7:250:ALA:HA	27:8:1622:XAT:H22	1.92	0.51
2:8:162:LEU:O	2:8:166:TYR:N	2.40	0.51
5:b:400:THR:HG22	5:b:410:THR:HG22	1.92	0.51
25:c:508:CLA:HBC3	25:c:510:CLA:H71	1.91	0.51
7:d:180:ARG:O	7:d:184:PHE:N	2.42	0.51
24:1:606:CHL:HBB1	24:1:607:CHL:HHC	1.91	0.51
4:A:192:ILE:HG13	4:A:293:MET:HE1	1.91	0.51
27:N:1622:XAT:H10	29:Y:2630:LHG:H223	1.93	0.51
25:Y:604:CLA:HAB	28:Y:1623:NEX:H362	1.92	0.51
2:9:228:LYS:HD3	2:9:232:GLN:HG2	1.92	0.51
5:b:367:PRO:HB2	7:d:345:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:h:74:LEU:HB2	10:h:77:VAL:HG12	1.92	0.51
4:A:343:LEU:HD23	6:C:389:LEU:HD21	1.93	0.51
16:O:204:ASP:OD1	16:O:208:ARG:N	2.38	0.51
2:n:195:PRO:HA	2:n:198:PHE:HB3	1.91	0.51
3:4:80:GLU:HG2	3:4:172:LEU:HD21	1.92	0.51
6:C:358:ARG:HA	6:C:363:LEU:HA	1.91	0.51
18:S:62:PRO:HD3	24:S:601:CHL:HHC	1.92	0.51
2:p:204:LYS:HD3	25:p:612:CLA:HAA2	1.91	0.51
18:s:62:PRO:HD3	24:s:601:CHL:HHC	1.92	0.51
6:C:225:HIS:HA	6:C:228:ILE:HG22	1.92	0.51
1:Y:236:ASP:O	1:Y:244:ASN:ND2	2.43	0.51
24:Y:608:CHL:HHC	24:Y:608:CHL:HBB1	1.92	0.51
25:0:611:CLA:HED3	25:0:611:CLA:H2A	1.91	0.51
1:7:46:ARG:NH2	1:7:61:LEU:O	2.42	0.51
8:E:55:TYR:O	8:E:60:ARG:NH2	2.44	0.51
3:G:143:ALA:HB3	24:G:605:CHL:HMC	1.92	0.51
2:p:45:ARG:HE	2:p:47:LYS:HE3	1.75	0.51
3:q:129:TYR:HB3	3:q:135:LEU:HD13	1.91	0.51
3:4:218:THR:HG21	3:4:225:ASN:HD21	1.76	0.51
1:6:211:LEU:HB3	29:6:2630:LHG:H242	1.92	0.51
17:r:133:PHE:HB3	25:r:602:CLA:HHB	1.91	0.51
4:A:136:ARG:NH1	11:I:27:ASP:OD1	2.44	0.51
18:S:109:ARG:NH1	24:S:608:CHL:OBD	2.41	0.51
1:7:172:PRO:HG2	24:7:608:CHL:HBB2	1.92	0.51
4:a:296:ASN:HB3	6:c:389:LEU:HA	1.92	0.51
18:S:58:LYS:HG3	24:S:601:CHL:CBC	2.40	0.51
1:0:43:GLY:O	1:0:46:ARG:NH1	2.39	0.51
25:y:604:CLA:HAB	28:y:1623:NEX:H362	1.92	0.51
16:o:135:MET:HE1	16:o:176:ILE:HD11	1.93	0.51
25:0:610:CLA:H2	26:0:1620:LUT:H28	1.93	0.50
4:a:301:ASN:HB3	6:c:395:VAL:HG21	1.93	0.50
24:n:601:CHL:HAC1	29:n:2630:LHG:HC11	1.93	0.50
2:5:60:TYR:OH	2:5:72:ASP:OD2	2.27	0.50
3:G:110:GLY:O	3:G:120:GLN:NE2	2.45	0.50
27:G:1622:XAT:H193	2:N:246:ALA:HB3	1.92	0.50
10:H:80:SER:HB3	10:H:82:GLU:HG2	1.92	0.50
2:N:71:TRP:HD1	2:N:73:THR:HG23	1.68	0.50
18:S:154:VAL:CG2	25:S:605:CLA:CHA	2.88	0.50
1:0:236:ASP:O	1:0:244:ASN:ND2	2.45	0.50
6:c:135:PHE:CD2	25:c:513:CLA:H3A	2.46	0.50
3:g:110:GLY:O	3:g:120:GLN:NE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:204:LYS:HD3	25:5:612:CLA:HAA2	1.93	0.50
2:p:52:TYR:OH	3:q:162:GLY:O	2.30	0.50
37:c:524:DGD:O2D	25:y:611:CLA:O1A	2.30	0.50
8:e:8:ARG:HB3	8:e:13:ILE:HD11	1.92	0.50
2:3:237:HIS:ND1	2:3:244:ASN:O	2.44	0.50
2:9:162:LEU:O	2:9:166:TYR:N	2.41	0.50
2:9:233:ASN:ND2	25:9:613:CLA:O1D	2.44	0.50
25:q:613:CLA:H2A	25:q:613:CLA:HED3	1.92	0.50
1:1:150:LEU:HD11	2:2:245:ASN:HD21	1.77	0.50
3:4:129:TYR:HB3	3:4:135:LEU:HD13	1.94	0.50
3:4:162:GLY:O	2:5:52:TYR:OH	2.30	0.50
1:0:60:TYR:OH	1:0:72:ASP:OD2	2.30	0.50
3:g:218:THR:HG21	3:g:225:ASN:HD21	1.77	0.50
2:3:58:PRO:HD2	2:3:61:LEU:HD12	1.93	0.50
1:0:81:GLU:OE2	1:0:84:LYS:NZ	2.45	0.50
4:a:136:ARG:NH1	11:i:27:ASP:OD1	2.44	0.50
18:S:156:TRP:HE1	25:S:605:CLA:HBB1	1.76	0.50
1:0:91:LEU:HD23	1:0:180:LEU:HD22	1.93	0.50
33:a:409:PHO:HBC3	7:d:279:LEU:HD12	1.94	0.50
35:a:412:SQD:H331	25:c:504:CLA:H191	1.94	0.50
23:z:57:LEU:HA	23:z:60:PHE:HD2	1.76	0.50
1:0:174:GLY:HA2	17:r:56:ASN:HD22	1.77	0.50
8:e:55:TYR:O	8:e:60:ARG:NH2	2.44	0.50
9:f:19:TRP:CD1	9:f:23:HIS:HD1	2.28	0.50
18:s:58:LYS:HE3	29:s:2630:LHG:C1	2.41	0.50
5:B:30:VAL:HG11	25:B:613:CLA:H112	1.93	0.50
6:C:135:PHE:CD2	25:C:513:CLA:H3A	2.46	0.50
23:Z:57:LEU:HA	23:Z:60:PHE:HD2	1.76	0.50
5:b:362:PHE:CE2	7:d:184:PHE:HZ	2.29	0.50
18:s:156:TRP:HH2	25:s:605:CLA:HMC3	1.72	0.50
2:3:187:ASP:OD1	26:3:1620:LUT:O23	2.30	0.49
3:4:228:ASP:HB3	3:4:236:VAL:HG11	1.94	0.49
6:C:454:VAL:HG21	7:D:248:THR:HG23	1.94	0.49
7:D:193:LEU:HA	7:D:198:MET:HE3	1.93	0.49
3:G:242:ALA:HA	27:Y:1622:XAT:H22	1.93	0.49
18:s:151:TYR:HE2	25:s:604:CLA:CGA	2.25	0.49
1:6:173:LEU:HB2	24:6:608:CHL:HBB1	1.95	0.49
6:c:332:SER:HB3	6:c:336:GLU:H	1.77	0.49
2:2:201:LEU:HD23	2:2:204:LYS:HD2	1.93	0.49
1:6:91:LEU:HD23	1:6:180:LEU:HD22	1.94	0.49
16:O:135:MET:HE1	16:O:176:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:603:CLA:HBB1	24:Y:609:CHL:H171	1.94	0.49
7:d:193:LEU:HA	7:d:198:MET:HE3	1.93	0.49
3:g:249:ALA:HB3	1:y:227:GLY:HA3	1.94	0.49
18:s:156:TRP:HE1	25:s:605:CLA:CBB	2.25	0.49
3:4:33:TYR:HD1	3:4:56:GLU:HA	1.78	0.49
1:0:99:LEU:HD13	25:0:604:CLA:HBB2	1.94	0.49
4:a:343:LEU:HD23	6:c:389:LEU:HD21	1.94	0.49
7:d:87:HIS:ND1	36:h:102:LMG:O2	2.46	0.49
3:g:242:ALA:HA	27:y:1622:XAT:H22	1.94	0.49
2:n:71:TRP:NE1	2:n:73:THR:HG23	2.28	0.49
2:2:42:GLY:O	2:2:45:ARG:NH1	2.43	0.49
4:A:254:TYR:HE2	7:D:142:ASN:HD22	1.59	0.49
1:0:105:ILE:HD11	1:0:231:LEU:HG	1.95	0.49
1:0:140:ASN:HD21	17:r:274:LEU:HA	1.76	0.49
1:0:156:GLN:HE22	24:0:607:CHL:HMC	1.78	0.49
5:b:160:GLY:HA3	5:b:180:PRO:HB3	1.95	0.49
25:b:602:CLA:H193	25:b:602:CLA:H141	1.95	0.49
27:n:1622:XAT:H10	29:y:2630:LHG:H223	1.93	0.49
1:1:225:VAL:O	1:1:252:LYS:NZ	2.46	0.49
4:A:199:MET:HE1	7:D:74:LEU:HD21	1.94	0.49
34:B:618:BCR:H322	36:B:622:LMG:H111	1.94	0.49
2:9:69:TYR:N	25:9:602:CLA:OBD	2.44	0.49
4:a:29:TYR:O	4:a:129:ARG:NH2	2.38	0.49
24:0:608:CHL:H12	26:0:1620:LUT:H383	1.94	0.49
5:b:30:VAL:HG11	25:b:613:CLA:H112	1.93	0.49
18:s:155:PRO:HD2	18:s:156:TRP:CD1	2.48	0.49
25:y:603:CLA:HBB1	24:y:609:CHL:H171	1.95	0.49
1:1:50:LEU:HB3	1:1:54:THR:HA	1.95	0.49
27:2:1622:XAT:H22	2:3:250:ALA:HA	1.93	0.49
2:3:45:ARG:NH1	2:3:68:ASP:O	2.46	0.49
24:7:606:CHL:HBB1	24:7:607:CHL:HHC	1.95	0.49
34:b:618:BCR:H322	36:b:622:LMG:H111	1.95	0.49
2:n:137:TYR:HB3	2:n:143:LEU:HD13	1.94	0.49
2:3:162:LEU:O	2:3:166:TYR:N	2.39	0.49
5:B:315:ILE:HD11	5:B:361:THR:HG23	1.94	0.49
2:9:220:PHE:HE2	25:9:603:CLA:HBB2	1.77	0.49
3:4:37:ARG:NH1	3:4:54:THR:O	2.46	0.48
5:B:3:LEU:HD13	5:B:8:VAL:HA	1.94	0.48
4:a:199:MET:HE1	7:d:74:LEU:HD21	1.94	0.48
5:b:364:GLU:OE1	5:b:364:GLU:HA	2.13	0.48
6:c:225:HIS:HA	6:c:228:ILE:HG22	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:246:PRO:HA	6:c:249:ARG:HE	1.78	0.48
25:y:610:CLA:H2	26:y:1620:LUT:H28	1.94	0.48
17:r:124:TYR:HB2	25:r:616:CLA:HED2	1.95	0.48
2:2:88:GLU:HA	2:2:180:LEU:HD21	1.95	0.48
2:3:60:TYR:OH	2:3:72:ASP:OD2	2.27	0.48
37:C:524:DGD:O2D	25:Y:611:CLA:O1A	2.30	0.48
16:O:139:PHE:HD1	16:O:149:LEU:HB3	1.77	0.48
18:s:109:ARG:NH1	24:s:608:CHL:OBD	2.41	0.48
17:r:249:PHE:CD2	27:r:622:XAT:H12	2.48	0.48
16:o:139:PHE:HD1	16:o:149:LEU:HB3	1.78	0.48
4:A:181:ASN:HD22	7:D:314:PHE:HD1	1.61	0.48
4:A:272:HIS:CE1	38:D:401:BCT:O2	2.65	0.48
5:B:321:LYS:HD3	5:B:361:THR:HG22	1.95	0.48
7:D:36:LEU:HB2	35:D:413:SQD:H182	1.96	0.48
34:D:404:BCR:H14C	9:F:32:PHE:CE2	2.47	0.48
17:R:124:TYR:HB2	25:R:616:CLA:HED2	1.95	0.48
18:S:54:GLY:O	18:S:57:ARG:CD	2.55	0.48
1:0:124:LYS:HA	24:0:607:CHL:HED2	1.95	0.48
1:0:131:GLN:NE2	1:0:134:GLY:O	2.40	0.48
1:7:106:PHE:HA	1:7:109:LEU:HB3	1.94	0.48
2:9:201:LEU:HD23	2:9:204:LYS:HD2	1.94	0.48
5:b:3:LEU:HD13	5:b:8:VAL:HA	1.94	0.48
2:n:245:ASN:HB2	25:n:614:CLA:HED3	1.95	0.48
18:s:258:GLU:OE1	18:s:263:ASN:ND2	2.46	0.48
33:A:409:PHO:HBC3	7:D:279:LEU:HD12	1.94	0.48
25:B:602:CLA:H193	25:B:602:CLA:H141	1.94	0.48
6:C:167:ALA:HA	6:C:172:GLY:HA2	1.96	0.48
17:R:249:PHE:CD2	27:R:622:XAT:H12	2.48	0.48
18:S:56:ASP:HA	18:S:68:ARG:HH12	1.78	0.48
18:S:275:ASN:H	18:S:278:THR:HG22	1.78	0.48
4:a:234:ASN:ND2	29:d:408:LHG:O2	2.47	0.48
27:g:1622:XAT:H10	29:n:2630:LHG:H212	1.95	0.48
18:s:275:ASN:H	18:s:278:THR:HG22	1.78	0.48
3:4:122:PHE:HZ	2:5:247:PHE:HB3	1.78	0.48
17:R:225:SER:OG	17:R:226:GLU:OE1	2.32	0.48
18:S:151:TYR:CD2	25:S:604:CLA:C1	2.97	0.48
18:S:196:ILE:HD11	18:S:198:LYS:HD2	1.95	0.48
1:7:50:LEU:HB3	1:7:54:THR:HA	1.95	0.48
2:8:144:VAL:HG13	24:8:605:CHL:C1D	2.44	0.48
4:a:25:GLU:OE1	6:c:458:ARG:NH2	2.47	0.48
5:b:275:TRP:CE2	5:b:315:ILE:HD13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:56:ASN:ND2	6:c:102:SER:OG	2.47	0.48
1:6:131:GLN:NE2	1:6:134:GLY:O	2.36	0.48
5:B:160:GLY:HA3	5:B:180:PRO:HB3	1.94	0.48
4:a:254:TYR:HE2	7:d:142:ASN:HD22	1.59	0.48
5:b:315:ILE:HG13	5:b:321:LYS:HG3	1.96	0.48
5:b:370:LEU:HD12	5:b:379:ALA:HB3	1.95	0.48
24:n:606:CHL:HHC	24:n:606:CHL:HBB1	1.96	0.48
16:o:125:MET:HB2	16:o:161:THR:HG23	1.94	0.48
16:o:194:VAL:HG21	16:o:267:PRO:HD2	1.96	0.48
1:6:99:LEU:HD13	25:6:604:CLA:HBB2	1.96	0.48
5:B:275:TRP:CE2	5:B:315:ILE:HD13	2.49	0.48
16:O:125:MET:HB2	16:O:161:THR:HG23	1.94	0.48
34:d:404:BCR:H14C	9:f:32:PHE:CE2	2.47	0.48
2:n:201:LEU:HD23	2:n:204:LYS:HD2	1.96	0.48
18:s:151:TYR:CD2	25:s:604:CLA:H11	2.48	0.48
3:4:237:ASN:HA	25:4:613:CLA:HAA1	1.95	0.48
2:9:129:ILE:HG21	2:9:149:ILE:HD12	1.96	0.48
17:r:124:TYR:OH	17:r:135:GLU:OE1	2.31	0.48
2:3:166:TYR:HD2	24:3:608:CHL:HBB1	1.79	0.48
4:A:270:SER:OG	35:A:412:SQD:O49	2.32	0.48
36:a:413:LMG:HO5	36:a:413:LMG:HO4	1.61	0.48
5:b:46:ASP:N	5:b:58:GLN:HE22	2.12	0.48
6:C:64:VAL:O	6:C:72:GLN:NE2	2.39	0.48
2:N:181:TYR:HB3	25:N:610:CLA:HED2	1.95	0.48
2:p:106:THR:HA	2:p:109:LEU:HD13	1.96	0.48
1:y:102:LEU:HD21	25:y:612:CLA:H202	1.96	0.48
25:1:614:CLA:H3A	25:1:614:CLA:HBA2	1.59	0.47
3:4:94:LEU:HA	3:4:97:ILE:HD12	1.95	0.47
24:G:601:CHL:HBA1	24:G:601:CHL:H3A	1.63	0.47
24:N:606:CHL:HHC	24:N:606:CHL:HBB1	1.96	0.47
17:R:124:TYR:OH	17:R:135:GLU:OE1	2.31	0.47
18:S:106:LEU:HG	24:S:608:CHL:HED1	1.96	0.47
18:S:135:THR:OG1	18:S:138:GLU:OE2	2.32	0.47
18:S:258:GLU:OE1	18:S:263:ASN:ND2	2.46	0.47
5:b:224:ARG:NH1	7:d:16:ASP:OD2	2.43	0.47
5:b:362:PHE:CZ	7:d:164:GLN:OE1	2.67	0.47
24:g:601:CHL:HBA1	24:g:601:CHL:H3A	1.65	0.47
24:g:608:CHL:HHC	24:g:608:CHL:HBB1	1.95	0.47
5:B:315:ILE:HG13	5:B:321:LYS:HG3	1.96	0.47
6:C:331:ARG:HH12	16:O:131:THR:HB	1.79	0.47
24:G:608:CHL:HHC	24:G:608:CHL:HBB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:45:ARG:NH1	2:8:68:ASP:O	2.47	0.47
4:a:153:ALA:HB1	25:a:405:CLA:HED1	1.96	0.47
28:n:1623:NEX:H15	28:n:1623:NEX:H201	1.78	0.47
1:6:60:TYR:OH	1:6:72:ASP:OD2	2.30	0.47
25:B:608:CLA:H203	14:L:36:ILE:HG13	1.95	0.47
34:C:516:BCR:H19C	13:K:38:VAL:HG21	1.96	0.47
3:G:218:THR:HG21	3:G:225:ASN:HD21	1.80	0.47
17:R:54:LEU:CD1	17:R:57:THR:HG23	2.43	0.47
4:a:16:ARG:HH11	4:a:16:ARG:CG	2.27	0.47
25:b:608:CLA:H203	14:l:36:ILE:HG13	1.95	0.47
25:c:511:CLA:HBA1	34:c:517:BCR:H271	1.95	0.47
18:s:106:LEU:HG	24:s:608:CHL:HED1	1.97	0.47
18:s:135:THR:OG1	18:s:138:GLU:OE2	2.32	0.47
25:s:602:CLA:CBB	26:s:1621:LUT:H32	2.45	0.47
6:C:424:PHE:O	6:C:428:GLY:N	2.46	0.47
7:D:188:PHE:O	7:D:294:ARG:NH2	2.48	0.47
29:D:409:LHG:H252	14:L:23:LEU:HD13	1.97	0.47
3:G:41:LEU:HB2	3:G:45:SER:HB3	1.96	0.47
10:H:75:ASP:OD2	22:X:64:ALA:N	2.48	0.47
24:9:601:CHL:H162	24:9:601:CHL:H122	1.71	0.47
6:c:331:ARG:HH12	16:o:131:THR:HB	1.79	0.47
4:A:153:ALA:HB1	25:A:405:CLA:HED1	1.97	0.47
2:9:67:GLY:HA3	2:9:206:ILE:HD11	1.95	0.47
4:a:190:HIS:ND1	4:a:298:ASN:OD1	2.40	0.47
7:d:192:THR:HG23	25:d:402:CLA:HBC2	1.96	0.47
1:1:85:ARG:NH2	2:2:72:ASP:O	2.48	0.47
25:S:602:CLA:CBB	26:S:1621:LUT:H32	2.45	0.47
1:7:162:ALA:O	1:7:166:TYR:N	2.47	0.47
7:d:36:LEU:HB2	35:d:413:SQD:H182	1.97	0.47
1:y:167:ARG:NH2	24:y:609:CHL:O1D	2.45	0.47
24:1:607:CHL:H151	24:1:607:CHL:H18	1.61	0.47
2:5:135:LEU:HD11	25:5:604:CLA:HAA2	1.97	0.47
24:6:608:CHL:H12	26:6:1620:LUT:H383	1.96	0.47
4:A:225:ARG:HD3	17:R:97:ALA:HB1	1.97	0.47
36:A:413:LMG:O4	36:A:413:LMG:O5	2.29	0.47
6:C:407:PHE:HA	37:C:519:DGD:HE4	1.97	0.47
7:D:26:ARG:NH1	9:F:17:VAL:HG21	2.30	0.47
10:H:74:LEU:HB2	10:H:77:VAL:HG22	1.97	0.47
24:7:601:CHL:HAC1	29:7:2630:LHG:HC32	1.96	0.47
2:9:163:VAL:O	2:9:167:ARG:N	2.46	0.47
2:p:236:ASP:HB3	2:p:244:ASN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:36:ILE:HG22	11:i:15:PHE:HB3	1.96	0.47
4:a:82:VAL:HB	4:a:174:LEU:HB2	1.96	0.47
5:b:192:PRO:HG3	10:h:68:TYR:CD1	2.50	0.47
5:b:379:ALA:HB1	5:b:392:ILE:HG22	1.95	0.47
6:c:167:ALA:HA	6:c:172:GLY:HA2	1.97	0.47
1:1:149:ILE:HG23	1:1:150:LEU:HD12	1.96	0.47
6:C:331:ARG:NH2	16:O:131:THR:O	2.48	0.47
3:G:249:ALA:HB3	1:Y:227:GLY:HA3	1.96	0.47
25:Y:603:CLA:HBB1	24:Y:609:CHL:H152	1.97	0.47
3:q:88:TRP:HA	3:q:91:LEU:HB3	1.97	0.47
37:c:524:DGD:HBF2	21:w:90:GLY:HA3	1.96	0.47
5:B:360:PRO:HD3	5:B:366:PHE:CD2	2.49	0.47
6:C:332:SER:HB3	6:C:336:GLU:H	1.79	0.47
10:H:67:ILE:HG22	10:H:79:MET:HE1	1.96	0.47
21:W:62:ASP:OD2	21:W:64:ARG:NH2	2.48	0.47
2:8:187:ASP:OD1	26:8:1620:LUT:O23	2.33	0.47
4:a:181:ASN:HD22	7:d:314:PHE:HD1	1.62	0.47
25:c:504:CLA:H41	25:c:504:CLA:H61	1.69	0.47
18:s:196:ILE:HD11	18:s:198:LYS:HD2	1.95	0.47
17:r:249:PHE:HA	17:r:252:TYR:CD2	2.50	0.47
2:3:61:LEU:HD11	2:3:72:ASP:HB2	1.97	0.47
3:4:35:PRO:HA	3:4:37:ARG:HH11	1.80	0.47
5:B:370:LEU:HD12	5:B:379:ALA:HB3	1.96	0.47
37:C:524:DGD:HBF2	21:W:90:GLY:HA3	1.96	0.47
7:D:192:THR:HG23	25:D:402:CLA:HBC2	1.96	0.47
2:N:137:TYR:HB3	2:N:143:LEU:HD13	1.96	0.47
18:S:103:ASN:O	18:S:107:HIS:ND1	2.40	0.47
18:S:151:TYR:CE2	25:S:604:CLA:C1	2.96	0.47
25:0:612:CLA:HED3	25:9:611:CLA:HBB2	1.97	0.47
2:5:161:GLY:HA2	24:5:609:CHL:HAB	1.96	0.46
16:O:159:ALA:HA	16:O:173:LEU:HA	1.97	0.46
1:Y:222:GLN:O	1:Y:226:THR:OG1	2.30	0.46
28:Y:1623:NEX:H15	28:Y:1623:NEX:H201	1.80	0.46
24:0:606:CHL:HHC	24:0:606:CHL:HBB1	1.97	0.46
6:c:331:ARG:NH2	16:o:131:THR:O	2.47	0.46
34:c:516:BCR:H19C	13:k:38:VAL:HG21	1.96	0.46
3:g:58:PRO:HG3	3:g:194:LYS:HD3	1.97	0.46
2:n:181:TYR:HB3	25:n:610:CLA:HED2	1.96	0.46
2:n:230:PRO:O	26:n:1620:LUT:O3	2.32	0.46
13:K:28:ILE:HD12	20:V:15:VAL:HG11	1.97	0.46
17:R:249:PHE:HA	17:R:252:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:102:LEU:HD21	25:Y:612:CLA:H202	1.96	0.46
1:0:75:GLY:HA3	2:p:85:ARG:HG3	1.97	0.46
27:1:1622:XAT:H15	27:1:1622:XAT:H201	1.78	0.46
1:6:195:PRO:HA	1:6:198:PHE:HB3	1.97	0.46
4:A:156:ALA:HA	4:A:160:VAL:HB	1.98	0.46
25:C:513:CLA:H62	25:C:513:CLA:H41	1.58	0.46
16:O:124:LEU:HA	16:O:162:VAL:HG23	1.98	0.46
1:0:119:GLU:H	1:0:128:GLN:HE21	1.64	0.46
2:9:121:VAL:O	2:9:125:ALA:N	2.48	0.46
25:y:613:CLA:H61	25:y:613:CLA:H2	1.72	0.46
2:2:173:ALA:HB2	24:2:608:CHL:HBB1	1.97	0.46
1:6:225:VAL:O	1:6:252:LYS:NZ	2.43	0.46
34:A:411:BCR:H15C	34:A:411:BCR:H351	1.81	0.46
2:N:71:TRP:NE1	2:N:73:THR:HG23	2.28	0.46
1:Y:161:GLY:HA2	24:Y:609:CHL:HAB	1.97	0.46
3:q:238:ALA:N	25:q:613:CLA:O1A	2.46	0.46
4:a:225:ARG:HD3	17:r:97:ALA:HB1	1.98	0.46
28:n:1623:NEX:H35	28:n:1623:NEX:H401	1.75	0.46
2:3:237:HIS:CG	25:3:613:CLA:HAA2	2.51	0.46
2:5:204:LYS:HD3	25:5:612:CLA:HBD	1.97	0.46
4:A:36:ILE:HG22	11:I:15:PHE:HB3	1.97	0.46
6:C:246:PRO:HA	6:C:249:ARG:HE	1.79	0.46
34:c:517:BCR:H351	34:c:517:BCR:H15C	1.82	0.46
8:e:57:THR:O	8:e:61:GLN:NE2	2.49	0.46
24:n:607:CHL:H141	24:n:607:CHL:H161	1.69	0.46
1:1:135:LEU:HD21	25:1:604:CLA:HAA1	1.98	0.46
25:4:603:CLA:H2A	25:4:603:CLA:HED2	1.97	0.46
1:6:84:LYS:HA	1:6:87:ARG:HE	1.80	0.46
4:A:82:VAL:HB	4:A:174:LEU:HB2	1.96	0.46
34:B:618:BCR:H24C	34:B:618:BCR:H371	1.76	0.46
6:C:408:VAL:HG13	6:C:413:TRP:HE1	1.81	0.46
25:Y:613:CLA:H61	25:Y:613:CLA:H2	1.73	0.46
1:7:85:ARG:NH2	2:9:72:ASP:O	2.49	0.46
6:c:424:PHE:O	6:c:428:GLY:N	2.44	0.46
3:g:210:GLY:O	3:g:214:GLN:HG3	2.15	0.46
16:o:124:LEU:HA	16:o:162:VAL:HG23	1.97	0.46
2:3:249:PHE:HB3	2:3:252:LYS:HB2	1.97	0.46
3:4:229:HIS:CG	25:4:613:CLA:HAA2	2.51	0.46
1:6:163:ILE:HD13	28:6:1623:NEX:H34	1.97	0.46
7:D:19:ASP:OD2	7:D:23:ARG:NH2	2.45	0.46
3:G:210:GLY:O	3:G:214:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:81:THR:HG21	16:O:85:LYS:H	1.80	0.46
18:S:245:SER:O	18:S:249:PHE:N	2.48	0.46
2:9:173:ALA:HB2	24:9:608:CHL:HBB1	1.97	0.46
2:p:181:TYR:HB3	25:p:610:CLA:HED2	1.97	0.46
6:c:64:VAL:O	6:c:72:GLN:NE2	2.39	0.46
24:1:608:CHL:HAB	25:R:611:CLA:H2	1.97	0.46
2:5:95:ARG:NH2	2:5:180:LEU:O	2.49	0.46
26:G:1620:LUT:H35	26:G:1620:LUT:H401	1.80	0.46
2:N:230:PRO:O	26:N:1620:LUT:O3	2.34	0.46
25:R:603:CLA:H2A	25:R:603:CLA:HED2	1.98	0.46
18:s:180:GLU:OE1	18:s:183:ARG:NH2	2.49	0.46
24:1:601:CHL:HAC1	29:1:2630:LHG:HC32	1.97	0.46
2:2:245:ASN:HA	25:2:613:CLA:HAA1	1.96	0.46
3:4:196:LYS:HD3	25:4:612:CLA:HAA2	1.97	0.46
6:C:56:ASN:ND2	6:C:102:SER:OG	2.47	0.46
8:E:66:ILE:HG22	8:E:68:ASP:H	1.80	0.46
3:G:173:HIS:HB3	25:G:610:CLA:HED2	1.97	0.46
2:N:247:PHE:HA	2:N:250:ALA:HB2	1.98	0.46
24:N:601:CHL:HAC1	29:N:2630:LHG:HC11	1.98	0.46
25:N:610:CLA:H92	25:N:610:CLA:H61	1.85	0.46
1:0:84:LYS:HA	1:0:87:ARG:HE	1.81	0.46
6:c:417:SER:HB3	37:c:519:DGD:HBT2	1.97	0.46
7:d:12:ARG:HH11	7:d:12:ARG:HB2	1.79	0.46
13:k:28:ILE:HD12	20:v:15:VAL:HG11	1.97	0.46
19:t:8:PHE:HD2	19:t:9:LEU:HD12	1.80	0.46
4:A:298:ASN:ND2	6:C:390:GLY:O	2.49	0.46
7:D:21:TRP:CZ2	22:X:93:VAL:HG11	2.51	0.46
14:L:27:VAL:HG11	29:L:101:LHG:H192	1.98	0.46
27:N:1622:XAT:H31	27:N:1622:XAT:H391	1.78	0.46
18:S:151:TYR:CD2	25:S:604:CLA:H11	2.50	0.46
2:8:216:MET:HE2	26:8:1621:LUT:H10	1.98	0.46
8:e:66:ILE:HG22	8:e:68:ASP:H	1.81	0.46
1:y:216:MET:HE2	26:y:1621:LUT:H10	1.97	0.46
2:2:121:VAL:O	2:2:125:ALA:N	2.49	0.45
1:6:175:GLU:OE1	17:R:56:ASN:ND2	2.49	0.45
27:G:1622:XAT:H31	27:G:1622:XAT:H391	1.80	0.45
10:H:79:MET:N	10:H:83:THR:HG21	2.31	0.45
2:N:218:GLY:O	2:N:222:GLN:HG3	2.16	0.45
1:7:221:VAL:HG11	25:7:613:CLA:HAC2	1.98	0.45
27:9:1622:XAT:H11	27:9:1622:XAT:H191	1.80	0.45
5:b:474:ILE:O	7:d:134:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:188:PHE:O	7:d:294:ARG:NH2	2.49	0.45
29:d:409:LHG:H252	14:l:23:LEU:HD13	1.97	0.45
17:r:225:SER:OG	17:r:226:GLU:OE1	2.31	0.45
2:2:76:LEU:HD11	25:2:602:CLA:H11	1.97	0.45
2:2:169:ASN:HA	2:3:55:ASN:HD21	1.81	0.45
2:3:156:GLN:HE22	24:3:607:CHL:HMC	1.81	0.45
1:6:206:ILE:O	1:6:210:ARG:N	2.40	0.45
8:E:57:THR:O	8:E:61:GLN:NE2	2.49	0.45
14:L:15:ARG:NH2	35:b:621:SQD:O2	2.49	0.45
1:0:194:ASP:O	1:0:198:PHE:N	2.43	0.45
25:9:602:CLA:HBA1	26:9:1621:LUT:H382	1.97	0.45
4:a:156:ALA:HA	4:a:160:VAL:HB	1.98	0.45
29:s:2630:LHG:H332	29:s:2630:LHG:H301	1.82	0.45
2:3:144:VAL:HG13	24:3:605:CHL:C1D	2.46	0.45
10:H:72:LEU:HA	22:X:68:SER:HB3	1.99	0.45
24:N:607:CHL:H141	24:N:607:CHL:H161	1.70	0.45
2:9:192:ALA:HB2	25:9:610:CLA:HAA1	1.98	0.45
5:b:138:ILE:O	5:b:142:HIS:ND1	2.49	0.45
26:n:1620:LUT:H35	26:n:1620:LUT:H401	1.85	0.45
24:y:609:CHL:H193	24:y:609:CHL:H162	1.84	0.45
25:N:613:CLA:H2	25:N:613:CLA:H61	1.66	0.45
16:O:194:VAL:HG21	16:O:267:PRO:HD2	1.98	0.45
25:R:613:CLA:H62	25:R:613:CLA:H41	1.73	0.45
26:7:1620:LUT:H35	26:7:1620:LUT:H401	1.82	0.45
3:g:173:HIS:HB3	25:g:610:CLA:HED2	1.98	0.45
13:k:29:PRO:HA	13:k:32:PHE:HD2	1.81	0.45
24:y:601:CHL:HMD1	29:y:2630:LHG:H251	1.99	0.45
25:6:610:CLA:H51	25:6:612:CLA:HMA3	1.97	0.45
5:B:46:ASP:N	5:B:58:GLN:HE22	2.15	0.45
5:B:138:ILE:O	5:B:142:HIS:ND1	2.49	0.45
19:T:8:PHE:HD2	19:T:9:LEU:HD12	1.80	0.45
1:Y:216:MET:HE2	26:Y:1621:LUT:H10	1.97	0.45
1:0:152:ILE:HG13	1:0:153:LEU:HD12	1.98	0.45
3:q:203:LEU:HD11	25:q:611:CLA:HAC2	1.99	0.45
5:b:46:ASP:H	5:b:58:GLN:HE22	1.64	0.45
26:g:1620:LUT:H15	26:g:1620:LUT:H201	1.79	0.45
10:h:82:GLU:HG2	10:h:82:GLU:H	1.48	0.45
2:n:71:TRP:HD1	2:n:73:THR:HG23	1.78	0.45
25:r:616:CLA:H3A	25:r:616:CLA:HBA2	1.69	0.45
4:A:234:ASN:HB3	7:D:263:ASN:HD21	1.82	0.45
5:B:362:PHE:CZ	7:D:184:PHE:HZ	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:1621:LUT:H15	26:G:1621:LUT:H201	1.78	0.45
18:S:58:LYS:HG2	24:S:601:CHL:HBC1	1.99	0.45
18:S:102:GLU:HA	18:S:210:LEU:HD21	1.99	0.45
34:a:411:BCR:H24C	34:a:411:BCR:H371	1.80	0.45
2:n:218:GLY:O	2:n:222:GLN:HG3	2.17	0.45
18:s:57:ARG:NH2	18:s:57:ARG:CG	2.73	0.45
26:2:1621:LUT:H15	26:2:1621:LUT:H201	1.79	0.45
6:C:176:THR:HA	6:C:182:GLY:HA3	1.99	0.45
13:K:29:PRO:HA	13:K:32:PHE:HD2	1.81	0.45
28:N:1623:NEX:H35	28:N:1623:NEX:H401	1.76	0.45
1:0:211:LEU:HB3	29:0:2630:LHG:H242	1.98	0.45
2:9:245:ASN:HA	25:9:613:CLA:HAA1	1.98	0.45
26:g:1621:LUT:H201	26:g:1621:LUT:H15	1.79	0.45
24:R:607:CHL:H61	24:R:607:CHL:H41	1.83	0.45
1:7:230:PRO:O	26:7:1620:LUT:O3	2.35	0.45
28:8:1623:NEX:H11	28:8:1623:NEX:H191	1.85	0.45
37:c:524:DGD:O5E	21:w:100:GLN:O	2.34	0.45
29:c:2630:LHG:O3	29:c:2630:LHG:O1	2.30	0.45
2:n:91:LEU:HD23	2:n:180:LEU:HD22	1.98	0.45
25:r:609:CLA:HMA2	25:r:616:CLA:HMD1	1.99	0.45
25:B:613:CLA:H3A	25:B:613:CLA:HBA2	1.28	0.45
24:R:606:CHL:HMC	24:R:607:CHL:C4C	2.47	0.45
18:S:154:VAL:HG23	25:S:605:CLA:CHA	2.46	0.45
27:Y:1622:XAT:H15	27:Y:1622:XAT:H201	1.77	0.45
2:8:61:LEU:HD11	2:8:72:ASP:HB2	1.99	0.45
34:c:515:BCR:H15C	34:c:515:BCR:H351	1.75	0.45
10:h:72:LEU:HA	22:x:68:SER:HB3	1.99	0.45
18:s:53:TYR:HE2	18:s:229:GLN:HG2	1.81	0.45
25:r:603:CLA:HED2	25:r:603:CLA:H2A	1.98	0.45
25:3:603:CLA:HED2	25:3:603:CLA:H2A	1.98	0.45
25:B:613:CLA:H122	25:B:613:CLA:H162	1.81	0.45
7:D:172:SER:HB2	7:D:177:ALA:HB1	1.99	0.45
25:g:602:CLA:H141	25:g:602:CLA:H193	1.99	0.45
26:s:1621:LUT:H35	26:s:1621:LUT:H401	1.81	0.45
24:r:606:CHL:HMC	24:r:607:CHL:C4C	2.47	0.45
25:r:613:CLA:H62	25:r:613:CLA:H41	1.68	0.45
3:4:187:PRO:HA	3:4:190:PHE:HB3	1.98	0.44
26:G:1620:LUT:H15	26:G:1620:LUT:H201	1.79	0.44
16:O:201:SER:HA	16:O:211:SER:HB3	1.99	0.44
18:S:154:VAL:HG21	25:S:605:CLA:O1D	2.17	0.44
2:8:166:TYR:HD2	24:8:608:CHL:HBB1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:249:PHE:HB3	2:8:252:LYS:HB2	1.99	0.44
2:p:245:ASN:HD22	25:p:614:CLA:HED2	1.81	0.44
25:p:602:CLA:HBA1	26:p:1621:LUT:H382	1.98	0.44
5:b:383:PHE:O	16:o:213:GLY:N	2.41	0.44
6:c:166:LYS:NZ	6:c:170:PHE:O	2.50	0.44
27:g:1622:XAT:H12	29:n:2630:LHG:H192	1.99	0.44
2:2:162:LEU:O	2:2:166:TYR:N	2.42	0.44
24:4:601:CHL:HHD	29:4:2630:LHG:HC41	1.99	0.44
1:6:108:GLU:OE2	1:6:232:GLN:N	2.51	0.44
5:B:274:GLN:NE2	10:H:81:TRP:NE1	2.57	0.44
5:B:474:ILE:O	7:D:134:ARG:NH1	2.49	0.44
6:C:221:ILE:O	6:C:225:HIS:ND1	2.45	0.44
7:D:87:HIS:ND1	36:H:102:LMG:O2	2.51	0.44
10:H:80:SER:OG	10:H:81:TRP:N	2.50	0.44
25:R:613:CLA:H92	25:R:613:CLA:H61	1.83	0.44
1:0:88:GLU:HG2	1:0:180:LEU:HD21	1.98	0.44
1:0:216:MET:HE2	26:0:1621:LUT:H10	1.99	0.44
25:7:602:CLA:H41	25:7:602:CLA:H61	1.63	0.44
2:9:88:GLU:HA	2:9:180:LEU:HD21	1.98	0.44
26:9:1620:LUT:H35	26:9:1620:LUT:H401	1.79	0.44
26:9:1621:LUT:H201	26:9:1621:LUT:H15	1.77	0.44
34:d:404:BCR:H292	12:j:27:LEU:HD21	2.00	0.44
14:l:27:VAL:HG11	29:l:101:LHG:H192	1.98	0.44
18:s:87:PRO:HD2	26:s:1621:LUT:H23	1.99	0.44
16:o:159:ALA:HA	16:o:173:LEU:HA	2.00	0.44
3:4:148:GLN:HE21	24:4:609:CHL:HMC	1.81	0.44
3:4:210:GLY:O	3:4:214:GLN:HG3	2.18	0.44
4:A:85:THR:HA	4:A:109:GLY:HA3	1.99	0.44
25:B:604:CLA:H61	25:B:604:CLA:H41	1.85	0.44
25:R:609:CLA:HMA2	25:R:616:CLA:HMD1	1.98	0.44
1:Y:143:LEU:HD23	24:Y:605:CHL:HED2	2.00	0.44
1:0:195:PRO:HA	1:0:198:PHE:HB3	1.98	0.44
1:0:225:VAL:HG22	1:0:253:PHE:HE2	1.81	0.44
2:9:49:LEU:HA	24:9:601:CHL:NB	2.33	0.44
5:b:10:THR:HG21	25:b:612:CLA:HED3	2.00	0.44
8:e:64:PRO:HB3	8:e:79:LEU:HD13	1.99	0.44
28:s:1623:NEX:H15	28:s:1623:NEX:H201	1.72	0.44
1:y:161:GLY:HA2	24:y:609:CHL:HAB	1.98	0.44
5:B:359:MET:HE3	5:B:359:MET:HB2	1.83	0.44
2:p:99:LEU:HB3	25:p:604:CLA:HBB2	2.00	0.44
25:y:603:CLA:HBB1	24:y:609:CHL:H152	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:609:CLA:H2	25:r:609:CLA:H62	1.78	0.44
36:A:413:LMG:H292	36:A:413:LMG:H321	1.81	0.44
34:B:620:BCR:H15C	34:B:620:BCR:H351	1.88	0.44
2:N:201:LEU:HD23	2:N:204:LYS:HD2	1.99	0.44
18:S:154:VAL:HG22	25:S:605:CLA:C4D	2.48	0.44
24:7:609:CHL:HAA1	2:9:73:THR:HG21	1.99	0.44
34:b:619:BCR:H15C	34:b:619:BCR:H351	1.73	0.44
6:c:264:LEU:HD23	6:c:267:ILE:HD11	1.99	0.44
25:g:603:CLA:H2A	25:g:603:CLA:HED2	2.00	0.44
26:r:620:LUT:H15	26:r:620:LUT:H201	1.76	0.44
24:1:606:CHL:HMB1	24:1:609:CHL:HAC1	2.00	0.44
26:N:1620:LUT:H15	26:N:1620:LUT:H201	1.88	0.44
18:S:87:PRO:HD2	26:S:1621:LUT:H23	1.99	0.44
25:Y:613:CLA:H8	25:Y:613:CLA:H122	1.81	0.44
2:8:55:ASN:HD21	2:9:169:ASN:HA	1.81	0.44
2:9:146:ALA:HB2	24:9:606:CHL:HMD3	2.00	0.44
2:9:172:PRO:HB2	24:9:608:CHL:HBB2	1.99	0.44
2:n:144:VAL:HG23	24:n:605:CHL:C1D	2.48	0.44
28:S:1623:NEX:H11	28:S:1623:NEX:H191	1.84	0.44
29:S:2630:LHG:H332	29:S:2630:LHG:H301	1.81	0.44
1:Y:230:PRO:O	26:Y:1620:LUT:O3	2.31	0.44
5:b:157:HIS:HA	5:b:163:GLY:HA3	2.00	0.44
28:y:1623:NEX:H11	28:y:1623:NEX:H191	1.85	0.44
1:1:160:MET:HA	1:1:163:ILE:HG22	2.00	0.44
2:2:66:PRO:HG3	2:2:202:LYS:HB3	1.99	0.44
2:2:91:LEU:HD23	2:2:180:LEU:HD22	1.99	0.44
37:C:524:DGD:O5E	21:W:100:GLN:O	2.34	0.44
34:D:404:BCR:H292	12:J:27:LEU:HD21	2.00	0.44
25:G:610:CLA:H92	25:G:610:CLA:H61	1.85	0.44
24:Y:609:CHL:H111	24:Y:609:CHL:H71	1.80	0.44
4:a:85:THR:HA	4:a:109:GLY:HA3	1.99	0.44
25:b:612:CLA:H142	25:b:612:CLA:H111	1.79	0.44
1:y:89:LEU:HD21	25:y:603:CLA:HBA1	1.99	0.44
16:o:81:THR:HG21	16:o:85:LYS:H	1.82	0.44
16:o:201:SER:HA	16:o:211:SER:HB3	2.00	0.44
2:2:183:GLY:O	2:2:187:ASP:N	2.49	0.44
35:A:412:SQD:H331	25:C:504:CLA:H191	2.00	0.44
5:B:363:PHE:HB3	7:D:326:ARG:HD2	2.00	0.44
34:B:620:BCR:H11C	34:B:620:BCR:H341	1.85	0.44
25:G:613:CLA:H143	29:G:2630:LHG:H341	2.00	0.44
24:Y:601:CHL:H141	24:Y:601:CHL:H162	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:1620:LUT:H35	26:Y:1620:LUT:H401	1.80	0.44
2:9:140:ASN:HB2	2:9:143:LEU:HG	1.99	0.44
2:p:60:TYR:OH	2:p:72:ASP:OD2	2.28	0.44
25:p:603:CLA:HBC1	24:p:609:CHL:HBC2	2.00	0.44
4:a:131:TRP:O	4:a:134:SER:OG	2.33	0.44
34:h:101:BCR:H24C	34:h:101:BCR:H371	1.80	0.44
18:s:90:LEU:HD12	25:s:602:CLA:H12	2.00	0.44
1:y:143:LEU:HD23	24:y:605:CHL:HED2	1.99	0.44
24:y:609:CHL:H71	24:y:609:CHL:H111	1.79	0.44
27:r:622:XAT:H15	27:r:622:XAT:H201	1.88	0.44
3:4:52:TYR:OH	3:4:64:ASP:OD2	2.33	0.43
3:4:184:ALA:HB2	25:4:610:CLA:HAA1	1.99	0.43
1:6:162:ALA:O	1:6:166:TYR:N	2.51	0.43
4:A:190:HIS:ND1	4:A:298:ASN:OD1	2.40	0.43
34:B:620:BCR:H20C	34:B:620:BCR:H361	1.85	0.43
35:B:621:SQD:O2	14:l:15:ARG:NH2	2.49	0.43
25:G:602:CLA:H141	25:G:602:CLA:H193	2.00	0.43
16:O:173:LEU:HD23	16:O:197:TYR:HA	2.00	0.43
24:Y:609:CHL:H193	24:Y:609:CHL:H162	1.85	0.43
27:7:1622:XAT:H11	27:7:1622:XAT:H191	1.81	0.43
25:b:613:CLA:H3A	25:b:613:CLA:HBA2	1.28	0.43
2:n:46:ALA:HB1	24:n:601:CHL:HBC1	2.00	0.43
18:s:154:VAL:HG23	25:s:605:CLA:CHA	2.48	0.43
1:y:230:PRO:O	26:y:1620:LUT:O3	2.36	0.43
16:o:173:LEU:HD23	16:o:197:TYR:HA	2.00	0.43
3:4:32:TRP:HZ3	3:4:192:GLU:HG3	1.83	0.43
25:A:406:CLA:H43	29:L:101:LHG:H223	1.99	0.43
5:B:177:ARG:NH1	5:B:179:GLN:OE1	2.51	0.43
25:B:603:CLA:H143	25:B:603:CLA:H161	1.85	0.43
34:B:619:BCR:H351	34:B:619:BCR:H15C	1.73	0.43
6:C:30:LEU:H	6:C:30:LEU:HG	1.73	0.43
6:C:264:LEU:HD23	6:C:267:ILE:HD11	1.99	0.43
37:C:523:DGD:HA22	37:C:524:DGD:HB31	2.00	0.43
26:R:620:LUT:H35	26:R:620:LUT:H401	1.88	0.43
1:Y:89:LEU:HD21	25:Y:603:CLA:HBA1	1.99	0.43
25:b:613:CLA:H61	25:b:613:CLA:H102	1.82	0.43
6:c:373:GLN:HB2	6:c:376:GLN:HG3	2.00	0.43
1:y:207:LYS:NZ	25:y:611:CLA:O1D	2.45	0.43
26:1:1621:LUT:H15	26:1:1621:LUT:H201	1.84	0.43
24:3:606:CHL:HMB1	24:3:609:CHL:HMC	2.00	0.43
1:6:98:MET:SD	25:6:610:CLA:HAB	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:106:PHE:HB2	1:6:110:LEU:HD13	2.00	0.43
25:C:509:CLA:H142	25:C:509:CLA:H112	1.86	0.43
25:C:511:CLA:HBA1	34:C:517:BCR:H271	1.99	0.43
27:G:1622:XAT:H15	27:G:1622:XAT:H201	1.86	0.43
27:G:1622:XAT:H12	29:N:2630:LHG:H192	2.00	0.43
2:N:206:ILE:H	2:N:206:ILE:HG13	1.56	0.43
4:a:270:SER:OG	35:a:412:SQD:O49	2.32	0.43
26:n:1621:LUT:H35	26:n:1621:LUT:H401	1.78	0.43
18:s:102:GLU:HA	18:s:210:LEU:HD21	1.99	0.43
6:C:308:ARG:HH21	6:C:311:ARG:HG3	1.82	0.43
25:D:402:CLA:H62	25:D:402:CLA:H41	1.66	0.43
2:N:206:ILE:HD12	2:N:207:LYS:HG3	2.01	0.43
21:W:110:ASP:N	21:W:110:ASP:OD1	2.50	0.43
24:Y:601:CHL:HMD1	29:Y:2630:LHG:H251	2.00	0.43
26:7:1620:LUT:H15	26:7:1620:LUT:H201	1.80	0.43
5:b:177:ARG:NH1	5:b:179:GLN:OE1	2.51	0.43
25:b:607:CLA:H52	34:b:620:BCR:H321	2.01	0.43
6:c:318:SER:HA	16:o:157:TYR:HE1	1.84	0.43
34:c:517:BCR:H11C	34:c:517:BCR:H341	1.88	0.43
10:h:75:ASP:OD2	22:x:64:ALA:N	2.51	0.43
2:n:247:PHE:HA	2:n:250:ALA:HB2	2.00	0.43
24:y:601:CHL:H102	24:y:601:CHL:H61	1.66	0.43
25:y:602:CLA:H51	26:y:1621:LUT:H28	2.01	0.43
25:1:603:CLA:HMD3	24:1:609:CHL:HBA2	1.99	0.43
2:5:50:GLY:HA2	24:5:601:CHL:HBC3	2.00	0.43
1:6:159:LEU:HD12	24:6:606:CHL:HMA2	1.99	0.43
5:B:10:THR:HG21	25:B:612:CLA:HED3	2.00	0.43
25:B:615:CLA:H152	36:B:622:LMG:H422	2.00	0.43
3:G:87:ARG:NH1	24:G:608:CHL:OBD	2.44	0.43
10:H:80:SER:H	10:H:83:THR:HG21	1.83	0.43
2:9:137:TYR:HB3	2:9:143:LEU:HD13	2.00	0.43
25:a:406:CLA:H43	29:l:101:LHG:H223	1.99	0.43
6:c:322:PRO:HG3	7:d:350:ASN:HD22	1.84	0.43
7:d:85:MET:SD	7:d:85:MET:N	2.91	0.43
34:d:404:BCR:H11C	34:d:404:BCR:H341	1.83	0.43
2:n:221:VAL:HA	2:n:224:ILE:HG22	2.00	0.43
18:s:154:VAL:CG2	25:s:605:CLA:CHA	2.96	0.43
2:3:77:SER:HB3	2:3:83:PHE:HB2	2.01	0.43
25:C:512:CLA:H41	25:C:512:CLA:H61	1.75	0.43
29:D:408:LHG:H262	29:D:408:LHG:H291	1.78	0.43
25:G:603:CLA:H2A	25:G:603:CLA:HED2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:180:GLU:OE1	18:S:183:ARG:NH2	2.49	0.43
29:Y:2630:LHG:H292	29:Y:2630:LHG:HC91	2.00	0.43
2:9:216:MET:HE3	2:9:216:MET:HB2	1.77	0.43
4:a:234:ASN:HB3	7:d:263:ASN:HD21	1.83	0.43
25:b:615:CLA:H162	25:b:615:CLA:H141	1.83	0.43
25:g:613:CLA:H143	29:g:2630:LHG:H341	2.00	0.43
25:r:616:CLA:H203	25:r:616:CLA:H162	1.86	0.43
25:B:613:CLA:H122	25:B:613:CLA:H8	1.80	0.43
7:D:8:TYR:CZ	7:D:10:GLU:HB3	2.53	0.43
8:E:64:PRO:HB3	8:E:79:LEU:HD13	2.01	0.43
29:G:2630:LHG:H262	29:G:2630:LHG:H291	1.77	0.43
2:N:245:ASN:HB2	25:N:614:CLA:HED3	2.00	0.43
25:Y:611:CLA:H122	25:Y:612:CLA:H141	2.01	0.43
25:7:614:CLA:HBA2	25:7:614:CLA:H3A	1.59	0.43
25:8:603:CLA:HMD3	24:8:609:CHL:HBA2	2.01	0.43
25:q:602:CLA:HBA1	26:q:1621:LUT:H382	2.01	0.43
25:c:505:CLA:H71	25:c:505:CLA:H112	1.81	0.43
25:c:512:CLA:H41	25:c:512:CLA:H61	1.81	0.43
37:c:519:DGD:HA22	37:c:519:DGD:HA52	1.80	0.43
7:d:172:SER:HB2	7:d:177:ALA:HB1	1.99	0.43
18:s:88:LEU:O	26:s:1621:LUT:O23	2.36	0.43
16:o:257:GLU:HA	16:o:289:GLN:HA	2.01	0.43
2:5:83:PHE:HA	2:5:86:TYR:HD2	1.84	0.43
25:5:602:CLA:HBA1	26:5:1621:LUT:H382	2.01	0.43
5:B:157:HIS:HA	5:B:163:GLY:HA3	2.00	0.43
39:D:405:PL9:H322	39:D:405:PL9:H28	1.81	0.43
24:G:601:CHL:H91	24:G:601:CHL:H112	1.81	0.43
2:N:135:LEU:HB3	2:N:146:ALA:HB3	2.01	0.43
24:N:608:CHL:H3A	36:S:2631:LMG:H192	2.01	0.43
16:O:257:GLU:HA	16:O:289:GLN:HA	2.01	0.43
25:Y:602:CLA:H51	26:Y:1621:LUT:H28	2.01	0.43
1:0:224:ILE:HA	3:q:247:PRO:HG3	2.00	0.43
24:8:606:CHL:HMB1	24:8:609:CHL:HMC	2.01	0.43
7:d:8:TYR:CZ	7:d:10:GLU:HB3	2.54	0.43
21:w:110:ASP:N	21:w:110:ASP:OD1	2.50	0.43
24:y:601:CHL:H203	24:y:601:CHL:H161	1.84	0.43
24:r:607:CHL:HBA1	24:r:607:CHL:H3A	1.91	0.43
24:r:608:CHL:H93	24:r:608:CHL:H61	1.89	0.43
28:r:623:NEX:H11	28:r:623:NEX:H191	1.80	0.43
2:2:63:GLY:N	2:2:68:ASP:OD2	2.51	0.43
3:4:53:LEU:HD13	3:4:62:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:165:LEU:HD13	24:4:608:CHL:HBB1	2.00	0.43
25:B:610:CLA:H141	25:B:610:CLA:H161	1.80	0.43
6:C:79:HIS:NE2	25:C:502:CLA:O1D	2.43	0.43
16:O:148:GLU:HB3	16:O:182:LYS:HG3	2.01	0.43
28:R:623:NEX:H35	28:R:623:NEX:H401	1.87	0.43
18:S:60:PHE:HB3	18:S:85:TYR:HB2	2.01	0.43
2:8:237:HIS:CG	25:8:613:CLA:HAA2	2.53	0.43
2:9:42:GLY:O	2:9:45:ARG:NH1	2.39	0.43
24:p:606:CHL:HHC	24:p:606:CHL:HBB1	2.00	0.43
25:b:603:CLA:H171	36:h:102:LMG:H411	2.01	0.43
25:y:610:CLA:H92	25:y:610:CLA:H61	1.89	0.43
1:1:172:PRO:HG2	24:1:608:CHL:HBB2	2.01	0.43
3:4:217:VAL:HG13	3:4:245:PHE:HE2	1.84	0.43
25:C:505:CLA:H92	25:C:505:CLA:H61	1.88	0.43
25:7:602:CLA:H62	25:7:603:CLA:H3A	2.00	0.43
2:8:63:GLY:HA2	2:8:68:ASP:HB3	2.00	0.43
25:b:615:CLA:H152	36:b:622:LMG:H422	2.00	0.43
18:s:156:TRP:CZ2	25:s:605:CLA:HHC	2.54	0.43
18:s:245:SER:O	18:s:249:PHE:N	2.50	0.43
26:y:1621:LUT:H15	26:y:1621:LUT:H201	1.83	0.43
2:3:63:GLY:HA2	2:3:68:ASP:HB3	2.01	0.42
4:A:221:SER:HA	7:D:139:ARG:HB2	2.01	0.42
26:R:620:LUT:H15	26:R:620:LUT:H201	1.76	0.42
24:Y:607:CHL:H92	24:Y:607:CHL:H62	1.82	0.42
1:0:160:MET:HE3	1:0:160:MET:HB3	1.68	0.42
2:p:91:LEU:HD23	2:p:180:LEU:HD22	2.01	0.42
35:b:621:SQD:H161	35:b:621:SQD:H191	1.88	0.42
27:g:1622:XAT:H11	27:g:1622:XAT:H191	1.91	0.42
29:g:2630:LHG:H262	29:g:2630:LHG:H291	1.76	0.42
28:1:1623:NEX:H15	28:1:1623:NEX:H201	1.78	0.42
2:2:169:ASN:OD1	2:3:55:ASN:ND2	2.53	0.42
25:3:602:CLA:CAB	26:3:1621:LUT:H32	2.49	0.42
5:B:192:PRO:HG3	10:H:68:TYR:CD1	2.54	0.42
5:B:360:PRO:HD3	5:B:366:PHE:HD2	1.84	0.42
25:B:603:CLA:H171	36:H:102:LMG:H411	2.00	0.42
25:B:615:CLA:H91	25:B:615:CLA:H112	1.85	0.42
16:O:184:THR:HG23	16:O:186:ASP:H	1.84	0.42
5:b:125:ASP:OD1	5:b:128:THR:OG1	2.37	0.42
6:c:333:PRO:HB3	16:o:127:ARG:HD3	2.01	0.42
7:d:141:TYR:OH	29:d:408:LHG:O4	2.32	0.42
26:g:1621:LUT:H35	26:g:1621:LUT:H401	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:r:623:NEX:H15	28:r:623:NEX:H201	1.90	0.42
24:1:608:CHL:HHC	24:1:608:CHL:HBB1	2.00	0.42
27:3:1622:XAT:H15	27:3:1622:XAT:H201	1.81	0.42
34:A:411:BCR:H371	34:A:411:BCR:H24C	1.80	0.42
34:C:517:BCR:H11C	34:C:517:BCR:H341	1.88	0.42
29:C:2630:LHG:H383	29:C:2630:LHG:H351	1.92	0.42
24:N:607:CHL:H141	24:N:607:CHL:H202	2.02	0.42
25:R:601:CLA:HBC2	29:R:2630:LHG:HC42	1.99	0.42
3:q:210:GLY:O	3:q:214:GLN:HG3	2.19	0.42
5:b:60:MET:HB3	5:b:60:MET:HE3	1.63	0.42
5:b:92:SER:OG	5:b:93:TYR:N	2.52	0.42
6:c:115:PHE:HA	25:c:511:CLA:H191	2.00	0.42
37:c:523:DGD:HA22	37:c:524:DGD:HB31	2.00	0.42
24:g:601:CHL:H62	24:g:601:CHL:H41	1.74	0.42
27:n:1622:XAT:H201	27:n:1622:XAT:H15	1.80	0.42
25:y:611:CLA:H142	25:y:611:CLA:H112	1.89	0.42
6:C:115:PHE:HA	25:C:511:CLA:H191	2.01	0.42
34:C:517:BCR:H371	34:C:517:BCR:H24C	1.72	0.42
27:R:622:XAT:H35	27:R:622:XAT:H401	1.86	0.42
28:7:1623:NEX:H191	28:7:1623:NEX:H11	1.77	0.42
25:q:604:CLA:HBA2	25:q:604:CLA:H3A	1.69	0.42
5:b:173:GLY:HA3	5:b:265:ILE:HD11	2.00	0.42
34:b:619:BCR:H24C	34:b:619:BCR:H371	1.78	0.42
3:g:129:TYR:HB3	3:g:135:LEU:HD13	2.01	0.42
2:2:85:ARG:HG3	2:3:75:GLY:HA3	2.01	0.42
25:B:602:CLA:H143	25:B:602:CLA:H161	1.90	0.42
25:B:609:CLA:H91	25:B:609:CLA:H112	1.86	0.42
37:C:518:DGD:HB62	37:C:518:DGD:HB91	1.88	0.42
26:G:1621:LUT:H372	25:Y:603:CLA:HED3	2.00	0.42
26:R:620:LUT:H31	26:R:620:LUT:H391	1.86	0.42
7:d:13:THR:CG2	10:h:44:TRP:NE1	2.62	0.42
25:d:402:CLA:H62	25:d:402:CLA:H41	1.66	0.42
34:d:404:BCR:H20C	34:d:404:BCR:H361	1.82	0.42
28:s:1623:NEX:H11	28:s:1623:NEX:H191	1.85	0.42
3:4:195:VAL:HG12	25:4:611:CLA:HED1	2.01	0.42
2:5:206:ILE:HG13	2:5:210:ARG:HG3	2.02	0.42
5:B:108:PHE:O	5:B:111:SER:OG	2.31	0.42
25:B:612:CLA:H142	25:B:612:CLA:H111	1.79	0.42
6:C:221:ILE:HG23	25:C:501:CLA:HMA3	2.01	0.42
3:G:68:LEU:HD13	25:G:602:CLA:H42	2.02	0.42
1:Y:50:LEU:O	24:Y:601:CHL:HBB1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:610:CLA:H2	26:Y:1620:LUT:H28	2.00	0.42
26:0:1621:LUT:H372	25:p:603:CLA:HED3	2.01	0.42
3:q:195:VAL:HG12	25:q:611:CLA:HED1	2.02	0.42
3:g:37:ARG:NH1	3:g:54:THR:O	2.52	0.42
27:n:1622:XAT:H31	27:n:1622:XAT:H391	1.79	0.42
25:y:611:CLA:H122	25:y:612:CLA:H141	2.01	0.42
27:y:1622:XAT:H31	27:y:1622:XAT:H391	1.78	0.42
25:r:601:CLA:HBC2	29:r:2630:LHG:HC42	2.01	0.42
26:2:1620:LUT:H11	26:2:1620:LUT:H191	1.85	0.42
2:3:105:ILE:HG23	2:3:109:LEU:HD13	2.01	0.42
25:5:603:CLA:HBC1	24:5:609:CHL:HBC2	2.00	0.42
25:B:607:CLA:H52	34:B:620:BCR:H321	2.02	0.42
6:C:318:SER:HA	16:O:157:TYR:HE1	1.84	0.42
3:G:87:ARG:NH2	3:G:197:GLU:OE2	2.52	0.42
2:N:50:GLY:O	2:N:53:SER:OG	2.31	0.42
1:Y:143:LEU:HD23	1:Y:143:LEU:HA	1.92	0.42
25:Y:602:CLA:H141	25:Y:602:CLA:H162	1.85	0.42
1:0:172:PRO:HB3	17:r:54:LEU:HD13	2.00	0.42
2:8:60:TYR:OH	2:8:72:ASP:OD2	2.29	0.42
25:8:602:CLA:CAB	26:8:1621:LUT:H32	2.49	0.42
26:8:1621:LUT:H11	26:8:1621:LUT:H191	1.92	0.42
26:9:1621:LUT:H35	26:9:1621:LUT:H401	1.79	0.42
34:a:411:BCR:H11C	34:a:411:BCR:H341	1.91	0.42
25:b:613:CLA:H122	25:b:613:CLA:H8	1.80	0.42
25:c:513:CLA:H62	25:c:513:CLA:H41	1.60	0.42
24:g:601:CHL:H91	24:g:601:CHL:H112	1.81	0.42
18:s:60:PHE:HB3	18:s:85:TYR:HB2	2.02	0.42
2:2:216:MET:HE3	2:2:216:MET:HB2	1.82	0.42
2:5:89:LEU:O	2:5:93:HIS:ND1	2.48	0.42
25:5:603:CLA:HED3	26:6:1621:LUT:H372	2.02	0.42
4:A:183:MET:HB3	25:A:405:CLA:HBC2	2.02	0.42
4:A:308:ASP:O	9:F:44:ARG:NH2	2.40	0.42
5:B:171:PRO:HG3	10:H:85:ALA:HB2	1.75	0.42
29:C:2630:LHG:O3	29:C:2630:LHG:O1	2.37	0.42
10:H:79:MET:HE3	10:H:79:MET:HB2	1.74	0.42
18:S:115:ALA:HA	18:S:249:PHE:HE2	1.85	0.42
28:Y:1623:NEX:H35	28:Y:1623:NEX:H401	1.87	0.42
26:7:1620:LUT:H31	26:7:1620:LUT:H391	1.96	0.42
2:p:167:ARG:HH21	24:p:609:CHL:HMA3	1.85	0.42
5:b:367:PRO:HB2	7:d:345:VAL:CG2	2.49	0.42
18:s:151:TYR:HE2	25:s:604:CLA:HBA2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:163:VAL:O	2:2:167:ARG:N	2.46	0.42
25:C:513:CLA:H13	29:C:2630:LHG:H181	2.02	0.42
34:C:516:BCR:HC7	23:Z:20:VAL:HG21	2.02	0.42
25:G:613:CLA:H111	29:G:2630:LHG:H341	2.02	0.42
2:N:143:LEU:HD23	2:N:143:LEU:HA	1.92	0.42
28:N:1623:NEX:H11	28:N:1623:NEX:H191	1.94	0.42
17:R:78:LEU:HD12	27:R:622:XAT:H23	2.01	0.42
18:S:90:LEU:HD12	25:S:602:CLA:H12	2.01	0.42
1:7:218:GLY:O	1:7:222:GLN:HG3	2.19	0.42
3:q:156:GLU:HB3	24:q:609:CHL:C1B	2.49	0.42
4:a:301:ASN:OD1	4:a:303:ASN:ND2	2.53	0.42
25:b:605:CLA:HMD2	25:b:613:CLA:H202	2.01	0.42
25:c:504:CLA:H112	25:c:504:CLA:H142	1.87	0.42
25:c:507:CLA:H112	25:c:507:CLA:H91	1.77	0.42
7:d:12:ARG:CB	7:d:12:ARG:NH1	2.83	0.42
3:g:37:ARG:NH2	3:g:60:ASP:OD2	2.53	0.42
3:g:80:GLU:HA	3:g:172:LEU:HD21	2.01	0.42
19:t:16:ILE:O	19:t:20:SER:N	2.51	0.42
1:y:50:LEU:O	24:y:601:CHL:HBB1	2.20	0.42
1:y:216:MET:HG2	26:y:1621:LUT:H12	2.02	0.42
29:y:2630:LHG:H182	29:y:2630:LHG:H152	1.90	0.42
17:r:54:LEU:CD1	17:r:57:THR:CG2	2.92	0.42
16:o:105:THR:O	16:o:281:LYS:N	2.52	0.42
16:o:148:GLU:HB3	16:o:182:LYS:HG3	2.02	0.42
1:1:189:LEU:HD12	26:1:1620:LUT:H222	2.02	0.42
3:4:144:THR:HG23	3:4:145:LEU:HD12	2.02	0.42
1:6:228:LYS:HD3	1:6:232:GLN:HG2	2.02	0.42
4:A:301:ASN:OD1	4:A:303:ASN:ND2	2.53	0.42
5:B:138:ILE:HG21	5:B:138:ILE:HD13	1.81	0.42
5:B:483:ASP:OD1	5:B:483:ASP:N	2.52	0.42
6:C:148:ILE:O	6:C:152:HIS:ND1	2.42	0.42
8:E:10:PHE:HA	8:E:13:ILE:HD12	2.01	0.42
24:G:607:CHL:HAA2	27:G:1622:XAT:H41	2.02	0.42
27:N:1622:XAT:H15	27:N:1622:XAT:H201	1.79	0.42
28:N:1623:NEX:H15	28:N:1623:NEX:H201	1.78	0.42
18:S:78:GLU:HG3	18:S:79:LEU:HD12	2.02	0.42
1:Y:222:GLN:HE22	26:Y:1620:LUT:H42	1.84	0.42
1:0:163:ILE:HA	1:0:166:TYR:HB2	2.01	0.42
34:c:517:BCR:H24C	34:c:517:BCR:H371	1.72	0.42
7:d:21:TRP:CZ2	22:x:93:VAL:HG11	2.54	0.42
3:g:68:LEU:HD13	25:g:602:CLA:H42	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:156:TRP:CD1	18:s:156:TRP:N	2.87	0.42
1:y:222:GLN:O	1:y:226:THR:OG1	2.30	0.42
24:y:607:CHL:H62	24:y:607:CHL:H92	1.75	0.42
17:r:78:LEU:HD12	27:r:622:XAT:H23	2.01	0.42
24:1:601:CHL:HMD1	29:1:2630:LHG:H251	2.02	0.41
3:4:65:THR:OG1	24:6:609:CHL:O1A	2.37	0.41
25:B:605:CLA:HMD2	25:B:613:CLA:H202	2.02	0.41
6:C:142:LYS:HE3	6:C:254:TRP:CD2	2.55	0.41
26:N:1621:LUT:H35	26:N:1621:LUT:H401	1.78	0.41
16:O:94:LEU:HB2	16:O:139:PHE:HB2	2.01	0.41
17:R:249:PHE:HA	17:R:252:TYR:HD2	1.85	0.41
18:S:88:LEU:O	26:S:1621:LUT:O23	2.37	0.41
24:7:607:CHL:H18	24:7:607:CHL:H151	1.62	0.41
24:8:601:CHL:HBA1	24:8:601:CHL:H3A	1.85	0.41
4:a:183:MET:HB3	25:a:405:CLA:HBC2	2.02	0.41
25:b:606:CLA:H92	25:b:606:CLA:H61	1.92	0.41
25:c:505:CLA:H171	37:c:518:DGD:HA61	2.02	0.41
25:g:613:CLA:H111	29:g:2630:LHG:H341	2.03	0.41
27:g:1622:XAT:H31	27:g:1622:XAT:H391	1.81	0.41
18:s:115:ALA:HA	18:s:249:PHE:HE2	1.85	0.41
24:y:601:CHL:HMA3	29:y:2630:LHG:H112	2.01	0.41
25:r:603:CLA:H71	25:r:603:CLA:H111	1.84	0.41
2:2:137:TYR:HB3	2:2:143:LEU:HD13	2.02	0.41
2:5:245:ASN:HA	25:5:613:CLA:HAA1	2.01	0.41
24:N:609:CHL:H161	24:N:609:CHL:H141	1.88	0.41
24:Y:609:CHL:H143	24:Y:609:CHL:H161	1.91	0.41
24:7:601:CHL:HMD1	29:7:2630:LHG:H251	2.02	0.41
6:c:142:LYS:HE3	6:c:254:TRP:CD2	2.55	0.41
1:6:221:VAL:HG11	25:6:613:CLA:HAC2	2.02	0.41
5:B:224:ARG:NH1	7:D:16:ASP:OD2	2.49	0.41
25:B:607:CLA:H111	25:B:607:CLA:H152	1.67	0.41
34:C:514:BCR:H15C	34:C:514:BCR:H351	1.83	0.41
27:G:1622:XAT:H10	29:N:2630:LHG:H212	2.02	0.41
18:S:58:LYS:HE2	29:S:2630:LHG:HC11	2.01	0.41
24:Y:601:CHL:H203	24:Y:601:CHL:H161	1.85	0.41
1:7:189:LEU:HD12	26:7:1620:LUT:H222	2.03	0.41
24:q:601:CHL:HBA1	24:q:601:CHL:H3A	1.81	0.41
4:a:221:SER:HA	7:d:139:ARG:HB2	2.02	0.41
1:1:163:ILE:HD11	24:1:608:CHL:C3B	2.50	0.41
2:5:85:ARG:HG3	1:6:75:GLY:HA3	2.02	0.41
28:6:1623:NEX:H15	28:6:1623:NEX:H201	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:409:PHO:H112	33:A:409:PHO:H72	1.85	0.41
5:B:125:ASP:OD1	5:B:128:THR:OG1	2.37	0.41
25:G:602:CLA:H192	26:G:1621:LUT:H393	2.02	0.41
25:N:603:CLA:H61	25:N:603:CLA:H2	1.85	0.41
24:7:607:CHL:H41	24:7:607:CHL:H61	1.85	0.41
26:8:1621:LUT:H35	26:8:1621:LUT:H401	1.83	0.41
33:a:408:PHO:H102	33:a:408:PHO:H13	1.87	0.41
25:b:614:CLA:H3A	25:b:614:CLA:HBA1	1.80	0.41
24:g:601:CHL:H122	24:y:607:CHL:H192	2.02	0.41
25:3:613:CLA:C3B	26:3:1620:LUT:H183	2.51	0.41
1:6:225:VAL:HG22	1:6:253:PHE:HE2	1.85	0.41
35:A:412:SQD:O8	35:A:412:SQD:O3	2.31	0.41
35:B:621:SQD:H161	35:B:621:SQD:H191	1.88	0.41
34:C:515:BCR:H351	34:C:515:BCR:H15C	1.76	0.41
37:C:524:DGD:HB71	25:Y:611:CLA:H93	2.02	0.41
7:D:145:ALA:HB2	7:D:272:LEU:HD11	2.03	0.41
1:0:98:MET:SD	25:0:610:CLA:HAB	2.60	0.41
27:7:1622:XAT:H31	27:7:1622:XAT:H391	1.87	0.41
26:8:1621:LUT:H15	26:8:1621:LUT:H201	1.86	0.41
2:9:91:LEU:HD23	2:9:180:LEU:HD22	2.01	0.41
2:p:226:THR:HG21	2:p:233:ASN:HD21	1.86	0.41
26:p:1621:LUT:H372	25:q:603:CLA:HED3	2.02	0.41
5:b:138:ILE:HG12	5:b:142:HIS:HE1	1.86	0.41
3:g:40:PHE:CG	3:g:63:TRP:HB2	2.55	0.41
17:r:255:GLN:HE22	26:r:620:LUT:H42	1.86	0.41
16:o:94:LEU:H	16:o:138:SER:HA	1.85	0.41
26:2:1621:LUT:H401	26:2:1621:LUT:H35	1.77	0.41
28:6:1623:NEX:H35	28:6:1623:NEX:H401	1.83	0.41
5:B:362:PHE:CZ	7:D:184:PHE:CZ	3.08	0.41
5:B:477:ASP:OD1	5:B:477:ASP:N	2.54	0.41
34:B:619:BCR:H11C	34:B:619:BCR:H341	1.82	0.41
34:C:517:BCR:H15C	34:C:517:BCR:H351	1.82	0.41
17:R:173:ALA:O	17:R:180:LEU:N	2.53	0.41
1:0:177:LEU:HD13	1:0:182:PRO:HB2	2.02	0.41
25:0:613:CLA:H2	25:0:613:CLA:H61	1.66	0.41
1:7:169:ASN:HD22	2:9:55:ASN:HB2	1.86	0.41
2:9:69:TYR:HB2	25:9:602:CLA:HMD3	2.02	0.41
25:9:603:CLA:H2	25:9:603:CLA:H61	1.81	0.41
25:b:607:CLA:H152	25:b:607:CLA:H111	1.68	0.41
25:b:610:CLA:H141	25:b:610:CLA:H161	1.80	0.41
37:c:524:DGD:HB71	25:y:611:CLA:H93	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:41:LEU:HB2	3:g:45:SER:HB3	2.01	0.41
25:g:610:CLA:H152	25:g:610:CLA:H111	1.88	0.41
25:n:613:CLA:H61	25:n:613:CLA:H2	1.67	0.41
1:y:88:GLU:HG3	24:y:609:CHL:HED1	2.02	0.41
16:o:94:LEU:HB2	16:o:139:PHE:HB2	2.02	0.41
28:1:1623:NEX:H11	28:1:1623:NEX:H191	1.81	0.41
4:A:232:SER:HB2	5:B:4:PRO:HG3	2.03	0.41
6:C:166:LYS:NZ	6:C:170:PHE:O	2.53	0.41
7:D:13:THR:CG2	10:H:44:TRP:HE1	2.31	0.41
26:G:1620:LUT:H31	26:G:1620:LUT:H391	1.91	0.41
26:G:1621:LUT:H35	26:G:1621:LUT:H401	1.77	0.41
24:N:607:CHL:H161	24:N:607:CHL:H202	1.77	0.41
25:R:603:CLA:H71	25:R:603:CLA:H111	1.84	0.41
25:Y:613:CLA:H112	25:Y:613:CLA:H152	1.94	0.41
2:8:143:LEU:HB3	2:8:144:VAL:H	1.67	0.41
2:9:49:LEU:HD23	2:9:53:SER:HB3	2.01	0.41
25:b:606:CLA:H162	25:b:606:CLA:H193	1.87	0.41
3:g:122:PHE:HZ	2:n:247:PHE:HB3	1.86	0.41
2:n:143:LEU:HD23	2:n:143:LEU:HA	1.88	0.41
23:z:47:TRP:HE3	23:z:48:LEU:HD22	1.86	0.41
25:2:603:CLA:H2	25:2:603:CLA:H61	1.83	0.41
3:4:111:GLU:O	3:4:120:GLN:NE2	2.53	0.41
1:6:42:TYR:OH	1:6:199:ALA:O	2.33	0.41
1:6:50:LEU:O	24:6:601:CHL:HBB1	2.21	0.41
24:6:606:CHL:HHC	24:6:606:CHL:HBB1	2.01	0.41
34:A:411:BCR:H11C	34:A:411:BCR:H341	1.91	0.41
25:B:610:CLA:H92	35:D:413:SQD:H292	2.03	0.41
25:C:505:CLA:H71	25:C:505:CLA:HAB	2.03	0.41
2:N:45:ARG:NH1	2:N:68:ASP:O	2.54	0.41
25:R:616:CLA:HBA2	25:R:616:CLA:H3A	1.69	0.41
28:S:1623:NEX:H15	28:S:1623:NEX:H201	1.73	0.41
2:p:129:ILE:HG13	2:p:135:LEU:HB2	2.03	0.41
7:d:145:ALA:HB2	7:d:272:LEU:HD11	2.03	0.41
39:d:405:PL9:H322	39:d:405:PL9:H28	1.81	0.41
29:d:408:LHG:H262	29:d:408:LHG:H291	1.78	0.41
18:s:58:LYS:HE3	29:s:2630:LHG:O1	2.20	0.41
18:s:176:MET:HA	18:s:179:VAL:HB	2.02	0.41
1:1:216:MET:HA	1:1:219:PHE:HB2	2.02	0.41
2:2:51:PRO:HD2	24:2:601:CHL:HBB1	2.02	0.41
25:3:603:CLA:HMD3	24:3:609:CHL:HBA2	2.03	0.41
26:3:1621:LUT:H401	26:3:1621:LUT:H35	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:119:GLU:HB3	1:6:128:GLN:HE21	1.86	0.41
4:A:283:ILE:HA	4:A:286:THR:HG22	2.03	0.41
6:C:373:GLN:HB2	6:C:376:GLN:HG3	2.02	0.41
25:C:506:CLA:H93	25:C:506:CLA:H111	1.94	0.41
25:C:513:CLA:H91	25:C:513:CLA:H111	1.87	0.41
7:D:53:THR:HA	7:D:67:TYR:HD2	1.86	0.41
34:D:404:BCR:H11C	34:D:404:BCR:H341	1.83	0.41
34:H:101:BCR:H15C	34:H:101:BCR:H351	1.78	0.41
17:R:255:GLN:HE22	26:R:620:LUT:H42	1.86	0.41
1:Y:167:ARG:NH2	24:Y:609:CHL:O1D	2.50	0.41
26:Y:1620:LUT:H11	26:Y:1620:LUT:H191	1.91	0.41
1:0:60:TYR:CZ	1:0:78:ALA:HA	2.56	0.41
28:0:1623:NEX:H11	28:0:1623:NEX:H191	1.90	0.41
3:q:225:ASN:ND2	25:q:613:CLA:O1D	2.53	0.41
4:a:283:ILE:HA	4:a:286:THR:HG22	2.03	0.41
25:b:603:CLA:H203	7:d:154:VAL:HG13	2.03	0.41
25:b:603:CLA:H143	25:b:603:CLA:H161	1.85	0.41
25:c:505:CLA:H71	25:c:505:CLA:HAB	2.03	0.41
34:c:516:BCR:HC7	23:z:20:VAL:HG21	2.02	0.41
34:d:404:BCR:H14C	9:f:32:PHE:CD2	2.56	0.41
3:g:214:GLN:HE22	26:g:1620:LUT:H42	1.86	0.41
25:g:602:CLA:H141	25:g:602:CLA:H161	1.88	0.41
29:l:101:LHG:H322	15:m:18:PRO:HB3	2.03	0.41
1:y:88:GLU:HG3	24:y:609:CHL:CED	2.51	0.41
24:y:601:CHL:H141	24:y:601:CHL:H162	1.84	0.41
26:y:1620:LUT:H15	26:y:1620:LUT:H201	1.88	0.41
27:r:622:XAT:H31	27:r:622:XAT:H391	1.97	0.41
1:1:230:PRO:O	26:1:1620:LUT:O3	2.38	0.41
5:B:359:MET:HA	5:B:366:PHE:HD2	1.86	0.41
6:C:333:PRO:HB3	16:O:127:ARG:HD3	2.02	0.41
29:L:101:LHG:H322	15:M:18:PRO:HB3	2.03	0.41
24:R:608:CHL:H91	24:R:608:CHL:H112	1.86	0.41
1:7:149:ILE:HG23	1:7:150:LEU:HD12	2.02	0.41
1:7:194:ASP:OD1	1:7:194:ASP:N	2.53	0.41
27:7:1622:XAT:H35	27:7:1622:XAT:H401	1.81	0.41
26:8:1620:LUT:H31	26:8:1620:LUT:H391	1.89	0.41
2:9:183:GLY:O	2:9:187:ASP:N	2.51	0.41
25:b:610:CLA:H92	35:d:413:SQD:H292	2.03	0.41
34:b:618:BCR:H371	34:b:618:BCR:H24C	1.76	0.41
34:c:516:BCR:H15C	34:c:516:BCR:H351	1.91	0.41
24:g:607:CHL:HAA2	27:g:1622:XAT:H41	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:101:BCR:H20C	34:h:101:BCR:H361	1.96	0.41
2:3:80:PRO:HA	2:3:83:PHE:HB3	2.02	0.40
5:B:366:PHE:CD1	5:B:367:PRO:CD	2.77	0.40
25:C:505:CLA:H171	37:C:518:DGD:HA61	2.01	0.40
25:D:403:CLA:H141	25:D:403:CLA:H162	1.89	0.40
25:D:403:CLA:H92	25:D:403:CLA:H61	1.87	0.40
3:G:80:GLU:HA	3:G:172:LEU:HD21	2.02	0.40
26:N:1621:LUT:H15	26:N:1621:LUT:H201	1.79	0.40
27:N:1622:XAT:H11	27:N:1622:XAT:H191	1.84	0.40
16:O:257:GLU:OE1	16:O:287:TYR:OH	2.39	0.40
36:a:413:LMG:H321	36:a:413:LMG:H292	1.81	0.40
5:b:243:ALA:HB2	5:b:466:HIS:CE1	2.57	0.40
6:c:407:PHE:HA	37:c:519:DGD:HE4	2.03	0.40
25:g:613:CLA:H2	25:g:613:CLA:H61	1.67	0.40
27:n:1622:XAT:H35	27:n:1622:XAT:H401	1.88	0.40
17:r:71:ARG:HG3	25:r:601:CLA:HAC2	2.04	0.40
25:1:602:CLA:H41	25:1:602:CLA:H61	1.72	0.40
27:1:1622:XAT:H35	27:1:1622:XAT:H401	1.81	0.40
3:4:51:ALA:O	3:4:54:THR:OG1	2.34	0.40
7:D:141:TYR:OH	29:D:408:LHG:O4	2.32	0.40
24:N:609:CHL:H91	24:N:609:CHL:H111	1.84	0.40
26:S:1621:LUT:H11	26:S:1621:LUT:H191	1.85	0.40
1:Y:222:GLN:NE2	26:Y:1620:LUT:H42	2.36	0.40
25:Y:603:CLA:H92	25:Y:603:CLA:H62	1.88	0.40
2:8:108:GLU:OE2	2:8:232:GLN:N	2.52	0.40
2:p:83:PHE:HA	2:p:86:TYR:HD2	1.86	0.40
3:q:80:GLU:HA	3:q:172:LEU:HD11	2.02	0.40
3:q:135:LEU:HD23	3:q:135:LEU:HA	1.93	0.40
5:b:280:PHE:CE2	5:b:312:TYR:HB3	2.57	0.40
6:c:397:GLY:HA3	6:c:401:GLU:HG2	2.04	0.40
37:c:518:DGD:HB91	37:c:518:DGD:HB62	1.88	0.40
25:y:613:CLA:H122	25:y:613:CLA:H8	1.81	0.40
27:1:1622:XAT:H191	27:1:1622:XAT:H11	1.80	0.40
2:2:222:GLN:HE22	26:2:1620:LUT:H42	1.87	0.40
28:3:1623:NEX:H11	28:3:1623:NEX:H191	1.86	0.40
1:6:173:LEU:HA	17:R:55:PRO:HB2	2.03	0.40
33:A:408:PHO:H102	33:A:408:PHO:H13	1.87	0.40
5:B:92:SER:OG	5:B:93:TYR:N	2.53	0.40
25:B:612:CLA:H72	25:B:612:CLA:H112	1.85	0.40
25:B:614:CLA:HBA1	25:B:614:CLA:H3A	1.80	0.40
36:H:102:LMG:H142	36:H:102:LMG:H111	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:171:ASP:OD1	17:R:171:ASP:N	2.54	0.40
18:S:58:LYS:HE2	29:S:2630:LHG:C1	2.51	0.40
27:Y:1622:XAT:H31	27:Y:1622:XAT:H391	1.78	0.40
25:b:612:CLA:H72	25:b:612:CLA:H112	1.85	0.40
6:c:408:VAL:HG23	6:c:413:TRP:HE1	1.86	0.40
26:n:1620:LUT:H15	26:n:1620:LUT:H201	1.85	0.40
25:y:602:CLA:H111	25:y:602:CLA:H93	1.84	0.40
26:y:1621:LUT:H35	26:y:1621:LUT:H401	1.82	0.40
17:r:249:PHE:HA	17:r:252:TYR:HD2	1.85	0.40
16:o:257:GLU:OE1	16:o:287:TYR:OH	2.38	0.40
27:1:1622:XAT:H31	27:1:1622:XAT:H391	1.86	0.40
2:2:200:GLU:HG2	2:2:204:LYS:HE3	2.03	0.40
25:B:603:CLA:H203	7:D:154:VAL:HG13	2.04	0.40
6:C:447:ILE:HB	7:D:223:PHE:HD1	1.86	0.40
25:C:511:CLA:H91	25:C:511:CLA:H112	1.88	0.40
25:N:603:CLA:H62	25:N:603:CLA:H92	1.85	0.40
18:S:143:MET:HG2	18:S:147:GLY:HA2	2.04	0.40
27:Y:1622:XAT:H11	27:Y:1622:XAT:H191	1.95	0.40
4:a:84:PRO:HA	4:a:112:TYR:CG	2.57	0.40
5:b:138:ILE:HD13	5:b:138:ILE:HG21	1.81	0.40
6:c:201:LEU:HD11	34:c:515:BCR:H373	2.03	0.40
34:c:515:BCR:H24C	34:c:515:BCR:H371	1.88	0.40
25:y:602:CLA:H141	25:y:602:CLA:H162	1.85	0.40
2:5:79:ASP:HB3	2:5:82:THR:HB	2.04	0.40
1:6:177:LEU:HD13	1:6:182:PRO:HB2	2.03	0.40
24:6:607:CHL:HBB2	24:6:609:CHL:HBC1	2.03	0.40
4:A:84:PRO:HA	4:A:112:TYR:CG	2.57	0.40
34:B:619:BCR:H371	34:B:619:BCR:H24C	1.78	0.40
36:B:622:LMG:H391	36:B:622:LMG:H421	1.83	0.40
6:C:397:GLY:HA3	6:C:401:GLU:HG2	2.04	0.40
25:C:508:CLA:H93	25:C:508:CLA:H111	1.88	0.40
34:D:404:BCR:H14C	9:F:32:PHE:CD2	2.56	0.40
3:G:214:GLN:HE22	26:G:1620:LUT:H42	1.86	0.40
27:R:622:XAT:H15	27:R:622:XAT:H201	1.88	0.40
18:S:130:ASN:OD1	18:S:158:ILE:HD13	2.22	0.40
2:8:77:SER:HB3	2:8:83:PHE:HB2	2.03	0.40
2:9:99:LEU:HB3	25:9:604:CLA:HBB2	2.02	0.40
2:p:73:THR:HG21	24:q:609:CHL:HAA1	2.04	0.40
7:d:8:TYR:HB2	17:r:107:ILE:HD11	2.04	0.40
26:n:1620:LUT:H31	26:n:1620:LUT:H391	1.91	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	0	214/256 (84%)	201 (94%)	13 (6%)	0	100	100
1	1	215/256 (84%)	201 (94%)	14 (6%)	0	100	100
1	6	214/256 (84%)	198 (92%)	16 (8%)	0	100	100
1	7	215/256 (84%)	198 (92%)	17 (8%)	0	100	100
1	Y	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
1	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
2	2	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	3	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	5	215/257 (84%)	195 (91%)	20 (9%)	0	100	100
2	8	216/257 (84%)	194 (90%)	22 (10%)	0	100	100
2	9	216/257 (84%)	196 (91%)	20 (9%)	0	100	100
2	N	217/257 (84%)	195 (90%)	22 (10%)	0	100	100
2	n	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
2	p	215/257 (84%)	199 (93%)	16 (7%)	0	100	100
3	4	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
3	G	217/249 (87%)	197 (91%)	20 (9%)	0	100	100
3	g	217/249 (87%)	199 (92%)	18 (8%)	0	100	100
3	q	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
4	A	334/352 (95%)	316 (95%)	18 (5%)	0	100	100
4	a	334/352 (95%)	318 (95%)	16 (5%)	0	100	100
5	B	488/508 (96%)	458 (94%)	30 (6%)	0	100	100
5	b	488/508 (96%)	460 (94%)	28 (6%)	0	100	100
6	C	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
6	c	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
7	D	344/352 (98%)	327 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	d	344/352 (98%)	326 (95%)	18 (5%)	0	100	100
8	E	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
8	e	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
9	F	29/44 (66%)	29 (100%)	0	0	100	100
9	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
10	H	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
10	h	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
11	I	33/37 (89%)	33 (100%)	0	0	100	100
11	i	33/37 (89%)	33 (100%)	0	0	100	100
12	J	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
12	j	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
13	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
13	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
14	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
14	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
15	M	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
15	m	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
16	O	226/291 (78%)	201 (89%)	25 (11%)	0	100	100
16	o	226/291 (78%)	202 (89%)	24 (11%)	0	100	100
17	R	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	30	59
17	r	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	30	59
18	S	250/289 (86%)	224 (90%)	26 (10%)	0	100	100
18	s	250/289 (86%)	223 (89%)	27 (11%)	0	100	100
19	T	28/31 (90%)	28 (100%)	0	0	100	100
19	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
20	V	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
20	v	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
21	W	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
21	w	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
22	X	32/101 (32%)	32 (100%)	0	0	100	100
22	x	32/101 (32%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
23	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	9614/11160 (86%)	8903 (93%)	709 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	R	100	ASN
17	r	100	ASN

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	0	165/196 (84%)	165 (100%)	0	100	100
1	1	166/196 (85%)	165 (99%)	1 (1%)	78	80
1	6	165/196 (84%)	165 (100%)	0	100	100
1	7	166/196 (85%)	164 (99%)	2 (1%)	63	72
1	Y	170/196 (87%)	170 (100%)	0	100	100
1	y	170/196 (87%)	169 (99%)	1 (1%)	78	80
2	2	169/194 (87%)	169 (100%)	0	100	100
2	3	169/194 (87%)	167 (99%)	2 (1%)	63	72
2	5	168/194 (87%)	168 (100%)	0	100	100
2	8	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	9	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	N	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	n	169/194 (87%)	169 (100%)	0	100	100
2	p	168/194 (87%)	168 (100%)	0	100	100
3	4	163/187 (87%)	162 (99%)	1 (1%)	78	80
3	G	164/187 (88%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g	164/187 (88%)	164 (100%)	0	100	100
3	q	163/187 (87%)	163 (100%)	0	100	100
4	A	274/289 (95%)	272 (99%)	2 (1%)	76	78
4	a	274/289 (95%)	272 (99%)	2 (1%)	76	78
5	B	392/407 (96%)	388 (99%)	4 (1%)	68	75
5	b	392/407 (96%)	387 (99%)	5 (1%)	61	71
6	C	351/362 (97%)	348 (99%)	3 (1%)	70	76
6	c	351/362 (97%)	348 (99%)	3 (1%)	70	76
7	D	276/281 (98%)	275 (100%)	1 (0%)	84	83
7	d	276/281 (98%)	273 (99%)	3 (1%)	65	74
8	E	67/71 (94%)	66 (98%)	1 (2%)	57	69
8	e	67/71 (94%)	66 (98%)	1 (2%)	57	69
9	F	25/37 (68%)	23 (92%)	2 (8%)	11	36
9	f	25/37 (68%)	24 (96%)	1 (4%)	28	53
10	H	58/75 (77%)	54 (93%)	4 (7%)	14	40
10	h	58/75 (77%)	55 (95%)	3 (5%)	21	48
11	I	32/34 (94%)	32 (100%)	0	100	100
11	i	32/34 (94%)	32 (100%)	0	100	100
12	J	26/32 (81%)	26 (100%)	0	100	100
12	j	26/32 (81%)	26 (100%)	0	100	100
13	K	31/38 (82%)	31 (100%)	0	100	100
13	k	31/38 (82%)	31 (100%)	0	100	100
14	L	34/35 (97%)	34 (100%)	0	100	100
14	l	34/35 (97%)	34 (100%)	0	100	100
15	M	26/30 (87%)	26 (100%)	0	100	100
15	m	26/30 (87%)	26 (100%)	0	100	100
16	O	190/222 (86%)	190 (100%)	0	100	100
16	o	190/222 (86%)	190 (100%)	0	100	100
17	R	187/218 (86%)	187 (100%)	0	100	100
17	r	187/218 (86%)	187 (100%)	0	100	100
18	S	189/217 (87%)	188 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	s	189/217 (87%)	188 (100%)	1 (0%)	81 81
19	T	27/28 (96%)	26 (96%)	1 (4%)	30 55
19	t	27/28 (96%)	26 (96%)	1 (4%)	30 55
20	V	27/27 (100%)	27 (100%)	0	100 100
20	v	27/27 (100%)	27 (100%)	0	100 100
21	W	44/87 (51%)	44 (100%)	0	100 100
21	w	44/87 (51%)	44 (100%)	0	100 100
22	X	24/67 (36%)	23 (96%)	1 (4%)	26 52
22	x	24/67 (36%)	23 (96%)	1 (4%)	26 52
23	Z	51/52 (98%)	51 (100%)	0	100 100
23	z	51/52 (98%)	51 (100%)	0	100 100
All	All	7668/8694 (88%)	7617 (99%)	51 (1%)	73 78

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	173	LEU
2	3	159	LEU
2	3	163	VAL
3	4	194	LYS
4	A	16	ARG
4	A	36	ILE
5	B	237	VAL
5	B	359	MET
5	B	362	PHE
5	B	363	PHE
6	C	30	LEU
6	C	108	ILE
6	C	128	LEU
7	D	346	LEU
8	E	38	VAL
9	F	18	ARG
9	F	20	LEU
10	H	82	GLU
10	H	83	THR
10	H	84	LEU
10	H	86	LYS
2	N	206	ILE

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Mol	Chain	Res	Type
18	S	57	ARG
19	T	16	ILE
22	X	90	ILE
1	7	152	ILE
1	7	173	LEU
2	8	163	VAL
2	9	224	ILE
4	a	16	ARG
4	a	36	ILE
5	b	237	VAL
5	b	272	ARG
5	b	361	THR
5	b	363	PHE
5	b	365	THR
6	c	30	LEU
6	c	108	ILE
6	c	128	LEU
7	d	13	THR
7	d	15	PHE
7	d	346	LEU
8	e	38	VAL
9	f	20	LEU
10	h	82	GLU
10	h	83	THR
10	h	84	LEU
18	s	57	ARG
19	t	16	ILE
22	x	90	ILE
1	y	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	169	ASN
2	2	245	ASN
2	3	55	ASN
3	4	120	GLN
3	4	139	GLN
3	4	148	GLN
2	5	147	GLN
2	5	245	ASN
1	6	128	GLN

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Mol	Chain	Res	Type
1	6	140	ASN
1	6	147	GLN
1	6	156	GLN
1	6	240	ASN
4	A	234	ASN
4	A	296	ASN
4	A	303	ASN
4	A	304	GLN
4	A	322	ASN
5	B	58	GLN
5	B	194	ASN
5	B	274	GLN
6	C	56	ASN
6	C	143	ASN
6	C	193	ASN
6	C	310	GLN
6	C	320	GLN
7	D	83	ASN
7	D	137	ASN
7	D	186	GLN
7	D	190	ASN
7	D	263	ASN
7	D	322	ASN
3	G	120	GLN
3	G	225	ASN
10	H	34	ASN
10	H	69	ASN
13	K	40	GLN
16	O	96	ASN
16	O	233	ASN
16	O	266	GLN
17	R	56	ASN
17	R	94	GLN
17	R	100	ASN
17	R	109	GLN
17	R	119	ASN
18	S	127	ASN
18	S	263	ASN
20	V	32	ASN
1	Y	240	ASN
1	0	140	ASN
1	0	145	HIS

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Mol	Chain	Res	Type
1	0	233	ASN
1	0	240	ASN
1	7	233	ASN
2	8	55	ASN
2	9	156	GLN
2	9	169	ASN
2	9	240	ASN
2	p	147	GLN
2	p	169	ASN
3	q	139	GLN
3	q	232	ASN
4	a	234	ASN
4	a	296	ASN
4	a	303	ASN
4	a	304	GLN
4	a	322	ASN
5	b	58	GLN
5	b	194	ASN
6	c	56	ASN
6	c	143	ASN
6	c	193	ASN
6	c	320	GLN
7	d	83	ASN
7	d	137	ASN
7	d	186	GLN
7	d	190	ASN
7	d	322	ASN
8	e	61	GLN
3	g	225	ASN
10	h	34	ASN
14	l	5	ASN
2	n	233	ASN
18	s	127	ASN
20	v	32	ASN
1	y	240	ASN
17	r	56	ASN
17	r	94	GLN
17	r	100	ASN
17	r	119	ASN
17	r	276	ASN
16	o	96	ASN
16	o	233	ASN

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Mol	Chain	Res	Type
16	o	266	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 560 ligands modelled in this entry, 4 are monoatomic - leaving 556 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	$\#\|Z\| > 2$
35	SQD	b	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
29	LHG	d	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
24	CHL	S	608	-	53,57,74	2.23	18 (33%)	59,93,114	3.24	23 (38%)
24	CHL	7	606	-	70,74,74	1.93	17 (24%)	80,114,114	2.77	26 (32%)
25	CLA	n	612	2	49,53,73	1.48	9 (18%)	59,89,113	1.44	8 (13%)
25	CLA	3	614	2	53,57,73	1.40	6 (11%)	62,93,113	1.21	8 (12%)
25	CLA	R	604	-	52,56,73	1.44	10 (19%)	62,92,113	1.37	6 (9%)
24	CHL	r	606	-	70,74,74	1.84	19 (27%)	80,114,114	2.95	26 (32%)
34	BCR	c	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
25	CLA	C	509	6	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	s	607	-	47,51,74	2.32	16 (34%)	52,86,114	3.13	21 (40%)
24	CHL	y	601	1	70,74,74	1.93	18 (25%)	80,114,114	2.97	28 (35%)
28	NEX	0	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.38	12 (24%)
26	LUT	G	1621	-	42,43,43	0.78	0	51,60,60	1.65	11 (21%)
26	LUT	N	1620	-	42,43,43	0.77	0	51,60,60	1.49	8 (15%)
25	CLA	Y	612	1	69,73,73	1.27	10 (14%)	83,113,113	1.29	10 (12%)
27	XAT	Y	1622	-	39,47,47	0.97	2 (5%)	54,74,74	4.30	23 (42%)
29	LHG	p	2630	25	48,48,48	0.95	2 (4%)	51,54,54	1.04	3 (5%)
25	CLA	B	603	5	69,73,73	1.24	11 (15%)	83,113,113	1.28	11 (13%)
28	NEX	9	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.33	12 (24%)
25	CLA	C	501	6	69,73,73	1.27	12 (17%)	83,113,113	1.23	6 (7%)
24	CHL	3	605	2	70,74,74	2.02	18 (25%)	80,114,114	2.71	23 (28%)
27	XAT	N	1622	-	39,47,47	1.04	3 (7%)	54,74,74	2.85	21 (38%)
38	BCT	D	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
36	LMG	D	412	-	46,46,55	0.95	2 (4%)	54,54,63	1.08	4 (7%)
25	CLA	7	611	29	69,73,73	1.25	10 (14%)	83,113,113	1.22	3 (3%)
26	LUT	q	1620	-	42,43,43	0.72	0	51,60,60	1.57	13 (25%)
35	SQD	B	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.13	4 (6%)
25	CLA	S	602	18	53,57,73	1.43	9 (16%)	62,93,113	1.41	8 (12%)
29	LHG	7	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	4 (7%)
25	CLA	B	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.11	4 (4%)
25	CLA	N	604	-	69,73,73	1.27	10 (14%)	83,113,113	1.21	6 (7%)
25	CLA	r	613	17	64,68,73	1.26	8 (12%)	77,107,113	1.31	7 (9%)
38	BCT	d	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
25	CLA	R	610	17	69,73,73	1.26	10 (14%)	83,113,113	1.27	6 (7%)
25	CLA	0	612	1	69,73,73	1.24	9 (13%)	83,113,113	1.21	7 (8%)
25	CLA	4	614	3	53,57,73	1.40	8 (15%)	62,93,113	1.27	7 (11%)
25	CLA	0	603	1	69,73,73	1.23	8 (11%)	83,113,113	1.32	5 (6%)
24	CHL	5	605	2	70,74,74	2.00	19 (27%)	80,114,114	2.91	28 (35%)
25	CLA	4	610	3	69,73,73	1.24	7 (10%)	83,113,113	1.18	5 (6%)
25	CLA	p	603	2	69,73,73	1.25	7 (10%)	83,113,113	1.25	4 (4%)
24	CHL	q	607	-	54,58,74	2.28	19 (35%)	59,94,114	3.09	21 (35%)
25	CLA	C	512	6	69,73,73	1.27	10 (14%)	83,113,113	1.33	7 (8%)
25	CLA	g	611	29	49,53,73	1.48	9 (18%)	59,89,113	1.41	6 (10%)
28	NEX	y	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.44	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	XAT	3	1622	-	39,47,47	0.92	0	54,74,74	2.60	20 (37%)
25	CLA	c	503	6	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
25	CLA	q	603	3	69,73,73	1.23	8 (11%)	83,113,113	1.26	7 (8%)
29	LHG	4	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)
25	CLA	G	610	3	69,73,73	1.22	8 (11%)	83,113,113	1.18	7 (8%)
25	CLA	A	406	-	69,73,73	1.24	11 (15%)	83,113,113	1.22	9 (10%)
26	LUT	6	1620	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
27	XAT	9	1622	-	39,47,47	0.91	0	54,74,74	2.65	19 (35%)
30	OEX	A	401	4,6	0,14,14	-	-	-		
24	CHL	9	601	2	70,74,74	1.93	20 (28%)	80,114,114	2.85	27 (33%)
25	CLA	Y	613	1	69,73,73	1.26	9 (13%)	83,113,113	1.19	6 (7%)
34	BCR	d	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)
25	CLA	n	614	2	53,57,73	1.40	9 (16%)	62,93,113	1.29	6 (9%)
25	CLA	6	611	29	69,73,73	1.25	6 (8%)	83,113,113	1.23	5 (6%)
25	CLA	q	612	3	47,51,73	1.47	6 (12%)	56,86,113	1.48	9 (16%)
35	SQD	a	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.79	9 (15%)
24	CHL	0	606	-	70,74,74	1.96	18 (25%)	80,114,114	2.76	25 (31%)
25	CLA	b	609	5	69,73,73	1.25	11 (15%)	83,113,113	1.27	8 (9%)
28	NEX	R	623	-	38,46,46	0.99	2 (5%)	50,70,70	2.39	15 (30%)
29	LHG	d	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	n	602	2	69,73,73	1.25	10 (14%)	83,113,113	1.18	8 (9%)
25	CLA	c	511	6	69,73,73	1.26	12 (17%)	83,113,113	1.37	10 (12%)
25	CLA	g	612	3	47,51,73	1.46	10 (21%)	56,86,113	1.32	7 (12%)
29	LHG	S	2630	25	44,44,48	0.94	2 (4%)	47,50,54	1.12	3 (6%)
25	CLA	s	603	18	46,50,73	1.48	7 (15%)	55,85,113	1.44	4 (7%)
25	CLA	6	604	-	69,73,73	1.26	9 (13%)	83,113,113	1.21	6 (7%)
25	CLA	S	611	29	53,57,73	1.39	10 (18%)	62,93,113	1.32	7 (11%)
26	LUT	s	1620	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
28	NEX	G	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.42	19 (38%)
25	CLA	6	603	1	69,73,73	1.23	8 (11%)	83,113,113	1.30	4 (4%)
24	CHL	8	601	2	70,74,74	1.91	18 (25%)	80,114,114	2.87	25 (31%)
27	XAT	0	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.20	22 (40%)
25	CLA	B	614	5	69,73,73	1.26	11 (15%)	83,113,113	1.25	6 (7%)
25	CLA	R	612	17	53,57,73	1.39	10 (18%)	62,93,113	1.40	7 (11%)
24	CHL	q	606	-	54,58,74	2.33	19 (35%)	59,94,114	2.98	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LUT	4	1621	-	42,43,43	0.76	0	51,60,60	1.50	11 (21%)
27	XAT	y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.30	23 (42%)
26	LUT	g	1620	-	42,43,43	0.78	0	51,60,60	1.47	6 (11%)
33	PHO	A	408	-	58,69,69	1.94	12 (20%)	56,99,99	1.71	10 (17%)
24	CHL	2	601	2	70,74,74	1.91	20 (28%)	80,114,114	2.84	26 (32%)
24	CHL	8	609	2	70,74,74	1.86	18 (25%)	80,114,114	2.82	26 (32%)
25	CLA	S	604	-	53,57,73	1.40	9 (16%)	62,93,113	1.30	8 (12%)
25	CLA	C	511	6	69,73,73	1.26	12 (17%)	83,113,113	1.38	11 (13%)
25	CLA	7	603	1	69,73,73	1.26	9 (13%)	83,113,113	1.22	4 (4%)
25	CLA	C	505	6	69,73,73	1.26	10 (14%)	83,113,113	1.25	10 (12%)
25	CLA	S	603	18	46,50,73	1.49	7 (15%)	55,85,113	1.45	5 (9%)
25	CLA	2	610	2	69,73,73	1.23	7 (10%)	83,113,113	1.16	8 (9%)
25	CLA	N	612	2	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
24	CHL	7	608	-	54,58,74	2.06	17 (31%)	59,94,114	3.32	20 (33%)
29	LHG	0	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	9	613	2	69,73,73	1.23	7 (10%)	83,113,113	1.20	4 (4%)
25	CLA	c	510	6	69,73,73	1.27	11 (15%)	83,113,113	1.30	7 (8%)
24	CHL	5	609	2	70,74,74	1.95	18 (25%)	80,114,114	2.81	23 (28%)
26	LUT	n	1620	-	42,43,43	0.78	0	51,60,60	1.53	10 (19%)
24	CHL	q	601	3	70,74,74	1.95	19 (27%)	80,114,114	2.86	28 (35%)
33	PHO	a	408	-	58,69,69	1.94	12 (20%)	56,99,99	1.72	10 (17%)
24	CHL	1	601	1	70,74,74	1.91	18 (25%)	80,114,114	3.00	29 (36%)
25	CLA	c	513	6	69,73,73	1.25	10 (14%)	83,113,113	1.22	5 (6%)
24	CHL	n	609	2	70,74,74	1.91	17 (24%)	80,114,114	2.87	27 (33%)
24	CHL	q	609	3	70,74,74	2.14	20 (28%)	80,114,114	2.73	23 (28%)
25	CLA	n	611	29	53,57,73	1.39	10 (18%)	62,93,113	1.34	5 (8%)
39	PL9	d	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.55	10 (14%)
25	CLA	a	410	4	64,68,73	1.31	10 (15%)	77,107,113	1.37	11 (14%)
25	CLA	B	605	5	69,73,73	1.25	11 (15%)	83,113,113	1.33	11 (13%)
28	NEX	1	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.45	17 (34%)
24	CHL	N	601	2	70,74,74	1.87	16 (22%)	80,114,114	2.98	29 (36%)
36	LMG	h	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.22	5 (8%)
27	XAT	G	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	20 (37%)
24	CHL	y	608	-	54,58,74	2.09	18 (33%)	59,94,114	3.34	23 (38%)
24	CHL	G	601	3	70,74,74	1.87	17 (24%)	80,114,114	2.98	31 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	p	606	-	50,54,74	2.39	18 (36%)	56,90,114	3.02	21 (37%)
26	LUT	4	1620	-	42,43,43	0.74	0	51,60,60	1.61	15 (29%)
25	CLA	s	612	18	49,53,73	1.47	9 (18%)	59,89,113	1.53	10 (16%)
26	LUT	g	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.62	7 (13%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	1.03	3 (3%)
25	CLA	S	610	18	53,57,73	1.41	9 (16%)	62,93,113	1.23	8 (12%)
25	CLA	5	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.14	7 (8%)
24	CHL	s	601	18	50,54,74	2.31	18 (36%)	56,90,114	3.26	24 (42%)
29	LHG	r	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
24	CHL	S	606	-	48,52,74	2.18	17 (35%)	53,87,114	3.45	23 (43%)
25	CLA	B	604	5	69,73,73	1.27	9 (13%)	83,113,113	1.21	7 (8%)
35	SQD	A	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.78	9 (15%)
24	CHL	Y	608	-	54,58,74	2.09	18 (33%)	59,94,114	3.33	23 (38%)
25	CLA	B	617	5	69,73,73	1.23	10 (14%)	83,113,113	1.36	10 (12%)
24	CHL	p	605	2	70,74,74	2.02	18 (25%)	80,114,114	2.83	26 (32%)
24	CHL	R	606	-	70,74,74	1.85	18 (25%)	80,114,114	2.95	26 (32%)
25	CLA	0	602	1	69,73,73	1.26	9 (13%)	83,113,113	1.15	6 (7%)
25	CLA	9	610	2	69,73,73	1.22	7 (10%)	83,113,113	1.14	9 (10%)
25	CLA	p	602	2	69,73,73	1.26	9 (13%)	83,113,113	1.15	7 (8%)
25	CLA	1	614	1	58,62,73	1.35	8 (13%)	69,99,113	1.21	4 (5%)
24	CHL	8	606	-	50,54,74	2.41	18 (36%)	56,90,114	3.13	22 (39%)
24	CHL	R	607	-	60,64,74	2.00	18 (30%)	68,102,114	3.12	24 (35%)
24	CHL	4	607	-	54,58,74	2.26	18 (33%)	59,94,114	3.16	22 (37%)
24	CHL	R	608	-	65,69,74	1.96	16 (24%)	74,108,114	2.91	27 (36%)
25	CLA	p	613	2	69,73,73	1.25	7 (10%)	83,113,113	1.18	4 (4%)
24	CHL	s	608	-	53,57,74	2.23	18 (33%)	59,93,114	3.24	23 (38%)
25	CLA	N	611	29	53,57,73	1.39	10 (18%)	62,93,113	1.32	5 (8%)
25	CLA	S	612	18	49,53,73	1.48	9 (18%)	59,89,113	1.53	10 (16%)
24	CHL	s	606	-	48,52,74	2.18	17 (35%)	53,87,114	3.45	23 (43%)
25	CLA	c	505	6	69,73,73	1.26	10 (14%)	83,113,113	1.25	11 (13%)
35	SQD	b	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.14	4 (6%)
25	CLA	G	613	3	69,73,73	1.26	10 (14%)	83,113,113	1.20	4 (4%)
25	CLA	q	604	-	53,57,73	1.41	8 (15%)	62,93,113	1.34	6 (9%)
25	CLA	a	406	-	69,73,73	1.24	11 (15%)	83,113,113	1.21	9 (10%)
25	CLA	b	610	5	69,73,73	1.23	10 (14%)	83,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	614	5	69,73,73	1.26	11 (15%)	83,113,113	1.24	6 (7%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.32	12 (24%)
34	BCR	b	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.98	16 (28%)
25	CLA	B	611	-	69,73,73	1.32	12 (17%)	83,113,113	1.43	7 (8%)
25	CLA	R	613	17	64,68,73	1.27	8 (12%)	77,107,113	1.32	7 (9%)
25	CLA	d	402	7	69,73,73	1.31	12 (17%)	83,113,113	1.32	8 (9%)
25	CLA	Y	614	1	58,62,73	1.35	9 (15%)	69,99,113	1.26	8 (11%)
24	CHL	3	601	2	70,74,74	1.90	17 (24%)	80,114,114	2.86	26 (32%)
26	LUT	8	1621	-	42,43,43	0.79	0	51,60,60	1.56	10 (19%)
24	CHL	0	605	1	50,54,74	2.26	20 (40%)	56,90,114	3.29	24 (42%)
24	CHL	6	607	-	70,74,74	1.90	18 (25%)	80,114,114	2.80	22 (27%)
25	CLA	G	604	-	53,57,73	1.41	10 (18%)	62,93,113	1.32	9 (14%)
25	CLA	B	616	5	69,73,73	1.28	11 (15%)	83,113,113	1.43	15 (18%)
25	CLA	c	509	6	69,73,73	1.26	10 (14%)	83,113,113	1.44	8 (9%)
25	CLA	9	603	2	69,73,73	1.24	9 (13%)	83,113,113	1.27	6 (7%)
25	CLA	n	603	2	69,73,73	1.25	12 (17%)	83,113,113	1.34	6 (7%)
24	CHL	n	607	-	70,74,74	1.87	17 (24%)	80,114,114	3.02	28 (35%)
24	CHL	n	608	-	54,58,74	2.06	17 (31%)	59,94,114	3.31	21 (35%)
25	CLA	r	609	17	62,66,73	1.33	9 (14%)	74,104,113	1.30	5 (6%)
24	CHL	5	601	2	70,74,74	1.91	18 (25%)	80,114,114	2.98	27 (33%)
25	CLA	s	602	18	53,57,73	1.42	9 (16%)	62,93,113	1.40	8 (12%)
25	CLA	4	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.23	6 (9%)
37	DGD	c	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
25	CLA	N	613	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	5 (6%)
25	CLA	5	604	-	69,73,73	1.23	7 (10%)	83,113,113	1.18	7 (8%)
24	CHL	2	609	2	70,74,74	1.95	20 (28%)	80,114,114	2.91	23 (28%)
24	CHL	N	608	-	54,58,74	2.07	17 (31%)	59,94,114	3.30	22 (37%)
25	CLA	6	612	1	69,73,73	1.25	8 (11%)	83,113,113	1.19	8 (9%)
25	CLA	b	608	-	69,73,73	1.26	11 (15%)	83,113,113	1.23	7 (8%)
26	LUT	p	1620	-	42,43,43	0.75	0	51,60,60	1.76	9 (17%)
26	LUT	q	1621	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
24	CHL	9	609	2	70,74,74	2.00	20 (28%)	80,114,114	2.89	23 (28%)
28	NEX	g	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.41	21 (42%)
24	CHL	1	609	1	70,74,74	1.87	19 (27%)	80,114,114	2.83	25 (31%)
26	LUT	1	1621	-	42,43,43	0.82	0	51,60,60	1.71	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	5	603	2	69,73,73	1.25	7 (10%)	83,113,113	1.24	4 (4%)
25	CLA	1	604	-	69,73,73	1.24	10 (14%)	83,113,113	1.19	8 (9%)
24	CHL	6	605	1	50,54,74	2.29	19 (38%)	56,90,114	3.21	24 (42%)
29	LHG	d	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
25	CLA	q	613	3	69,73,73	1.23	6 (8%)	83,113,113	1.29	5 (6%)
34	BCR	a	411	-	41,41,41	0.82	0	56,56,56	1.71	12 (21%)
25	CLA	7	602	1	69,73,73	1.24	10 (14%)	83,113,113	1.18	7 (8%)
24	CHL	q	605	3	52,56,74	2.31	18 (34%)	58,92,114	3.27	23 (39%)
28	NEX	n	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.37	15 (30%)
35	SQD	B	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
25	CLA	3	612	2	49,53,73	1.47	7 (14%)	59,89,113	1.46	6 (10%)
25	CLA	b	616	5	69,73,73	1.27	12 (17%)	83,113,113	1.44	14 (16%)
34	BCR	b	620	-	41,41,41	0.83	1 (2%)	56,56,56	1.87	19 (33%)
25	CLA	s	611	29	53,57,73	1.40	10 (18%)	62,93,113	1.33	6 (9%)
24	CHL	S	607	-	47,51,74	2.32	16 (34%)	52,86,114	3.12	22 (42%)
25	CLA	5	610	2	69,73,73	1.24	7 (10%)	83,113,113	1.09	5 (6%)
24	CHL	y	609	1	70,74,74	1.88	16 (22%)	80,114,114	2.91	26 (32%)
36	LMG	H	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.26	5 (8%)
25	CLA	1	610	1	69,73,73	1.21	8 (11%)	83,113,113	1.16	8 (9%)
25	CLA	6	613	1	69,73,73	1.25	7 (10%)	83,113,113	1.23	4 (4%)
26	LUT	7	1621	-	42,43,43	0.77	0	51,60,60	1.60	11 (21%)
25	CLA	7	613	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
26	LUT	R	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
25	CLA	C	504	-	69,73,73	1.25	11 (15%)	83,113,113	1.22	6 (7%)
25	CLA	S	609	18	45,49,73	1.48	8 (17%)	54,84,113	1.34	6 (11%)
24	CHL	7	601	1	70,74,74	1.91	18 (25%)	80,114,114	3.01	29 (36%)
24	CHL	G	606	-	54,58,74	2.15	18 (33%)	59,94,114	3.24	26 (44%)
24	CHL	g	605	3	52,56,74	2.24	18 (34%)	58,92,114	3.27	24 (41%)
25	CLA	4	612	3	47,51,73	1.47	7 (14%)	56,86,113	1.49	10 (17%)
24	CHL	Y	606	-	70,74,74	1.87	19 (27%)	80,114,114	2.91	23 (28%)
24	CHL	G	609	3	70,74,74	1.95	17 (24%)	80,114,114	2.71	23 (28%)
25	CLA	N	614	2	53,57,73	1.40	9 (16%)	62,93,113	1.29	6 (9%)
25	CLA	7	604	-	69,73,73	1.26	11 (15%)	83,113,113	1.24	8 (9%)
24	CHL	p	601	2	70,74,74	1.91	19 (27%)	80,114,114	2.96	27 (33%)
25	CLA	G	614	3	53,57,73	1.41	9 (16%)	62,93,113	1.22	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LMG	d	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.13	3 (5%)
33	PHO	a	409	-	58,69,69	1.91	11 (18%)	56,99,99	1.89	10 (17%)
25	CLA	r	604	-	52,56,73	1.44	10 (19%)	62,92,113	1.37	6 (9%)
25	CLA	g	613	3	69,73,73	1.26	10 (14%)	83,113,113	1.20	4 (4%)
25	CLA	B	610	5	69,73,73	1.24	12 (17%)	83,113,113	1.26	7 (8%)
25	CLA	y	612	1	69,73,73	1.27	10 (14%)	83,113,113	1.29	10 (12%)
24	CHL	9	607	-	54,58,74	2.22	18 (33%)	59,94,114	3.17	22 (37%)
24	CHL	9	608	-	48,52,74	2.20	18 (37%)	53,87,114	3.39	20 (37%)
29	LHG	c	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.04	3 (6%)
34	BCR	D	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)
24	CHL	N	607	-	70,74,74	1.87	18 (25%)	80,114,114	3.03	28 (35%)
24	CHL	2	606	-	54,58,74	2.22	18 (33%)	59,94,114	3.07	21 (35%)
26	LUT	0	1621	-	42,43,43	0.79	0	51,60,60	1.61	10 (19%)
34	BCR	c	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)
25	CLA	3	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.18	7 (8%)
27	XAT	1	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.22	24 (44%)
25	CLA	c	507	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	12 (14%)
27	XAT	r	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.48	17 (31%)
25	CLA	0	614	1	58,62,73	1.35	6 (10%)	69,99,113	1.30	4 (5%)
29	LHG	2	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
25	CLA	Y	603	1	69,73,73	1.26	12 (17%)	83,113,113	1.37	8 (9%)
24	CHL	3	608	-	54,58,74	2.16	18 (33%)	59,94,114	3.20	23 (38%)
27	XAT	n	1622	-	39,47,47	1.05	3 (7%)	54,74,74	2.82	22 (40%)
25	CLA	9	602	2	69,73,73	1.23	9 (13%)	83,113,113	1.25	9 (10%)
25	CLA	B	613	5	69,73,73	1.26	11 (15%)	83,113,113	1.43	8 (9%)
24	CHL	4	606	-	54,58,74	2.30	19 (35%)	59,94,114	3.03	21 (35%)
29	LHG	C	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.02	3 (6%)
33	PHO	A	409	-	58,69,69	1.90	11 (18%)	56,99,99	1.89	10 (17%)
24	CHL	7	607	-	70,74,74	1.91	17 (24%)	80,114,114	2.77	28 (35%)
25	CLA	7	610	1	69,73,73	1.22	8 (11%)	83,113,113	1.16	8 (9%)
24	CHL	7	605	1	50,54,74	2.28	17 (34%)	56,90,114	3.21	20 (35%)
25	CLA	r	610	17	69,73,73	1.25	10 (14%)	83,113,113	1.26	5 (6%)
24	CHL	N	609	2	70,74,74	1.89	17 (24%)	80,114,114	2.90	26 (32%)
29	LHG	n	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.10	3 (5%)
25	CLA	q	614	3	53,57,73	1.39	7 (13%)	62,93,113	1.26	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	p	610	2	69,73,73	1.23	7 (10%)	83,113,113	1.15	5 (6%)
28	NEX	N	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.36	14 (28%)
25	CLA	s	613	18	53,57,73	1.42	9 (16%)	62,93,113	1.34	6 (9%)
25	CLA	8	612	2	49,53,73	1.47	7 (14%)	59,89,113	1.44	5 (8%)
25	CLA	y	610	1	69,73,73	1.22	9 (13%)	83,113,113	1.15	8 (9%)
30	OEX	a	401	4,6	0,14,14	-	-	-		
34	BCR	C	515	-	41,41,41	0.92	2 (4%)	56,56,56	1.73	11 (19%)
25	CLA	B	606	5	69,73,73	1.27	11 (15%)	83,113,113	1.13	7 (8%)
24	CHL	n	606	-	50,54,74	2.22	17 (34%)	56,90,114	3.40	24 (42%)
25	CLA	3	611	29	53,57,73	1.41	7 (13%)	62,93,113	1.31	9 (14%)
37	DGD	C	520	-	60,60,67	0.85	2 (3%)	74,74,81	0.99	4 (5%)
25	CLA	R	601	17	53,57,73	1.42	9 (16%)	62,93,113	1.57	8 (12%)
36	LMG	C	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
24	CHL	0	601	1	70,74,74	1.92	18 (25%)	80,114,114	2.81	24 (30%)
25	CLA	5	614	2	53,57,73	1.43	7 (13%)	62,93,113	1.28	7 (11%)
26	LUT	6	1621	-	42,43,43	0.80	0	51,60,60	1.61	9 (17%)
24	CHL	y	606	-	70,74,74	1.87	17 (24%)	80,114,114	2.91	23 (28%)
25	CLA	A	410	4	64,68,73	1.30	10 (15%)	77,107,113	1.37	11 (14%)
25	CLA	b	606	5	69,73,73	1.26	11 (15%)	83,113,113	1.13	7 (8%)
25	CLA	8	614	2	53,57,73	1.41	6 (11%)	62,93,113	1.21	8 (12%)
25	CLA	N	603	2	69,73,73	1.25	12 (17%)	83,113,113	1.34	6 (7%)
25	CLA	0	604	-	69,73,73	1.23	9 (13%)	83,113,113	1.15	7 (8%)
25	CLA	n	613	2	69,73,73	1.23	8 (11%)	83,113,113	1.31	4 (4%)
24	CHL	8	607	-	70,74,74	1.90	18 (25%)	80,114,114	2.97	27 (33%)
37	DGD	C	523	-	67,67,67	0.82	2 (2%)	81,81,81	1.02	4 (4%)
25	CLA	c	512	6	69,73,73	1.27	10 (14%)	83,113,113	1.34	6 (7%)
24	CHL	2	607	-	54,58,74	2.24	19 (35%)	59,94,114	3.13	23 (38%)
29	LHG	9	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	2 (3%)
24	CHL	5	606	-	50,54,74	2.32	19 (38%)	56,90,114	3.08	21 (37%)
28	NEX	p	1623	-	38,46,46	0.88	1 (2%)	50,70,70	2.39	16 (32%)
25	CLA	C	507	-	69,73,73	1.25	12 (17%)	83,113,113	1.33	11 (13%)
25	CLA	S	605	18	54,58,73	1.38	9 (16%)	65,95,113	1.18	6 (9%)
29	LHG	D	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
25	CLA	y	603	1	69,73,73	1.26	12 (17%)	83,113,113	1.36	7 (8%)
27	XAT	7	1622	-	39,47,47	0.94	0	54,74,74	4.18	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	G	611	29	49,53,73	1.47	9 (18%)	59,89,113	1.42	6 (10%)
25	CLA	S	614	18	52,56,73	1.41	9 (17%)	62,92,113	1.30	10 (16%)
25	CLA	Y	604	-	69,73,73	1.27	11 (15%)	83,113,113	1.29	8 (9%)
28	NEX	q	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.34	17 (34%)
25	CLA	c	506	6	69,73,73	1.27	11 (15%)	83,113,113	1.32	6 (7%)
25	CLA	A	407	-	53,57,73	1.39	12 (22%)	62,93,113	1.33	5 (8%)
35	SQD	D	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
25	CLA	4	611	29	49,53,73	1.46	8 (16%)	59,89,113	1.32	3 (5%)
24	CHL	3	609	2	70,74,74	1.85	18 (25%)	80,114,114	2.84	26 (32%)
26	LUT	3	1620	-	42,43,43	0.73	0	51,60,60	1.67	12 (23%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	b	604	5	69,73,73	1.27	9 (13%)	83,113,113	1.21	7 (8%)
34	BCR	c	515	-	41,41,41	0.91	2 (4%)	56,56,56	1.74	11 (19%)
24	CHL	p	607	-	70,74,74	1.96	19 (27%)	80,114,114	2.76	25 (31%)
25	CLA	y	604	-	69,73,73	1.27	11 (15%)	83,113,113	1.29	8 (9%)
25	CLA	y	611	29	69,73,73	1.25	10 (14%)	83,113,113	1.24	6 (7%)
25	CLA	2	614	2	53,57,73	1.40	7 (13%)	62,93,113	1.25	7 (11%)
25	CLA	1	612	1	69,73,73	1.23	10 (14%)	83,113,113	1.23	10 (12%)
36	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
36	LMG	s	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.11	4 (6%)
25	CLA	B	607	5	69,73,73	1.25	8 (11%)	83,113,113	1.32	11 (13%)
28	NEX	s	1623	-	38,46,46	1.03	3 (7%)	50,70,70	2.55	18 (36%)
25	CLA	n	610	2	69,73,73	1.22	9 (13%)	83,113,113	1.12	7 (8%)
24	CHL	8	608	-	54,58,74	2.16	19 (35%)	59,94,114	3.20	24 (40%)
25	CLA	6	614	1	58,62,73	1.36	6 (10%)	69,99,113	1.29	5 (7%)
29	LHG	5	2630	25	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	b	612	5	69,73,73	1.29	9 (13%)	83,113,113	1.31	9 (10%)
24	CHL	2	608	-	48,52,74	2.19	20 (41%)	53,87,114	3.44	22 (41%)
26	LUT	N	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.58	9 (17%)
25	CLA	3	603	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
25	CLA	c	508	6	69,73,73	1.29	9 (13%)	83,113,113	1.32	9 (10%)
25	CLA	C	506	6	69,73,73	1.26	10 (14%)	83,113,113	1.32	7 (8%)
25	CLA	9	604	-	53,57,73	1.40	8 (15%)	62,93,113	1.31	5 (8%)
34	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
24	CHL	6	601	1	70,74,74	1.90	18 (25%)	80,114,114	2.87	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	7	614	1	58,62,73	1.36	8 (13%)	69,99,113	1.22	5 (7%)
25	CLA	c	502	6	69,73,73	1.33	11 (15%)	83,113,113	1.62	10 (12%)
25	CLA	2	603	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
29	LHG	Y	2630	25	48,48,48	0.88	2 (4%)	51,54,54	1.21	5 (9%)
25	CLA	Y	602	1	69,73,73	1.25	10 (14%)	83,113,113	1.20	7 (8%)
29	LHG	8	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
25	CLA	A	405	4	69,73,73	1.30	10 (14%)	83,113,113	1.33	8 (9%)
25	CLA	r	612	17	53,57,73	1.39	10 (18%)	62,93,113	1.41	7 (11%)
26	LUT	s	1621	-	42,43,43	0.82	0	51,60,60	1.80	14 (27%)
37	DGD	c	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
26	LUT	5	1620	-	42,43,43	0.76	0	51,60,60	1.83	13 (25%)
34	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
24	CHL	1	608	-	54,58,74	2.08	18 (33%)	59,94,114	3.34	22 (37%)
24	CHL	g	601	3	70,74,74	1.86	18 (25%)	80,114,114	2.97	33 (41%)
29	LHG	s	2630	25	44,44,48	0.95	2 (4%)	47,50,54	1.12	3 (6%)
25	CLA	4	613	3	69,73,73	1.23	7 (10%)	83,113,113	1.22	6 (7%)
36	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
29	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	4 (7%)
28	NEX	S	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.46	16 (32%)
25	CLA	c	501	6	69,73,73	1.26	12 (17%)	83,113,113	1.24	6 (7%)
25	CLA	5	613	2	69,73,73	1.24	7 (10%)	83,113,113	1.33	4 (4%)
34	BCR	h	101	-	41,41,41	0.81	0	56,56,56	2.03	17 (30%)
26	LUT	3	1621	-	42,43,43	0.77	0	51,60,60	1.56	11 (21%)
25	CLA	g	610	3	69,73,73	1.22	8 (11%)	83,113,113	1.18	7 (8%)
25	CLA	8	611	29	53,57,73	1.40	7 (13%)	62,93,113	1.31	8 (12%)
25	CLA	8	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.21	7 (8%)
25	CLA	0	610	1	69,73,73	1.23	9 (13%)	83,113,113	1.10	6 (7%)
26	LUT	G	1620	-	42,43,43	0.78	0	51,60,60	1.48	6 (11%)
25	CLA	2	611	29	49,53,73	1.47	9 (18%)	59,89,113	1.36	7 (11%)
25	CLA	2	604	-	53,57,73	1.39	7 (13%)	62,93,113	1.32	7 (11%)
29	LHG	1	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	5 (9%)
26	LUT	9	1621	-	42,43,43	0.77	0	51,60,60	1.74	13 (25%)
28	NEX	3	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.35	13 (26%)
29	LHG	D	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
24	CHL	n	605	2	70,74,74	1.90	17 (24%)	80,114,114	2.83	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	405	4	69,73,73	1.30	10 (14%)	83,113,113	1.34	8 (9%)
29	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	C	502	6	69,73,73	1.33	11 (15%)	83,113,113	1.61	11 (13%)
24	CHL	0	609	1	70,74,74	1.98	20 (28%)	80,114,114	2.82	24 (30%)
24	CHL	9	606	-	54,58,74	2.23	18 (33%)	59,94,114	3.02	22 (37%)
25	CLA	C	513	6	69,73,73	1.24	10 (14%)	83,113,113	1.20	5 (6%)
25	CLA	G	612	3	47,51,73	1.47	10 (21%)	56,86,113	1.32	7 (12%)
27	XAT	6	1622	-	39,47,47	0.92	2 (5%)	54,74,74	4.25	21 (38%)
25	CLA	b	603	5	69,73,73	1.24	11 (15%)	83,113,113	1.28	11 (13%)
25	CLA	1	602	1	69,73,73	1.24	9 (13%)	83,113,113	1.18	6 (7%)
25	CLA	Y	611	29	69,73,73	1.25	10 (14%)	83,113,113	1.25	6 (7%)
25	CLA	b	605	5	69,73,73	1.25	10 (14%)	83,113,113	1.33	11 (13%)
25	CLA	1	611	29	69,73,73	1.25	10 (14%)	83,113,113	1.20	3 (3%)
25	CLA	B	612	5	69,73,73	1.29	9 (13%)	83,113,113	1.31	9 (10%)
24	CHL	7	609	1	70,74,74	1.87	18 (25%)	80,114,114	2.85	23 (28%)
34	BCR	B	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.97	17 (30%)
25	CLA	N	602	2	69,73,73	1.25	10 (14%)	83,113,113	1.19	7 (8%)
25	CLA	4	603	3	69,73,73	1.23	8 (11%)	83,113,113	1.32	8 (9%)
24	CHL	5	608	-	54,58,74	2.13	18 (33%)	59,94,114	3.31	20 (33%)
24	CHL	Y	607	-	70,74,74	1.90	18 (25%)	80,114,114	3.12	29 (36%)
35	SQD	d	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
26	LUT	y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.67	14 (27%)
24	CHL	S	601	18	50,54,74	2.31	18 (36%)	56,90,114	3.27	25 (44%)
27	XAT	g	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	19 (35%)
34	BCR	b	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)
25	CLA	R	611	29	53,57,73	1.38	10 (18%)	62,93,113	1.32	4 (6%)
25	CLA	y	602	1	69,73,73	1.25	10 (14%)	83,113,113	1.20	7 (8%)
26	LUT	8	1620	-	42,43,43	0.72	0	51,60,60	1.62	12 (23%)
25	CLA	G	603	3	69,73,73	1.25	10 (14%)	83,113,113	1.27	5 (6%)
25	CLA	s	610	18	53,57,73	1.41	9 (16%)	62,93,113	1.23	7 (11%)
36	LMG	S	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.10	4 (6%)
25	CLA	R	609	17	62,66,73	1.33	8 (12%)	74,104,113	1.31	5 (6%)
26	LUT	2	1620	-	42,43,43	0.77	0	51,60,60	1.55	10 (19%)
25	CLA	b	617	5	69,73,73	1.23	11 (15%)	83,113,113	1.36	10 (12%)
27	XAT	R	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.47	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	4	601	3	70,74,74	1.97	18 (25%)	80,114,114	2.77	26 (32%)
24	CHL	r	608	-	65,69,74	1.97	18 (27%)	74,108,114	2.90	27 (36%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.98	4 (5%)
24	CHL	Y	605	1	50,54,74	2.20	17 (34%)	56,90,114	3.35	23 (41%)
25	CLA	a	407	-	53,57,73	1.39	12 (22%)	62,93,113	1.33	5 (8%)
34	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
25	CLA	R	603	17	64,68,73	1.29	10 (15%)	77,107,113	1.41	5 (6%)
36	LMG	c	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
34	BCR	H	101	-	41,41,41	0.81	0	56,56,56	2.03	16 (28%)
26	LUT	1	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	9 (17%)
24	CHL	3	607	-	70,74,74	1.90	18 (25%)	80,114,114	3.00	27 (33%)
24	CHL	5	607	-	70,74,74	1.91	18 (25%)	80,114,114	2.77	24 (30%)
24	CHL	p	609	2	70,74,74	1.93	18 (25%)	80,114,114	2.83	23 (28%)
25	CLA	8	603	2	69,73,73	1.24	7 (10%)	83,113,113	1.32	7 (8%)
25	CLA	Y	610	1	69,73,73	1.23	9 (13%)	83,113,113	1.14	8 (9%)
28	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.40	16 (32%)
34	BCR	C	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)
25	CLA	8	613	2	69,73,73	1.23	6 (8%)	83,113,113	1.34	5 (6%)
25	CLA	2	612	2	47,51,73	1.47	8 (17%)	56,86,113	1.42	5 (8%)
26	LUT	2	1621	-	42,43,43	0.76	0	51,60,60	1.78	11 (21%)
37	DGD	C	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
39	PL9	D	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.54	11 (16%)
25	CLA	s	605	18	54,58,73	1.37	8 (14%)	65,95,113	1.18	4 (6%)
26	LUT	r	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
24	CHL	4	608	-	48,52,74	2.29	17 (35%)	53,87,114	3.35	20 (37%)
24	CHL	1	607	-	70,74,74	1.90	17 (24%)	80,114,114	2.76	28 (35%)
24	CHL	4	605	3	52,56,74	2.33	19 (36%)	58,92,114	3.21	24 (41%)
25	CLA	s	609	18	45,49,73	1.48	7 (15%)	54,84,113	1.33	6 (11%)
26	LUT	5	1621	-	42,43,43	0.74	0	51,60,60	1.58	11 (21%)
29	LHG	G	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	r	611	29	53,57,73	1.39	10 (18%)	62,93,113	1.33	4 (6%)
25	CLA	b	615	5	69,73,73	1.25	11 (15%)	83,113,113	1.16	7 (8%)
25	CLA	1	603	1	69,73,73	1.26	9 (13%)	83,113,113	1.23	4 (4%)
25	CLA	2	602	2	69,73,73	1.23	10 (14%)	83,113,113	1.22	8 (9%)
25	CLA	9	612	2	47,51,73	1.48	7 (14%)	56,86,113	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	g	609	3	70,74,74	1.94	17 (24%)	80,114,114	2.69	22 (27%)
28	NEX	5	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.54	15 (30%)
24	CHL	9	605	2	52,56,74	2.31	19 (36%)	58,92,114	3.14	24 (41%)
28	NEX	8	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.31	12 (24%)
25	CLA	g	604	-	53,57,73	1.41	9 (16%)	62,93,113	1.31	10 (16%)
26	LUT	7	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	8 (15%)
27	XAT	q	1622	-	39,47,47	0.89	0	54,74,74	2.58	17 (31%)
26	LUT	p	1621	-	42,43,43	0.73	0	51,60,60	1.55	9 (17%)
28	NEX	2	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.35	13 (26%)
26	LUT	Y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	16 (31%)
25	CLA	9	614	2	53,57,73	1.41	8 (15%)	62,93,113	1.25	7 (11%)
25	CLA	6	610	1	69,73,73	1.21	9 (13%)	83,113,113	1.09	7 (8%)
24	CHL	6	609	1	70,74,74	1.91	19 (27%)	80,114,114	2.81	25 (31%)
25	CLA	S	613	18	53,57,73	1.42	9 (16%)	62,93,113	1.34	6 (9%)
25	CLA	q	610	3	69,73,73	1.23	6 (8%)	83,113,113	1.16	7 (8%)
25	CLA	s	604	-	53,57,73	1.40	9 (16%)	62,93,113	1.31	7 (11%)
25	CLA	3	613	2	69,73,73	1.22	6 (8%)	83,113,113	1.34	5 (6%)
36	LMG	d	412	-	46,46,55	0.94	2 (4%)	54,54,63	1.09	4 (7%)
25	CLA	g	614	3	53,57,73	1.42	9 (16%)	62,93,113	1.23	8 (12%)
25	CLA	b	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.11	4 (4%)
24	CHL	y	605	1	50,54,74	2.21	17 (34%)	56,90,114	3.35	23 (41%)
27	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.65	18 (33%)
25	CLA	0	611	29	69,73,73	1.25	7 (10%)	83,113,113	1.25	5 (6%)
24	CHL	G	607	-	54,58,74	2.12	18 (33%)	59,94,114	3.32	24 (40%)
24	CHL	G	608	-	48,52,74	2.24	15 (31%)	53,87,114	3.21	21 (39%)
25	CLA	D	402	7	69,73,73	1.31	11 (15%)	83,113,113	1.32	10 (12%)
25	CLA	0	613	1	69,73,73	1.22	6 (8%)	83,113,113	1.20	6 (7%)
25	CLA	3	604	-	69,73,73	1.25	9 (13%)	83,113,113	1.22	7 (8%)
28	NEX	4	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.36	18 (36%)
24	CHL	g	606	-	54,58,74	2.15	18 (33%)	59,94,114	3.26	26 (44%)
25	CLA	p	612	2	49,53,73	1.48	6 (12%)	59,89,113	1.43	8 (13%)
26	LUT	n	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	9 (17%)
25	CLA	d	403	7	69,73,73	1.24	11 (15%)	83,113,113	1.18	7 (8%)
25	CLA	G	602	3	69,73,73	1.25	11 (15%)	83,113,113	1.27	9 (10%)
25	CLA	r	603	17	64,68,73	1.29	11 (17%)	77,107,113	1.41	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	XAT	p	1622	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
24	CHL	G	605	3	52,56,74	2.24	18 (34%)	58,92,114	3.26	23 (39%)
24	CHL	8	605	2	70,74,74	2.02	18 (25%)	80,114,114	2.73	23 (28%)
24	CHL	n	601	2	70,74,74	1.86	17 (24%)	80,114,114	3.01	32 (40%)
25	CLA	p	614	2	53,57,73	1.43	7 (13%)	62,93,113	1.25	5 (8%)
24	CHL	2	605	2	52,56,74	2.30	20 (38%)	58,92,114	3.14	24 (41%)
28	NEX	7	1623	-	38,46,46	1.03	2 (5%)	50,70,70	2.38	20 (40%)
24	CHL	Y	609	1	70,74,74	1.88	16 (22%)	80,114,114	2.91	26 (32%)
25	CLA	n	604	-	69,73,73	1.28	10 (14%)	83,113,113	1.20	6 (7%)
25	CLA	5	612	2	49,53,73	1.48	8 (16%)	59,89,113	1.43	6 (10%)
25	CLA	b	611	-	69,73,73	1.32	12 (17%)	83,113,113	1.43	6 (7%)
29	LHG	R	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
25	CLA	R	602	17	64,68,73	1.31	10 (15%)	77,107,113	1.32	7 (9%)
25	CLA	b	613	5	69,73,73	1.26	11 (15%)	83,113,113	1.43	8 (9%)
25	CLA	3	610	2	69,73,73	1.24	8 (11%)	83,113,113	1.11	5 (6%)
25	CLA	C	503	6	69,73,73	1.27	11 (15%)	83,113,113	1.26	7 (8%)
25	CLA	r	601	17	53,57,73	1.42	9 (16%)	62,93,113	1.58	8 (12%)
24	CHL	p	608	-	54,58,74	2.14	18 (33%)	59,94,114	3.31	21 (35%)
25	CLA	y	613	1	69,73,73	1.27	9 (13%)	83,113,113	1.20	6 (7%)
26	LUT	0	1620	-	42,43,43	0.76	0	51,60,60	1.59	11 (21%)
25	CLA	s	614	18	52,56,73	1.41	9 (17%)	62,92,113	1.29	10 (16%)
25	CLA	8	602	2	69,73,73	1.25	9 (13%)	83,113,113	1.18	7 (8%)
27	XAT	2	1622	-	39,47,47	0.90	0	54,74,74	2.68	19 (35%)
37	DGD	C	518	-	56,56,67	0.89	2 (3%)	70,70,81	1.12	6 (8%)
29	LHG	g	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	g	602	3	69,73,73	1.25	10 (14%)	83,113,113	1.26	9 (10%)
24	CHL	3	606	-	50,54,74	2.41	18 (36%)	56,90,114	3.12	20 (35%)
25	CLA	9	611	29	49,53,73	1.46	9 (18%)	59,89,113	1.35	7 (11%)
25	CLA	r	616	17	69,73,73	1.24	9 (13%)	83,113,113	1.20	7 (8%)
29	LHG	y	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.18	5 (9%)
26	LUT	9	1620	-	42,43,43	0.77	0	51,60,60	1.61	13 (25%)
25	CLA	7	612	1	69,73,73	1.24	10 (14%)	83,113,113	1.23	9 (10%)
34	BCR	B	620	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	19 (33%)
25	CLA	D	403	7	69,73,73	1.24	11 (15%)	83,113,113	1.19	6 (7%)
26	LUT	Y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.66	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	N	610	2	69,73,73	1.22	9 (13%)	83,113,113	1.13	7 (8%)
29	LHG	6	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
24	CHL	0	607	-	70,74,74	1.86	17 (24%)	80,114,114	2.87	22 (27%)
24	CHL	0	608	-	54,58,74	2.17	17 (31%)	59,94,114	3.23	22 (37%)
24	CHL	1	606	-	70,74,74	1.94	18 (25%)	80,114,114	2.79	24 (30%)
34	BCR	B	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)
40	HEM	F	101	8,9	50,50,50	1.31	4 (8%)	66,82,82	1.08	5 (7%)
26	LUT	y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	17 (33%)
24	CHL	N	606	-	50,54,74	2.22	17 (34%)	56,90,114	3.36	23 (41%)
27	XAT	4	1622	-	39,47,47	0.89	0	54,74,74	2.60	16 (29%)
25	CLA	C	510	6	69,73,73	1.26	11 (15%)	83,113,113	1.30	7 (8%)
24	CHL	6	608	-	54,58,74	2.16	18 (33%)	59,94,114	3.26	23 (38%)
29	LHG	3	2630	25	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	C	508	6	69,73,73	1.28	9 (13%)	83,113,113	1.32	9 (10%)
25	CLA	2	613	2	69,73,73	1.24	8 (11%)	83,113,113	1.21	4 (4%)
24	CHL	q	608	-	48,52,74	2.38	18 (37%)	53,87,114	3.31	18 (33%)
36	LMG	D	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.12	3 (5%)
25	CLA	c	504	-	69,73,73	1.25	10 (14%)	83,113,113	1.21	6 (7%)
25	CLA	4	602	3	69,73,73	1.25	7 (10%)	83,113,113	1.16	7 (8%)
25	CLA	y	614	1	58,62,73	1.35	9 (15%)	69,99,113	1.26	8 (11%)
25	CLA	R	616	17	69,73,73	1.24	9 (13%)	83,113,113	1.21	8 (9%)
25	CLA	5	611	29	53,57,73	1.41	8 (15%)	62,93,113	1.26	5 (8%)
25	CLA	B	608	-	69,73,73	1.26	11 (15%)	83,113,113	1.21	6 (7%)
37	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
34	BCR	A	411	-	41,41,41	0.82	0	56,56,56	1.70	12 (21%)
36	LMG	A	413	-	48,48,55	0.93	2 (4%)	56,56,63	1.15	4 (7%)
24	CHL	4	609	3	70,74,74	2.12	20 (28%)	80,114,114	2.65	21 (26%)
26	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.55	11 (21%)
25	CLA	1	613	1	69,73,73	1.23	9 (13%)	83,113,113	1.34	7 (8%)
24	CHL	Y	601	1	70,74,74	1.92	18 (25%)	80,114,114	2.91	29 (36%)
29	LHG	q	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)
24	CHL	1	605	1	50,54,74	2.28	17 (34%)	56,90,114	3.21	20 (35%)
24	CHL	y	607	-	70,74,74	1.90	18 (25%)	80,114,114	3.12	29 (36%)
25	CLA	p	604	-	69,73,73	1.25	7 (10%)	83,113,113	1.14	5 (6%)
25	CLA	p	611	29	53,57,73	1.40	7 (13%)	62,93,113	1.31	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	N	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	3 (5%)
24	CHL	r	607	-	60,64,74	1.99	17 (28%)	68,102,114	3.14	24 (35%)
40	HEM	f	101	8,9	50,50,50	1.36	6 (12%)	66,82,82	1.07	3 (4%)
25	CLA	b	607	5	69,73,73	1.24	8 (11%)	83,113,113	1.32	11 (13%)
24	CHL	g	607	-	54,58,74	2.13	18 (33%)	59,94,114	3.31	25 (42%)
24	CHL	g	608	-	48,52,74	2.22	15 (31%)	53,87,114	3.25	21 (39%)
26	LUT	S	1621	-	42,43,43	0.81	0	51,60,60	1.79	14 (27%)
24	CHL	N	605	2	70,74,74	1.91	18 (25%)	80,114,114	2.84	26 (32%)
25	CLA	6	602	1	69,73,73	1.26	9 (13%)	83,113,113	1.13	6 (7%)
29	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
28	NEX	Y	1623	-	38,46,46	1.04	3 (7%)	50,70,70	2.39	16 (32%)
27	XAT	8	1622	-	39,47,47	0.92	0	54,74,74	2.62	19 (35%)
25	CLA	q	602	3	69,73,73	1.25	8 (11%)	83,113,113	1.18	8 (9%)
25	CLA	g	603	3	69,73,73	1.25	10 (14%)	83,113,113	1.27	5 (6%)
25	CLA	q	611	29	49,53,73	1.45	8 (16%)	59,89,113	1.36	3 (5%)
24	CHL	6	606	-	70,74,74	1.93	18 (25%)	80,114,114	2.79	25 (31%)
25	CLA	B	615	5	69,73,73	1.25	11 (15%)	83,113,113	1.16	7 (8%)
36	LMG	a	413	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	B	609	5	69,73,73	1.24	11 (15%)	83,113,113	1.27	8 (9%)
25	CLA	r	602	17	64,68,73	1.30	10 (15%)	77,107,113	1.33	7 (9%)
25	CLA	8	610	2	69,73,73	1.24	8 (11%)	83,113,113	1.10	6 (7%)

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
35	SQD	b	623	-	-	14/45/65/69	0/1/1/1
29	LHG	d	408	-	-	10/48/48/53	-
24	CHL	S	608	-	-	13/21/97/117	-
24	CHL	7	606	-	-	20/41/117/117	-
25	CLA	n	612	2	-	8/15/91/115	-
25	CLA	3	614	2	-	10/20/96/115	-
25	CLA	R	604	-	-	10/19/95/115	-
24	CHL	r	606	-	-	24/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
25	CLA	C	509	6	-	4/39/115/115	-
24	CHL	s	607	-	-	4/14/90/117	-
24	CHL	y	601	1	-	16/41/117/117	-
28	NEX	0	1623	-	-	5/27/83/83	0/3/3/3
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	Y	612	1	-	17/39/115/115	-
27	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
29	LHG	p	2630	25	-	12/53/53/53	-
25	CLA	B	603	5	-	13/39/115/115	-
28	NEX	9	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	C	501	6	-	16/39/115/115	-
24	CHL	3	605	2	-	17/41/117/117	-
27	XAT	N	1622	-	-	0/31/93/93	0/4/4/4
36	LMG	D	412	-	-	5/41/61/70	0/1/1/1
25	CLA	7	611	29	-	10/39/115/115	-
26	LUT	q	1620	-	-	2/29/67/67	0/2/2/2
35	SQD	B	621	-	-	17/49/69/69	0/1/1/1
25	CLA	S	602	18	-	12/20/96/115	-
29	LHG	7	2630	25	-	18/53/53/53	-
25	CLA	B	602	-	-	19/39/115/115	-
25	CLA	N	604	-	-	11/39/115/115	-
25	CLA	r	613	17	-	17/33/109/115	-
25	CLA	R	610	17	-	16/39/115/115	-
25	CLA	0	612	1	-	13/39/115/115	-
25	CLA	4	614	3	-	10/20/96/115	-
25	CLA	0	603	1	-	13/39/115/115	-
24	CHL	5	605	2	-	22/41/117/117	-
25	CLA	4	610	3	-	14/39/115/115	-
25	CLA	p	603	2	-	16/39/115/115	-
24	CHL	q	607	-	-	15/22/98/117	-
25	CLA	C	512	6	-	17/39/115/115	-
25	CLA	g	611	29	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	y	1623	-	-	5/27/83/83	0/3/3/3
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	c	503	6	-	14/39/115/115	-
25	CLA	q	603	3	-	19/39/115/115	-
29	LHG	4	2630	25	-	19/53/53/53	-
25	CLA	G	610	3	-	12/39/115/115	-
25	CLA	A	406	-	-	3/39/115/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
27	XAT	9	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	9	601	2	-	23/41/117/117	-
25	CLA	Y	613	1	-	11/39/115/115	-
34	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	CLA	n	614	2	-	8/20/96/115	-
25	CLA	6	611	29	-	14/39/115/115	-
25	CLA	q	612	3	-	8/13/89/115	-
35	SQD	a	412	-	-	18/46/66/69	0/1/1/1
24	CHL	0	606	-	-	21/41/117/117	-
25	CLA	b	609	5	-	12/39/115/115	-
28	NEX	R	623	-	-	2/27/83/83	0/3/3/3
29	LHG	d	409	-	-	12/53/53/53	-
25	CLA	n	602	2	-	8/39/115/115	-
25	CLA	c	511	6	-	14/39/115/115	-
25	CLA	g	612	3	-	6/13/89/115	-
29	LHG	S	2630	25	-	16/49/49/53	-
25	CLA	s	603	18	-	7/12/88/115	-
25	CLA	6	604	-	-	20/39/115/115	-
25	CLA	S	611	29	-	8/20/96/115	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
28	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	6	603	1	-	12/39/115/115	-
24	CHL	8	601	2	-	26/41/117/117	-
27	XAT	0	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	B	614	5	-	10/39/115/115	-
25	CLA	R	612	17	-	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	q	606	-	-	7/22/98/117	-
26	LUT	4	1621	-	-	7/29/67/67	0/2/2/2
27	XAT	y	1622	-	-	0/31/93/93	0/4/4/4
26	LUT	g	1620	-	-	3/29/67/67	0/2/2/2
33	PHO	A	408	-	-	10/37/103/103	0/5/6/6
24	CHL	2	601	2	-	26/41/117/117	-
24	CHL	8	609	2	-	22/41/117/117	-
25	CLA	S	604	-	-	10/20/96/115	-
25	CLA	C	511	6	-	14/39/115/115	-
25	CLA	7	603	1	-	17/39/115/115	-
25	CLA	C	505	6	-	18/39/115/115	-
25	CLA	S	603	18	-	7/12/88/115	-
25	CLA	2	610	2	-	6/39/115/115	-
25	CLA	N	612	2	-	8/15/91/115	-
24	CHL	7	608	-	-	14/22/98/117	-
29	LHG	0	2630	25	-	18/53/53/53	-
25	CLA	9	613	2	-	10/39/115/115	-
25	CLA	c	510	6	-	10/39/115/115	-
24	CHL	5	609	2	-	20/41/117/117	-
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	q	601	3	-	19/41/117/117	-
33	PHO	a	408	-	-	10/37/103/103	0/5/6/6
24	CHL	1	601	1	-	16/41/117/117	-
25	CLA	c	513	6	-	20/39/115/115	-
24	CHL	n	609	2	-	22/41/117/117	-
24	CHL	q	609	3	-	20/41/117/117	-
25	CLA	n	611	29	-	11/20/96/115	-
39	PL9	d	405	-	-	14/53/73/73	0/1/1/1
25	CLA	a	410	4	-	6/33/109/115	-
25	CLA	B	605	5	-	15/39/115/115	-
28	NEX	1	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	N	601	2	-	10/41/117/117	-
36	LMG	h	102	-	-	14/43/63/70	0/1/1/1
27	XAT	G	1622	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	y	608	-	-	4/22/98/117	-
24	CHL	G	601	3	-	18/41/117/117	-
24	CHL	p	606	-	-	5/17/93/117	-
26	LUT	4	1620	-	-	6/29/67/67	0/2/2/2
25	CLA	s	612	18	-	5/15/91/115	-
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
37	DGD	c	523	-	-	12/55/95/95	0/2/2/2
25	CLA	S	610	18	-	11/20/96/115	-
25	CLA	5	602	2	-	18/39/115/115	-
24	CHL	s	601	18	-	11/17/93/117	-
29	LHG	r	2630	25	-	16/42/42/53	-
24	CHL	S	606	-	-	12/15/91/117	-
25	CLA	B	604	5	-	13/39/115/115	-
35	SQD	A	412	-	-	18/46/66/69	0/1/1/1
24	CHL	Y	608	-	-	4/22/98/117	-
25	CLA	B	617	5	-	10/39/115/115	-
24	CHL	p	605	2	-	19/41/117/117	-
24	CHL	R	606	-	-	24/41/117/117	-
25	CLA	0	602	1	-	13/39/115/115	-
25	CLA	9	610	2	-	6/39/115/115	-
25	CLA	p	602	2	-	14/39/115/115	-
25	CLA	1	614	1	-	15/26/102/115	-
24	CHL	8	606	-	-	10/17/93/117	-
24	CHL	R	607	-	-	19/29/105/117	-
24	CHL	4	607	-	-	15/22/98/117	-
24	CHL	R	608	-	-	17/35/111/117	-
25	CLA	p	613	2	-	13/39/115/115	-
24	CHL	s	608	-	-	13/21/97/117	-
25	CLA	N	611	29	-	11/20/96/115	-
25	CLA	S	612	18	-	5/15/91/115	-
24	CHL	s	606	-	-	12/15/91/117	-
25	CLA	c	505	6	-	18/39/115/115	-
35	SQD	b	621	-	-	17/49/69/69	0/1/1/1
25	CLA	G	613	3	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	q	604	-	-	14/20/96/115	-
25	CLA	a	406	-	-	3/39/115/115	-
25	CLA	b	610	5	-	8/39/115/115	-
25	CLA	b	614	5	-	10/39/115/115	-
28	NEX	6	1623	-	-	3/27/83/83	0/3/3/3
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	CLA	B	611	-	-	9/39/115/115	-
25	CLA	R	613	17	-	17/33/109/115	-
25	CLA	d	402	7	-	16/39/115/115	-
25	CLA	Y	614	1	-	12/26/102/115	-
24	CHL	3	601	2	-	26/41/117/117	-
26	LUT	8	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	0	605	1	-	9/17/93/117	-
24	CHL	6	607	-	-	27/41/117/117	-
25	CLA	G	604	-	-	9/20/96/115	-
25	CLA	B	616	5	-	10/39/115/115	-
25	CLA	c	509	6	-	5/39/115/115	-
25	CLA	9	603	2	-	23/39/115/115	-
25	CLA	n	603	2	-	9/39/115/115	-
24	CHL	n	607	-	-	16/41/117/117	-
24	CHL	n	608	-	-	12/22/98/117	-
25	CLA	r	609	17	-	8/31/107/115	-
24	CHL	5	601	2	-	20/41/117/117	-
25	CLA	s	602	18	-	9/20/96/115	-
25	CLA	4	604	-	-	15/20/96/115	-
37	DGD	c	524	-	-	9/55/95/95	0/2/2/2
25	CLA	N	613	2	-	16/39/115/115	-
25	CLA	5	604	-	-	18/39/115/115	-
24	CHL	2	609	2	-	22/41/117/117	-
24	CHL	N	608	-	-	6/22/98/117	-
25	CLA	6	612	1	-	13/39/115/115	-
25	CLA	b	608	-	-	19/39/115/115	-
26	LUT	p	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	q	1621	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	9	609	2	-	21/41/117/117	-
28	NEX	g	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	1	609	1	-	17/41/117/117	-
26	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	5	603	2	-	15/39/115/115	-
25	CLA	1	604	-	-	17/39/115/115	-
24	CHL	6	605	1	-	7/17/93/117	-
29	LHG	d	410	-	-	12/43/43/53	-
25	CLA	q	613	3	-	16/39/115/115	-
34	BCR	a	411	-	-	2/29/63/63	0/2/2/2
25	CLA	7	602	1	-	15/39/115/115	-
24	CHL	q	605	3	-	8/20/96/117	-
28	NEX	n	1623	-	-	2/27/83/83	0/3/3/3
35	SQD	B	623	-	-	11/45/65/69	0/1/1/1
25	CLA	3	612	2	-	10/15/91/115	-
25	CLA	b	616	5	-	10/39/115/115	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
25	CLA	s	611	29	-	8/20/96/115	-
24	CHL	S	607	-	-	4/14/90/117	-
25	CLA	5	610	2	-	10/39/115/115	-
24	CHL	y	609	1	-	19/41/117/117	-
36	LMG	H	102	-	-	15/43/63/70	0/1/1/1
25	CLA	1	610	1	-	14/39/115/115	-
25	CLA	6	613	1	-	22/39/115/115	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	7	613	1	-	15/39/115/115	-
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
25	CLA	C	504	-	-	17/39/115/115	-
25	CLA	S	609	18	-	6/10/86/115	-
24	CHL	7	601	1	-	18/41/117/117	-
24	CHL	G	606	-	-	5/22/98/117	-
24	CHL	g	605	3	-	9/20/96/117	-
25	CLA	4	612	3	-	9/13/89/115	-
24	CHL	Y	606	-	-	23/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	G	609	3	-	16/41/117/117	-
25	CLA	N	614	2	-	8/20/96/115	-
25	CLA	7	604	-	-	19/39/115/115	-
24	CHL	p	601	2	-	18/41/117/117	-
25	CLA	G	614	3	-	11/20/96/115	-
36	LMG	d	411	-	-	8/41/61/70	0/1/1/1
33	PHO	a	409	-	-	9/37/103/103	0/5/6/6
25	CLA	r	604	-	-	10/19/95/115	-
25	CLA	g	613	3	-	14/39/115/115	-
25	CLA	B	610	5	-	8/39/115/115	-
25	CLA	y	612	1	-	17/39/115/115	-
24	CHL	9	607	-	-	13/22/98/117	-
24	CHL	9	608	-	-	6/15/91/117	-
29	LHG	c	2630	-	-	15/51/51/53	-
34	BCR	D	404	-	-	4/29/63/63	0/2/2/2
24	CHL	N	607	-	-	16/41/117/117	-
24	CHL	2	606	-	-	11/22/98/117	-
26	LUT	0	1621	-	-	3/29/67/67	0/2/2/2
34	BCR	c	517	-	-	0/29/63/63	0/2/2/2
25	CLA	3	602	2	-	12/39/115/115	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	c	507	-	-	12/39/115/115	-
27	XAT	r	622	-	-	0/31/93/93	0/4/4/4
25	CLA	0	614	1	-	11/26/102/115	-
29	LHG	2	2630	25	-	22/53/53/53	-
25	CLA	Y	603	1	-	16/39/115/115	-
24	CHL	3	608	-	-	11/22/98/117	-
27	XAT	n	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	9	602	2	-	18/39/115/115	-
25	CLA	B	613	5	-	14/39/115/115	-
24	CHL	4	606	-	-	10/22/98/117	-
29	LHG	C	2630	-	-	19/51/51/53	-
33	PHO	A	409	-	-	9/37/103/103	0/5/6/6
24	CHL	7	607	-	-	21/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	7	610	1	-	15/39/115/115	-
24	CHL	7	605	1	-	10/17/93/117	-
25	CLA	r	610	17	-	16/39/115/115	-
24	CHL	N	609	2	-	21/41/117/117	-
29	LHG	n	2630	25	-	15/53/53/53	-
25	CLA	q	614	3	-	10/20/96/115	-
25	CLA	p	610	2	-	11/39/115/115	-
28	NEX	N	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	s	613	18	-	11/20/96/115	-
25	CLA	8	612	2	-	9/15/91/115	-
25	CLA	y	610	1	-	11/39/115/115	-
34	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	B	606	5	-	14/39/115/115	-
24	CHL	n	606	-	-	9/17/93/117	-
25	CLA	3	611	29	-	10/20/96/115	-
37	DGD	C	520	-	-	10/48/88/95	0/2/2/2
25	CLA	R	601	17	-	10/20/96/115	-
36	LMG	C	521	-	-	10/46/66/70	0/1/1/1
24	CHL	0	601	1	-	13/41/117/117	-
25	CLA	5	614	2	-	10/20/96/115	-
26	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
24	CHL	y	606	-	-	23/41/117/117	-
25	CLA	A	410	4	-	6/33/109/115	-
25	CLA	b	606	5	-	14/39/115/115	-
25	CLA	8	614	2	-	10/20/96/115	-
25	CLA	N	603	2	-	8/39/115/115	-
25	CLA	0	604	-	-	19/39/115/115	-
25	CLA	n	613	2	-	16/39/115/115	-
24	CHL	8	607	-	-	26/41/117/117	-
37	DGD	C	523	-	-	12/55/95/95	0/2/2/2
25	CLA	c	512	6	-	15/39/115/115	-
24	CHL	2	607	-	-	12/22/98/117	-
29	LHG	9	2630	25	-	20/53/53/53	-
24	CHL	5	606	-	-	4/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	p	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	C	507	-	-	11/39/115/115	-
25	CLA	S	605	18	-	11/21/97/115	-
29	LHG	D	410	-	-	10/43/43/53	-
25	CLA	y	603	1	-	17/39/115/115	-
27	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	G	611	29	-	8/15/91/115	-
25	CLA	S	614	18	-	7/19/95/115	-
25	CLA	Y	604	-	-	20/39/115/115	-
28	NEX	q	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	c	506	6	-	22/39/115/115	-
25	CLA	A	407	-	-	6/20/96/115	-
35	SQD	D	413	-	-	10/47/67/69	0/1/1/1
25	CLA	4	611	29	-	9/15/91/115	-
24	CHL	3	609	2	-	18/41/117/117	-
26	LUT	3	1620	-	-	6/29/67/67	0/2/2/2
37	DGD	c	518	-	-	7/44/84/95	0/2/2/2
25	CLA	b	604	5	-	13/39/115/115	-
34	BCR	c	515	-	-	4/29/63/63	0/2/2/2
24	CHL	p	607	-	-	24/41/117/117	-
25	CLA	y	604	-	-	20/39/115/115	-
25	CLA	y	611	29	-	10/39/115/115	-
25	CLA	2	614	2	-	9/20/96/115	-
25	CLA	1	612	1	-	17/39/115/115	-
36	LMG	B	622	-	-	9/46/66/70	0/1/1/1
36	LMG	s	2631	-	-	10/47/67/70	0/1/1/1
25	CLA	B	607	5	-	17/39/115/115	-
28	NEX	s	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	n	610	2	-	8/39/115/115	-
24	CHL	8	608	-	-	11/22/98/117	-
25	CLA	6	614	1	-	9/26/102/115	-
29	LHG	5	2630	25	-	13/53/53/53	-
25	CLA	b	612	5	-	9/39/115/115	-
24	CHL	2	608	-	-	7/15/91/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	N	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	3	603	2	-	15/39/115/115	-
25	CLA	c	508	6	-	13/39/115/115	-
25	CLA	C	506	6	-	22/39/115/115	-
25	CLA	9	604	-	-	10/20/96/115	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
24	CHL	6	601	1	-	12/41/117/117	-
25	CLA	7	614	1	-	15/26/102/115	-
25	CLA	c	502	6	-	19/39/115/115	-
25	CLA	2	603	2	-	22/39/115/115	-
29	LHG	Y	2630	25	-	23/53/53/53	-
25	CLA	Y	602	1	-	12/39/115/115	-
29	LHG	8	2630	25	-	10/53/53/53	-
25	CLA	A	405	4	-	13/39/115/115	-
25	CLA	r	612	17	-	10/20/96/115	-
26	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
37	DGD	c	519	-	-	20/51/91/95	0/2/2/2
26	LUT	5	1620	-	-	4/29/67/67	0/2/2/2
34	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	CHL	1	608	-	-	9/22/98/117	-
24	CHL	g	601	3	-	19/41/117/117	-
29	LHG	s	2630	25	-	18/49/49/53	-
25	CLA	4	613	3	-	17/39/115/115	-
36	LMG	b	622	-	-	8/46/66/70	0/1/1/1
29	LHG	l	101	-	-	18/53/53/53	-
28	NEX	S	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	c	501	6	-	16/39/115/115	-
25	CLA	5	613	2	-	14/39/115/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
26	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	g	610	3	-	12/39/115/115	-
25	CLA	8	611	29	-	10/20/96/115	-
25	CLA	8	604	-	-	10/39/115/115	-
25	CLA	0	610	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	G	1620	-	-	3/29/67/67	0/2/2/2
25	CLA	2	611	29	-	10/15/91/115	-
25	CLA	2	604	-	-	11/20/96/115	-
29	LHG	1	2630	25	-	16/53/53/53	-
26	LUT	9	1621	-	-	3/29/67/67	0/2/2/2
28	NEX	3	1623	-	-	5/27/83/83	0/3/3/3
29	LHG	D	408	-	-	10/48/48/53	-
24	CHL	n	605	2	-	22/41/117/117	-
25	CLA	a	405	4	-	13/39/115/115	-
29	LHG	L	101	-	-	17/53/53/53	-
25	CLA	C	502	6	-	20/39/115/115	-
24	CHL	0	609	1	-	21/41/117/117	-
24	CHL	9	606	-	-	12/22/98/117	-
25	CLA	C	513	6	-	19/39/115/115	-
25	CLA	G	612	3	-	6/13/89/115	-
27	XAT	6	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	b	603	5	-	13/39/115/115	-
25	CLA	1	602	1	-	13/39/115/115	-
25	CLA	Y	611	29	-	10/39/115/115	-
25	CLA	b	605	5	-	15/39/115/115	-
25	CLA	1	611	29	-	10/39/115/115	-
25	CLA	B	612	5	-	9/39/115/115	-
24	CHL	7	609	1	-	17/41/117/117	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	CLA	N	602	2	-	8/39/115/115	-
25	CLA	4	603	3	-	18/39/115/115	-
24	CHL	5	608	-	-	13/22/98/117	-
24	CHL	Y	607	-	-	21/41/117/117	-
35	SQD	d	413	-	-	9/47/67/69	0/1/1/1
26	LUT	y	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	S	601	18	-	11/17/93/117	-
27	XAT	g	1622	-	-	0/31/93/93	0/4/4/4
34	BCR	b	618	-	-	5/29/63/63	0/2/2/2
25	CLA	R	611	29	-	11/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	y	602	1	-	12/39/115/115	-
26	LUT	8	1620	-	-	4/29/67/67	0/2/2/2
25	CLA	G	603	3	-	9/39/115/115	-
25	CLA	s	610	18	-	11/20/96/115	-
36	LMG	S	2631	-	-	12/47/67/70	0/1/1/1
25	CLA	R	609	17	-	8/31/107/115	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	b	617	5	-	11/39/115/115	-
27	XAT	R	622	-	-	0/31/93/93	0/4/4/4
24	CHL	4	601	3	-	18/41/117/117	-
24	CHL	r	608	-	-	17/35/111/117	-
37	DGD	c	520	-	-	10/48/88/95	0/2/2/2
24	CHL	Y	605	1	-	8/17/93/117	-
25	CLA	a	407	-	-	6/20/96/115	-
34	BCR	C	514	-	-	4/29/63/63	0/2/2/2
25	CLA	R	603	17	-	12/33/109/115	-
36	LMG	c	521	-	-	10/46/66/70	0/1/1/1
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	3	607	-	-	26/41/117/117	-
24	CHL	5	607	-	-	19/41/117/117	-
24	CHL	p	609	2	-	21/41/117/117	-
25	CLA	8	603	2	-	16/39/115/115	-
25	CLA	Y	610	1	-	11/39/115/115	-
28	NEX	r	623	-	-	2/27/83/83	0/3/3/3
34	BCR	C	517	-	-	0/29/63/63	0/2/2/2
25	CLA	8	613	2	-	17/39/115/115	-
25	CLA	2	612	2	-	6/13/89/115	-
26	LUT	2	1621	-	-	6/29/67/67	0/2/2/2
37	DGD	C	524	-	-	9/55/95/95	0/2/2/2
39	PL9	D	405	-	-	14/53/73/73	0/1/1/1
25	CLA	s	605	18	-	10/21/97/115	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
24	CHL	4	608	-	-	4/15/91/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	1	607	-	-	21/41/117/117	-
24	CHL	4	605	3	-	12/20/96/117	-
25	CLA	s	609	18	-	6/10/86/115	-
26	LUT	5	1621	-	-	2/29/67/67	0/2/2/2
29	LHG	G	2630	25	-	12/53/53/53	-
25	CLA	r	611	29	-	12/20/96/115	-
25	CLA	b	615	5	-	16/39/115/115	-
25	CLA	1	603	1	-	19/39/115/115	-
25	CLA	2	602	2	-	13/39/115/115	-
25	CLA	9	612	2	-	6/13/89/115	-
24	CHL	g	609	3	-	17/41/117/117	-
28	NEX	5	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	9	605	2	-	8/20/96/117	-
28	NEX	8	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	g	604	-	-	10/20/96/115	-
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
27	XAT	q	1622	-	-	3/31/93/93	0/4/4/4
26	LUT	p	1621	-	-	4/29/67/67	0/2/2/2
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	9	614	2	-	10/20/96/115	-
25	CLA	6	610	1	-	8/39/115/115	-
24	CHL	6	609	1	-	21/41/117/117	-
25	CLA	S	613	18	-	11/20/96/115	-
25	CLA	q	610	3	-	11/39/115/115	-
25	CLA	s	604	-	-	10/20/96/115	-
25	CLA	3	613	2	-	16/39/115/115	-
36	LMG	d	412	-	-	5/41/61/70	0/1/1/1
25	CLA	g	614	3	-	11/20/96/115	-
25	CLA	b	602	-	-	19/39/115/115	-
24	CHL	y	605	1	-	8/17/93/117	-
27	XAT	5	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	0	611	29	-	9/39/115/115	-
24	CHL	G	607	-	-	9/22/98/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	G	608	-	-	6/15/91/117	-
25	CLA	D	402	7	-	16/39/115/115	-
25	CLA	0	613	1	-	18/39/115/115	-
25	CLA	3	604	-	-	8/39/115/115	-
28	NEX	4	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	g	606	-	-	5/22/98/117	-
25	CLA	p	612	2	-	6/15/91/115	-
26	LUT	n	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	d	403	7	-	14/39/115/115	-
25	CLA	G	602	3	-	11/39/115/115	-
25	CLA	r	603	17	-	12/33/109/115	-
27	XAT	p	1622	-	-	0/31/93/93	0/4/4/4
24	CHL	G	605	3	-	11/20/96/117	-
24	CHL	8	605	2	-	15/41/117/117	-
24	CHL	n	601	2	-	10/41/117/117	-
25	CLA	p	614	2	-	9/20/96/115	-
24	CHL	2	605	2	-	8/20/96/117	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	Y	609	1	-	19/41/117/117	-
25	CLA	n	604	-	-	11/39/115/115	-
25	CLA	5	612	2	-	8/15/91/115	-
25	CLA	b	611	-	-	9/39/115/115	-
29	LHG	R	2630	25	-	16/42/42/53	-
25	CLA	R	602	17	-	8/33/109/115	-
25	CLA	b	613	5	-	14/39/115/115	-
25	CLA	3	610	2	-	8/39/115/115	-
25	CLA	C	503	6	-	10/39/115/115	-
25	CLA	r	601	17	-	10/20/96/115	-
24	CHL	p	608	-	-	15/22/98/117	-
25	CLA	y	613	1	-	11/39/115/115	-
26	LUT	0	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	s	614	18	-	7/19/95/115	-
25	CLA	8	602	2	-	12/39/115/115	-
27	XAT	2	1622	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	518	-	-	7/44/84/95	0/2/2/2
29	LHG	g	2630	25	-	12/53/53/53	-
25	CLA	g	602	3	-	11/39/115/115	-
24	CHL	3	606	-	-	10/17/93/117	-
25	CLA	9	611	29	-	10/15/91/115	-
25	CLA	r	616	17	-	24/39/115/115	-
29	LHG	y	2630	25	-	24/53/53/53	-
26	LUT	9	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	7	612	1	-	15/39/115/115	-
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
25	CLA	D	403	7	-	14/39/115/115	-
26	LUT	Y	1621	-	-	4/29/67/67	0/2/2/2
25	CLA	N	610	2	-	8/39/115/115	-
29	LHG	6	2630	25	-	19/53/53/53	-
24	CHL	0	607	-	-	24/41/117/117	-
24	CHL	0	608	-	-	8/22/98/117	-
24	CHL	1	606	-	-	19/41/117/117	-
34	BCR	B	618	-	-	5/29/63/63	0/2/2/2
40	HEM	F	101	8,9	-	4/14/54/54	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	N	606	-	-	9/17/93/117	-
27	XAT	4	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	C	510	6	-	10/39/115/115	-
24	CHL	6	608	-	-	10/22/98/117	-
29	LHG	3	2630	25	-	12/53/53/53	-
25	CLA	C	508	6	-	16/39/115/115	-
25	CLA	2	613	2	-	10/39/115/115	-
24	CHL	q	608	-	-	6/15/91/117	-
36	LMG	D	411	-	-	8/41/61/70	0/1/1/1
25	CLA	c	504	-	-	17/39/115/115	-
25	CLA	4	602	3	-	12/39/115/115	-
25	CLA	y	614	1	-	12/26/102/115	-
25	CLA	R	616	17	-	24/39/115/115	-
25	CLA	5	611	29	-	13/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	608	-	-	18/39/115/115	-
37	DGD	C	519	-	-	20/51/91/95	0/2/2/2
34	BCR	A	411	-	-	2/29/63/63	0/2/2/2
36	LMG	A	413	-	-	12/43/63/70	0/1/1/1
24	CHL	4	609	3	-	20/41/117/117	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	1	613	1	-	14/39/115/115	-
24	CHL	Y	601	1	-	15/41/117/117	-
29	LHG	q	2630	25	-	17/53/53/53	-
24	CHL	1	605	1	-	10/17/93/117	-
24	CHL	y	607	-	-	18/41/117/117	-
25	CLA	p	604	-	-	17/39/115/115	-
25	CLA	p	611	29	-	8/20/96/115	-
29	LHG	N	2630	25	-	15/53/53/53	-
24	CHL	r	607	-	-	19/29/105/117	-
40	HEM	f	101	8,9	-	4/14/54/54	-
25	CLA	b	607	5	-	17/39/115/115	-
24	CHL	g	607	-	-	12/22/98/117	-
24	CHL	g	608	-	-	3/15/91/117	-
26	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	N	605	2	-	25/41/117/117	-
25	CLA	6	602	1	-	14/39/115/115	-
29	LHG	D	409	-	-	12/53/53/53	-
28	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3
27	XAT	8	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	q	602	3	-	17/39/115/115	-
25	CLA	g	603	3	-	9/39/115/115	-
25	CLA	q	611	29	-	9/15/91/115	-
24	CHL	6	606	-	-	22/41/117/117	-
25	CLA	B	615	5	-	17/39/115/115	-
36	LMG	a	413	-	-	12/43/63/70	0/1/1/1
25	CLA	B	609	5	-	12/39/115/115	-
25	CLA	r	602	17	-	8/33/109/115	-
25	CLA	8	610	2	-	11/39/115/115	-

All (4830) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	409	PHO	C1B-C2B	8.37	1.48	1.39
33	A	409	PHO	C1B-C2B	8.32	1.48	1.39
33	a	408	PHO	C1B-C2B	8.21	1.48	1.39
33	A	408	PHO	C1B-C2B	8.16	1.48	1.39
33	A	408	PHO	C3B-C4B	6.96	1.49	1.41
33	a	408	PHO	C3B-C4B	6.92	1.49	1.41
39	d	405	PL9	C7-C3	-6.82	1.44	1.51
33	a	409	PHO	C3B-C4B	6.71	1.49	1.41
39	D	405	PL9	C7-C3	-6.71	1.44	1.51
33	A	409	PHO	C3B-C4B	6.71	1.49	1.41
39	D	405	PL9	C3-C4	-6.12	1.39	1.49
39	d	405	PL9	C3-C4	-6.03	1.39	1.49
24	G	609	CHL	C3D-C4D	-5.77	1.31	1.44
24	G	601	CHL	C3D-C4D	-5.77	1.31	1.44
24	g	609	CHL	C3D-C4D	-5.76	1.31	1.44
24	g	601	CHL	C3D-C4D	-5.73	1.31	1.44
24	y	609	CHL	C3D-C4D	-5.67	1.31	1.44
24	y	601	CHL	C3D-C4D	-5.67	1.31	1.44
24	Y	601	CHL	C3D-C4D	-5.67	1.31	1.44
24	Y	609	CHL	C3D-C4D	-5.63	1.31	1.44
24	R	608	CHL	C3D-C4D	-5.55	1.31	1.44
24	r	608	CHL	C3D-C4D	-5.55	1.31	1.44
24	Y	608	CHL	C3D-C4D	-5.46	1.31	1.44
24	N	607	CHL	C3D-C4D	-5.44	1.31	1.44
24	y	608	CHL	C3D-C4D	-5.43	1.31	1.44
24	N	609	CHL	C3D-C4D	-5.42	1.31	1.44
24	n	607	CHL	C3D-C4D	-5.42	1.32	1.44
24	N	601	CHL	C3D-C4D	-5.39	1.32	1.44
24	r	606	CHL	C3D-C4D	-5.38	1.32	1.44
24	n	609	CHL	C3D-C4D	-5.37	1.32	1.44
24	n	601	CHL	C3D-C4D	-5.36	1.32	1.44
24	1	606	CHL	C3D-C4D	-5.36	1.32	1.44
24	R	606	CHL	C3D-C4D	-5.35	1.32	1.44
24	7	601	CHL	C3D-C4D	-5.34	1.32	1.44
24	q	606	CHL	CHC-C1C	5.34	1.49	1.38
24	1	601	CHL	C3D-C4D	-5.34	1.32	1.44
24	7	606	CHL	C3D-C4D	-5.33	1.32	1.44
24	9	605	CHL	O2D-CGD	5.31	1.46	1.33
24	R	607	CHL	C3D-C4D	-5.31	1.32	1.44
24	q	605	CHL	O2D-CGD	5.30	1.46	1.33
24	y	607	CHL	C3D-C4D	-5.30	1.32	1.44
24	5	605	CHL	O2D-CGD	5.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	605	CHL	O2D-CGD	5.29	1.46	1.33
24	1	609	CHL	C3D-C4D	-5.28	1.32	1.44
24	Y	607	CHL	C3D-C4D	-5.28	1.32	1.44
24	4	609	CHL	C3D-C4D	-5.27	1.32	1.44
24	y	606	CHL	C3D-C4D	-5.27	1.32	1.44
24	G	606	CHL	C3D-C4D	-5.26	1.32	1.44
24	p	605	CHL	O2D-CGD	5.26	1.46	1.33
24	4	605	CHL	O2D-CGD	5.26	1.46	1.33
24	7	609	CHL	C3D-C4D	-5.25	1.32	1.44
24	Y	606	CHL	C3D-C4D	-5.25	1.32	1.44
24	g	606	CHL	C3D-C4D	-5.25	1.32	1.44
24	r	607	CHL	C3D-C4D	-5.25	1.32	1.44
24	p	606	CHL	O2D-CGD	5.24	1.46	1.33
24	n	606	CHL	C3D-C4D	-5.24	1.32	1.44
24	N	605	CHL	C3D-C4D	-5.24	1.32	1.44
24	3	606	CHL	C3D-C4D	-5.24	1.32	1.44
24	8	606	CHL	C3D-C4D	-5.23	1.32	1.44
24	n	605	CHL	C3D-C4D	-5.23	1.32	1.44
24	s	601	CHL	C3D-C4D	-5.23	1.32	1.44
24	3	605	CHL	O2D-CGD	5.22	1.45	1.33
24	N	606	CHL	C3D-C4D	-5.21	1.32	1.44
24	q	601	CHL	C3D-C4D	-5.21	1.32	1.44
24	4	606	CHL	CHC-C1C	5.21	1.49	1.38
24	8	605	CHL	O2D-CGD	5.21	1.45	1.33
24	N	608	CHL	C3D-C4D	-5.21	1.32	1.44
24	2	601	CHL	C3D-C4D	-5.20	1.32	1.44
24	S	601	CHL	C3D-C4D	-5.20	1.32	1.44
24	6	601	CHL	O2D-CGD	5.19	1.45	1.33
24	p	608	CHL	O2D-CGD	5.19	1.45	1.33
24	5	606	CHL	O2D-CGD	5.18	1.45	1.33
24	q	606	CHL	O2D-CGD	5.18	1.45	1.33
24	q	609	CHL	C3D-C4D	-5.18	1.32	1.44
39	d	405	PL9	C6-C1	-5.17	1.39	1.48
24	7	605	CHL	C3D-C4D	-5.17	1.32	1.44
24	4	606	CHL	O2D-CGD	5.16	1.45	1.33
24	0	606	CHL	C3D-C4D	-5.16	1.32	1.44
24	6	608	CHL	C3D-C4D	-5.16	1.32	1.44
24	s	607	CHL	C3D-C4D	-5.15	1.32	1.44
24	9	606	CHL	O2D-CGD	5.15	1.45	1.33
24	p	601	CHL	O2D-CGD	5.15	1.45	1.33
24	1	605	CHL	C3D-C4D	-5.14	1.32	1.44
24	5	608	CHL	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	C3D-C4D	-5.14	1.32	1.44
24	8	606	CHL	O2D-CGD	5.14	1.45	1.33
24	s	608	CHL	C3D-C4D	-5.14	1.32	1.44
24	n	608	CHL	C3D-C4D	-5.13	1.32	1.44
24	2	606	CHL	O2D-CGD	5.13	1.45	1.33
24	0	605	CHL	O2D-CGD	5.13	1.45	1.33
24	p	607	CHL	O2D-CGD	5.13	1.45	1.33
24	4	609	CHL	CHC-C1C	5.13	1.48	1.38
24	G	605	CHL	O2D-CGD	5.12	1.45	1.33
24	g	605	CHL	O2D-CGD	5.12	1.45	1.33
24	0	601	CHL	O2D-CGD	5.12	1.45	1.33
24	9	601	CHL	C3D-C4D	-5.12	1.32	1.44
24	0	608	CHL	C3D-C4D	-5.12	1.32	1.44
24	q	607	CHL	O2D-CGD	5.12	1.45	1.33
24	3	606	CHL	O2D-CGD	5.11	1.45	1.33
39	D	405	PL9	C6-C1	-5.11	1.39	1.48
24	5	601	CHL	O2D-CGD	5.11	1.45	1.33
24	S	607	CHL	C3D-C4D	-5.11	1.32	1.44
24	s	601	CHL	O2D-CGD	5.11	1.45	1.33
24	q	609	CHL	CHC-C1C	5.11	1.48	1.38
24	S	601	CHL	O2D-CGD	5.11	1.45	1.33
24	6	605	CHL	O2D-CGD	5.10	1.45	1.33
24	4	607	CHL	O2D-CGD	5.10	1.45	1.33
24	9	607	CHL	O2D-CGD	5.09	1.45	1.33
24	2	607	CHL	O2D-CGD	5.09	1.45	1.33
24	5	609	CHL	O2D-CGD	5.09	1.45	1.33
24	5	607	CHL	O2D-CGD	5.09	1.45	1.33
24	S	606	CHL	C3D-C4D	-5.08	1.32	1.44
24	9	608	CHL	O2D-CGD	5.07	1.45	1.33
24	p	609	CHL	O2D-CGD	5.07	1.45	1.33
24	4	601	CHL	C3D-C4D	-5.06	1.32	1.44
24	g	608	CHL	C3D-C4D	-5.06	1.32	1.44
24	6	606	CHL	C3D-C4D	-5.05	1.32	1.44
24	q	609	CHL	C2C-C3C	5.04	1.47	1.36
24	G	608	CHL	C3D-C4D	-5.04	1.32	1.44
24	g	607	CHL	C3D-C4D	-5.04	1.32	1.44
24	7	608	CHL	C3D-C4D	-5.04	1.32	1.44
24	p	606	CHL	C3D-C4D	-5.03	1.32	1.44
24	3	608	CHL	O2D-CGD	5.03	1.45	1.33
24	0	608	CHL	O2D-CGD	5.03	1.45	1.33
24	s	606	CHL	C3D-C4D	-5.02	1.32	1.44
24	q	609	CHL	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	607	CHL	O2D-CGD	5.02	1.45	1.33
24	8	601	CHL	C3D-C4D	-5.01	1.32	1.44
24	4	609	CHL	O2D-CGD	5.01	1.45	1.33
24	3	601	CHL	C3D-C4D	-5.01	1.32	1.44
24	9	609	CHL	C2C-C3C	5.01	1.47	1.36
24	8	608	CHL	O2D-CGD	5.01	1.45	1.33
24	Y	605	CHL	C3D-C4D	-5.00	1.32	1.44
24	y	605	CHL	C3D-C4D	-5.00	1.32	1.44
24	1	606	CHL	O2D-CGD	5.00	1.45	1.33
24	7	607	CHL	O2D-CGD	4.99	1.45	1.33
24	6	608	CHL	O2D-CGD	4.99	1.45	1.33
24	5	609	CHL	C3D-C4D	-4.99	1.32	1.44
24	q	601	CHL	O2D-CGD	4.98	1.45	1.33
24	q	608	CHL	O2D-CGD	4.98	1.45	1.33
24	3	607	CHL	O2D-CGD	4.98	1.45	1.33
24	0	609	CHL	O2D-CGD	4.98	1.45	1.33
24	6	609	CHL	O2D-CGD	4.98	1.45	1.33
24	1	608	CHL	C3D-C4D	-4.98	1.32	1.44
24	s	606	CHL	O2D-CGD	4.98	1.45	1.33
24	2	606	CHL	C3D-C4D	-4.98	1.32	1.44
24	q	609	CHL	CHD-C1D	4.98	1.48	1.38
24	G	607	CHL	C3D-C4D	-4.98	1.32	1.44
24	7	606	CHL	O2D-CGD	4.97	1.45	1.33
24	6	609	CHL	C3D-C4D	-4.97	1.33	1.44
24	1	607	CHL	C3D-C4D	-4.97	1.33	1.44
24	7	607	CHL	C3D-C4D	-4.97	1.33	1.44
24	3	609	CHL	O2D-CGD	4.97	1.45	1.33
24	3	609	CHL	C3D-C4D	-4.96	1.33	1.44
24	S	606	CHL	O2D-CGD	4.96	1.45	1.33
24	3	601	CHL	O2D-CGD	4.95	1.45	1.33
24	5	606	CHL	C3D-C4D	-4.95	1.33	1.44
24	p	609	CHL	C3D-C4D	-4.95	1.33	1.44
24	8	609	CHL	O2D-CGD	4.95	1.45	1.33
24	n	606	CHL	O2D-CGD	4.95	1.45	1.33
24	G	609	CHL	O2D-CGD	4.94	1.45	1.33
24	G	606	CHL	O2D-CGD	4.94	1.45	1.33
24	9	606	CHL	C3D-C4D	-4.94	1.33	1.44
24	2	608	CHL	O2D-CGD	4.94	1.45	1.33
24	0	609	CHL	C3D-C4D	-4.94	1.33	1.44
24	4	608	CHL	O2D-CGD	4.94	1.45	1.33
24	4	601	CHL	O2D-CGD	4.93	1.45	1.33
24	g	606	CHL	O2D-CGD	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	609	CHL	C3D-C4D	-4.93	1.33	1.44
24	8	607	CHL	O2D-CGD	4.93	1.45	1.33
24	6	601	CHL	C3D-C4D	-4.92	1.33	1.44
24	8	609	CHL	C3D-C4D	-4.92	1.33	1.44
24	3	606	CHL	CHC-C1C	4.91	1.48	1.38
35	A	412	SQD	O8-S	4.91	1.65	1.47
24	N	606	CHL	O2D-CGD	4.91	1.45	1.33
24	8	601	CHL	O2D-CGD	4.91	1.45	1.33
24	6	607	CHL	C3D-C4D	-4.91	1.33	1.44
24	4	609	CHL	C2C-C3C	4.91	1.47	1.36
24	2	609	CHL	O2D-CGD	4.90	1.45	1.33
24	7	605	CHL	O2D-CGD	4.90	1.45	1.33
24	g	608	CHL	O2D-CGD	4.90	1.45	1.33
24	p	605	CHL	C3D-C4D	-4.90	1.33	1.44
24	q	608	CHL	CHC-C1C	4.90	1.48	1.38
24	g	609	CHL	O2D-CGD	4.90	1.45	1.33
24	s	607	CHL	O2D-CGD	4.90	1.45	1.33
24	G	608	CHL	O2D-CGD	4.89	1.45	1.33
24	S	607	CHL	O2D-CGD	4.89	1.45	1.33
24	9	609	CHL	O2D-CGD	4.89	1.45	1.33
35	a	412	SQD	O8-S	4.89	1.64	1.47
24	4	607	CHL	C3D-C4D	-4.88	1.33	1.44
24	1	605	CHL	O2D-CGD	4.88	1.45	1.33
24	1	608	CHL	O2D-CGD	4.88	1.45	1.33
24	7	608	CHL	O2D-CGD	4.88	1.45	1.33
24	2	609	CHL	C2C-C3C	4.87	1.47	1.36
24	S	608	CHL	O2D-CGD	4.87	1.45	1.33
24	s	608	CHL	O2D-CGD	4.87	1.45	1.33
24	2	609	CHL	C3D-C4D	-4.87	1.33	1.44
24	q	608	CHL	C2C-C3C	4.86	1.47	1.36
24	2	601	CHL	O2D-CGD	4.86	1.45	1.33
24	Y	605	CHL	O2D-CGD	4.86	1.45	1.33
24	y	605	CHL	O2D-CGD	4.86	1.45	1.33
24	4	608	CHL	C3D-C4D	-4.86	1.33	1.44
24	0	601	CHL	C3D-C4D	-4.85	1.33	1.44
24	5	605	CHL	C2C-C3C	4.85	1.47	1.36
24	8	608	CHL	C3D-C4D	-4.85	1.33	1.44
24	5	601	CHL	C3D-C4D	-4.85	1.33	1.44
24	4	606	CHL	C3D-C4D	-4.84	1.33	1.44
24	p	605	CHL	CHD-C1D	4.84	1.47	1.38
24	7	609	CHL	O2D-CGD	4.84	1.45	1.33
24	y	609	CHL	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	607	CHL	O2D-CGD	4.84	1.45	1.33
24	8	605	CHL	C2C-C3C	4.84	1.47	1.36
24	q	607	CHL	C3D-C4D	-4.84	1.33	1.44
24	2	608	CHL	C3D-C4D	-4.84	1.33	1.44
24	3	605	CHL	CHC-C1C	4.83	1.48	1.38
24	S	601	CHL	CHC-C1C	4.83	1.48	1.38
24	9	601	CHL	O2D-CGD	4.83	1.45	1.33
24	4	609	CHL	CHD-C1D	4.82	1.47	1.38
24	0	606	CHL	O2D-CGD	4.82	1.45	1.33
24	2	607	CHL	C3D-C4D	-4.82	1.33	1.44
24	8	605	CHL	CHC-C1C	4.82	1.48	1.38
24	8	607	CHL	C3D-C4D	-4.82	1.33	1.44
24	9	607	CHL	C3D-C4D	-4.81	1.33	1.44
24	3	605	CHL	C2C-C3C	4.81	1.47	1.36
24	3	608	CHL	C3D-C4D	-4.81	1.33	1.44
24	5	607	CHL	C3D-C4D	-4.81	1.33	1.44
24	s	601	CHL	CHC-C1C	4.81	1.48	1.38
24	q	606	CHL	C3D-C4D	-4.81	1.33	1.44
24	8	606	CHL	CHC-C1C	4.80	1.48	1.38
24	0	607	CHL	O2D-CGD	4.80	1.44	1.33
24	p	607	CHL	C3D-C4D	-4.79	1.33	1.44
24	0	607	CHL	C3D-C4D	-4.79	1.33	1.44
24	n	607	CHL	O2D-CGD	4.79	1.44	1.33
24	q	605	CHL	C3D-C4D	-4.79	1.33	1.44
24	9	608	CHL	C3D-C4D	-4.79	1.33	1.44
24	R	606	CHL	O2D-CGD	4.79	1.44	1.33
24	Y	607	CHL	O2D-CGD	4.79	1.44	1.33
24	r	606	CHL	O2D-CGD	4.78	1.44	1.33
24	4	608	CHL	CHC-C1C	4.78	1.48	1.38
24	4	605	CHL	C3D-C4D	-4.78	1.33	1.44
24	4	607	CHL	CHC-C1C	4.78	1.48	1.38
24	5	605	CHL	C3D-C4D	-4.78	1.33	1.44
24	7	601	CHL	O2D-CGD	4.78	1.44	1.33
24	8	605	CHL	C3D-C4D	-4.77	1.33	1.44
24	p	606	CHL	CHD-C1D	4.77	1.47	1.38
24	y	607	CHL	O2D-CGD	4.77	1.44	1.33
24	3	607	CHL	C3D-C4D	-4.77	1.33	1.44
24	p	601	CHL	C3D-C4D	-4.77	1.33	1.44
24	g	607	CHL	O2D-CGD	4.77	1.44	1.33
24	3	606	CHL	CHD-C1D	4.77	1.47	1.38
24	5	609	CHL	C2C-C3C	4.76	1.47	1.36
24	p	605	CHL	C2C-C3C	4.76	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	607	CHL	O2D-CGD	4.76	1.44	1.33
24	q	607	CHL	CHC-C1C	4.76	1.48	1.38
24	6	606	CHL	O2D-CGD	4.76	1.44	1.33
24	6	607	CHL	O2D-CGD	4.76	1.44	1.33
24	q	608	CHL	C3D-C4D	-4.76	1.33	1.44
24	1	601	CHL	O2D-CGD	4.76	1.44	1.33
24	p	609	CHL	C2C-C3C	4.76	1.46	1.36
24	N	605	CHL	O2D-CGD	4.76	1.44	1.33
24	8	606	CHL	CHD-C1D	4.75	1.47	1.38
24	2	607	CHL	C2C-C3C	4.74	1.46	1.36
24	5	605	CHL	CHC-C1C	4.74	1.48	1.38
24	Y	606	CHL	O2D-CGD	4.74	1.44	1.33
24	y	606	CHL	O2D-CGD	4.74	1.44	1.33
24	3	605	CHL	C3D-C4D	-4.73	1.33	1.44
24	9	609	CHL	CHD-C1D	4.72	1.47	1.38
24	q	605	CHL	CHD-C1D	4.71	1.47	1.38
24	G	605	CHL	C3D-C4D	-4.71	1.33	1.44
24	9	606	CHL	C2C-C3C	4.71	1.46	1.36
24	6	605	CHL	C3D-C4D	-4.71	1.33	1.44
24	n	601	CHL	O2D-CGD	4.71	1.44	1.33
24	q	606	CHL	CHD-C1D	4.71	1.47	1.38
24	0	605	CHL	C3D-C4D	-4.70	1.33	1.44
24	1	609	CHL	O2D-CGD	4.70	1.44	1.33
24	Y	609	CHL	O2D-CGD	4.70	1.44	1.33
24	q	606	CHL	C2C-C3C	4.70	1.46	1.36
24	p	605	CHL	CHC-C1C	4.69	1.48	1.38
24	8	606	CHL	C2C-C3C	4.69	1.46	1.36
24	n	605	CHL	O2D-CGD	4.69	1.44	1.33
24	9	605	CHL	CHC-C1C	4.69	1.48	1.38
24	2	605	CHL	CHC-C1C	4.69	1.48	1.38
24	2	605	CHL	CHD-C1D	4.68	1.47	1.38
24	N	601	CHL	O2D-CGD	4.68	1.44	1.33
24	5	606	CHL	CHC-C1C	4.67	1.48	1.38
24	g	605	CHL	C3D-C4D	-4.67	1.33	1.44
24	n	608	CHL	O2D-CGD	4.67	1.44	1.33
24	N	608	CHL	O2D-CGD	4.67	1.44	1.33
24	p	607	CHL	C2C-C3C	4.66	1.46	1.36
24	3	606	CHL	C2C-C3C	4.66	1.46	1.36
24	9	605	CHL	CHD-C1D	4.65	1.47	1.38
24	4	605	CHL	CHC-C1C	4.65	1.48	1.38
24	2	606	CHL	C2C-C3C	4.65	1.46	1.36
24	9	605	CHL	C2C-C3C	4.65	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	609	CHL	O2D-CGD	4.65	1.44	1.33
24	4	605	CHL	CHD-C1D	4.65	1.47	1.38
24	9	607	CHL	C2C-C3C	4.65	1.46	1.36
24	9	601	CHL	C2C-C3C	4.64	1.46	1.36
24	p	606	CHL	C2C-C3C	4.64	1.46	1.36
24	q	605	CHL	C2C-C3C	4.64	1.46	1.36
24	g	605	CHL	C2C-C3C	4.64	1.46	1.36
24	p	606	CHL	CHC-C1C	4.64	1.47	1.38
24	q	607	CHL	CHD-C1D	4.63	1.47	1.38
24	p	608	CHL	C3D-C4D	-4.63	1.33	1.44
24	G	605	CHL	C2C-C3C	4.63	1.46	1.36
24	6	605	CHL	C2C-C3C	4.62	1.46	1.36
24	0	609	CHL	CHC-C1C	4.62	1.47	1.38
24	5	609	CHL	CHD-C1D	4.62	1.47	1.38
24	S	608	CHL	C2C-C3C	4.62	1.46	1.36
24	s	608	CHL	C2C-C3C	4.61	1.46	1.36
24	9	608	CHL	C2C-C3C	4.61	1.46	1.36
24	5	608	CHL	C3D-C4D	-4.61	1.33	1.44
24	N	609	CHL	O2D-CGD	4.61	1.44	1.33
24	4	606	CHL	C2C-C3C	4.60	1.46	1.36
35	B	621	SQD	O8-S	4.60	1.63	1.47
24	4	601	CHL	C2C-C3C	4.60	1.46	1.36
24	2	605	CHL	C2C-C3C	4.59	1.46	1.36
24	5	607	CHL	C2C-C3C	4.59	1.46	1.36
24	9	608	CHL	CHC-C1C	4.59	1.47	1.38
24	9	601	CHL	CHD-C1D	4.59	1.47	1.38
24	4	605	CHL	C2C-C3C	4.59	1.46	1.36
24	0	605	CHL	C2C-C3C	4.59	1.46	1.36
24	y	608	CHL	O2D-CGD	4.58	1.44	1.33
35	b	623	SQD	O8-S	4.58	1.63	1.47
24	2	609	CHL	CHD-C1D	4.58	1.47	1.38
24	3	605	CHL	CHD-C1D	4.58	1.47	1.38
24	8	605	CHL	CHD-C1D	4.57	1.47	1.38
35	B	623	SQD	O8-S	4.57	1.63	1.47
35	b	621	SQD	O8-S	4.57	1.63	1.47
24	Y	608	CHL	O2D-CGD	4.57	1.44	1.33
24	0	609	CHL	C2C-C3C	4.57	1.46	1.36
24	2	605	CHL	C3D-C4D	-4.57	1.33	1.44
24	p	609	CHL	CHD-C1D	4.57	1.47	1.38
24	p	608	CHL	C2C-C3C	4.57	1.46	1.36
24	2	601	CHL	C2C-C3C	4.56	1.46	1.36
24	2	607	CHL	CHC-C1C	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	607	CHL	CHC-C1C	4.56	1.47	1.38
24	9	605	CHL	C3D-C4D	-4.56	1.33	1.44
24	r	607	CHL	O2D-CGD	4.56	1.44	1.33
24	6	605	CHL	CHC-C1C	4.55	1.47	1.38
24	2	608	CHL	C2C-C3C	4.55	1.46	1.36
24	4	608	CHL	C2C-C3C	4.55	1.46	1.36
24	s	607	CHL	C2C-C3C	4.55	1.46	1.36
24	q	607	CHL	C2C-C3C	4.55	1.46	1.36
24	q	605	CHL	CHC-C1C	4.54	1.47	1.38
24	0	605	CHL	CHC-C1C	4.54	1.47	1.38
24	4	606	CHL	CHD-C1D	4.54	1.47	1.38
24	R	607	CHL	O2D-CGD	4.53	1.44	1.33
24	2	608	CHL	CHC-C1C	4.53	1.47	1.38
24	6	601	CHL	C2C-C3C	4.53	1.46	1.36
24	6	606	CHL	C2C-C3C	4.53	1.46	1.36
24	8	607	CHL	CHC-C1C	4.53	1.47	1.38
24	q	601	CHL	C2C-C3C	4.52	1.46	1.36
24	Y	601	CHL	O2D-CGD	4.52	1.44	1.33
24	0	606	CHL	C2C-C3C	4.52	1.46	1.36
24	y	601	CHL	O2D-CGD	4.52	1.44	1.33
24	5	606	CHL	C2C-C3C	4.51	1.46	1.36
35	D	413	SQD	O8-S	4.51	1.63	1.47
24	8	609	CHL	C2C-C3C	4.51	1.46	1.36
24	3	609	CHL	C2C-C3C	4.51	1.46	1.36
24	S	607	CHL	C2C-C3C	4.51	1.46	1.36
24	9	607	CHL	CHC-C1C	4.51	1.47	1.38
35	d	413	SQD	O8-S	4.50	1.63	1.47
24	p	607	CHL	CHC-C1C	4.50	1.47	1.38
24	1	609	CHL	O2A-CGA	4.50	1.46	1.33
24	1	606	CHL	O2A-CGA	4.50	1.46	1.33
24	5	605	CHL	O2A-CGA	4.50	1.46	1.33
24	8	601	CHL	O2A-CGA	4.50	1.46	1.33
24	1	605	CHL	C2C-C3C	4.50	1.46	1.36
24	8	606	CHL	O2A-CGA	4.50	1.45	1.30
24	s	601	CHL	O2A-CGA	4.50	1.45	1.30
24	7	607	CHL	CHC-C1C	4.50	1.47	1.38
24	0	601	CHL	CHC-C1C	4.49	1.47	1.38
24	7	605	CHL	C2C-C3C	4.49	1.46	1.36
24	7	609	CHL	O2A-CGA	4.49	1.46	1.33
24	y	607	CHL	O2A-CGA	4.49	1.46	1.33
24	4	607	CHL	CHD-C1D	4.49	1.47	1.38
24	p	601	CHL	O2A-CGA	4.49	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	601	CHL	C2C-C3C	4.49	1.46	1.36
24	g	601	CHL	O2D-CGD	4.48	1.44	1.33
24	5	608	CHL	CHC-C1C	4.48	1.47	1.38
24	8	607	CHL	O2A-CGA	4.48	1.46	1.33
24	G	601	CHL	O2D-CGD	4.48	1.44	1.33
24	8	601	CHL	C2C-C3C	4.48	1.46	1.36
24	5	608	CHL	C2C-C3C	4.47	1.46	1.36
24	S	601	CHL	O2A-CGA	4.47	1.45	1.30
24	3	606	CHL	O2A-CGA	4.47	1.45	1.30
24	3	601	CHL	O2A-CGA	4.47	1.46	1.33
24	7	605	CHL	O2A-CGA	4.47	1.45	1.30
24	3	608	CHL	CHC-C1C	4.47	1.47	1.38
24	1	605	CHL	O2A-CGA	4.47	1.45	1.30
24	4	601	CHL	CHC-C1C	4.46	1.47	1.38
24	2	606	CHL	CHC-C1C	4.46	1.47	1.38
24	r	608	CHL	O2D-CGD	4.46	1.44	1.33
24	7	606	CHL	O2A-CGA	4.46	1.46	1.33
24	S	608	CHL	CHC-C1C	4.46	1.47	1.38
24	5	606	CHL	O2A-CGA	4.46	1.45	1.30
24	G	605	CHL	CHD-C1D	4.46	1.47	1.38
24	S	607	CHL	CHC-C1C	4.46	1.47	1.38
24	R	608	CHL	O2D-CGD	4.46	1.44	1.33
24	n	607	CHL	CHC-C1C	4.46	1.47	1.38
24	s	607	CHL	CHC-C1C	4.46	1.47	1.38
24	3	608	CHL	C2C-C3C	4.45	1.46	1.36
24	1	607	CHL	CHC-C1C	4.45	1.47	1.38
24	q	609	CHL	O2A-CGA	4.45	1.46	1.33
24	3	607	CHL	O2A-CGA	4.45	1.46	1.33
24	s	608	CHL	CHC-C1C	4.44	1.47	1.38
24	y	601	CHL	CHC-C1C	4.44	1.47	1.38
24	Y	605	CHL	O2A-CGA	4.44	1.45	1.30
24	Y	601	CHL	CHC-C1C	4.44	1.47	1.38
24	Y	607	CHL	CHC-C1C	4.44	1.47	1.38
24	n	606	CHL	O2A-CGA	4.44	1.45	1.30
24	Y	607	CHL	O2A-CGA	4.43	1.46	1.33
24	S	601	CHL	C2C-C3C	4.43	1.46	1.36
24	p	605	CHL	O2A-CGA	4.43	1.46	1.33
24	0	605	CHL	O2A-CGA	4.43	1.45	1.30
24	5	605	CHL	CHD-C1D	4.43	1.47	1.38
24	8	608	CHL	CHC-C1C	4.43	1.47	1.38
24	y	607	CHL	CHC-C1C	4.43	1.47	1.38
24	N	606	CHL	O2A-CGA	4.43	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	606	CHL	CHD-C1D	4.43	1.47	1.38
24	2	607	CHL	CHD-C1D	4.43	1.47	1.38
24	6	605	CHL	CHD-C1D	4.42	1.47	1.38
24	y	601	CHL	O2A-CGA	4.42	1.46	1.33
24	y	609	CHL	O2A-CGA	4.42	1.46	1.33
24	Y	609	CHL	O2A-CGA	4.42	1.46	1.33
24	4	607	CHL	C2C-C3C	4.42	1.46	1.36
24	q	608	CHL	CHD-C1D	4.42	1.47	1.38
24	y	605	CHL	O2A-CGA	4.42	1.45	1.30
24	5	607	CHL	CHC-C1C	4.42	1.47	1.38
24	9	607	CHL	CHD-C1D	4.42	1.47	1.38
24	6	608	CHL	C2C-C3C	4.42	1.46	1.36
24	3	609	CHL	O2A-CGA	4.42	1.46	1.33
24	1	608	CHL	O2A-CGA	4.42	1.46	1.33
24	g	605	CHL	CHD-C1D	4.42	1.47	1.38
24	1	605	CHL	CHC-C1C	4.42	1.47	1.38
24	8	608	CHL	C2C-C3C	4.41	1.46	1.36
24	s	601	CHL	CHD-C1D	4.41	1.47	1.38
24	7	605	CHL	CHD-C1D	4.41	1.46	1.38
24	0	608	CHL	C2C-C3C	4.40	1.46	1.36
24	N	607	CHL	CHC-C1C	4.40	1.47	1.38
24	Y	609	CHL	C2C-C3C	4.40	1.46	1.36
24	p	606	CHL	O2A-CGA	4.40	1.45	1.30
24	9	606	CHL	CHC-C1C	4.40	1.47	1.38
24	6	605	CHL	O2A-CGA	4.40	1.45	1.30
24	S	607	CHL	CHD-C1D	4.40	1.46	1.38
24	q	601	CHL	CHC-C1C	4.39	1.47	1.38
24	4	601	CHL	O2A-CGA	4.39	1.46	1.33
24	y	609	CHL	C2C-C3C	4.38	1.46	1.36
24	7	605	CHL	CHC-C1C	4.38	1.47	1.38
24	6	609	CHL	C2C-C3C	4.38	1.46	1.36
24	s	607	CHL	CHD-C1D	4.38	1.46	1.38
24	3	607	CHL	C2C-C3C	4.38	1.46	1.36
24	0	606	CHL	O2A-CGA	4.37	1.46	1.33
24	p	608	CHL	CHC-C1C	4.37	1.47	1.38
24	S	608	CHL	O2A-CGA	4.37	1.46	1.33
24	G	608	CHL	C2C-C3C	4.37	1.46	1.36
24	7	608	CHL	O2A-CGA	4.37	1.46	1.33
24	6	608	CHL	CHC-C1C	4.37	1.47	1.38
24	5	601	CHL	O2A-CGA	4.37	1.46	1.33
24	5	601	CHL	C2C-C3C	4.37	1.46	1.36
24	s	601	CHL	C2C-C3C	4.37	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	CHD-C1D	4.37	1.46	1.38
24	G	609	CHL	O2A-CGA	4.36	1.46	1.33
24	g	609	CHL	O2A-CGA	4.36	1.46	1.33
24	0	608	CHL	CHC-C1C	4.35	1.47	1.38
24	p	609	CHL	O2A-CGA	4.35	1.46	1.33
24	6	606	CHL	O2A-CGA	4.35	1.46	1.33
24	q	606	CHL	O2A-CGA	4.35	1.46	1.33
24	2	606	CHL	CHD-C1D	4.34	1.46	1.38
24	G	608	CHL	CHC-C1C	4.34	1.47	1.38
24	s	608	CHL	O2A-CGA	4.34	1.46	1.33
24	4	605	CHL	O2A-CGA	4.34	1.46	1.33
24	Y	605	CHL	CHC-C1C	4.34	1.47	1.38
24	q	601	CHL	O2A-CGA	4.34	1.46	1.33
24	5	609	CHL	O2A-CGA	4.34	1.46	1.33
24	q	605	CHL	O2A-CGA	4.34	1.46	1.33
24	5	601	CHL	CHD-C1D	4.34	1.46	1.38
24	y	605	CHL	CHC-C1C	4.34	1.47	1.38
24	G	606	CHL	O2A-CGA	4.33	1.46	1.33
24	8	607	CHL	C2C-C3C	4.33	1.46	1.36
24	G	605	CHL	O2A-CGA	4.33	1.46	1.33
24	4	608	CHL	CHD-C1D	4.33	1.46	1.38
24	4	609	CHL	O2A-CGA	4.33	1.46	1.33
24	g	606	CHL	O2A-CGA	4.33	1.46	1.33
24	8	609	CHL	O2A-CGA	4.32	1.46	1.33
24	g	607	CHL	O2A-CGA	4.32	1.46	1.33
24	g	608	CHL	C2C-C3C	4.32	1.46	1.36
24	1	605	CHL	CHD-C1D	4.32	1.46	1.38
24	9	609	CHL	CHC-C1C	4.32	1.47	1.38
24	N	605	CHL	C2C-C3C	4.32	1.46	1.36
24	3	601	CHL	C2C-C3C	4.31	1.46	1.36
24	7	601	CHL	CHD-C1D	4.31	1.46	1.38
24	q	607	CHL	O2A-CGA	4.31	1.45	1.33
24	g	605	CHL	O2A-CGA	4.31	1.45	1.33
24	9	606	CHL	CHD-C1D	4.31	1.46	1.38
24	n	608	CHL	O2A-CGA	4.31	1.45	1.33
24	q	609	CHL	CHD-C4C	4.30	1.49	1.39
24	g	606	CHL	CHC-C1C	4.30	1.47	1.38
24	y	606	CHL	O2A-CGA	4.30	1.45	1.33
24	0	606	CHL	CHC-C1C	4.29	1.47	1.38
24	6	601	CHL	CHC-C1C	4.29	1.47	1.38
24	6	607	CHL	O2A-CGA	4.29	1.45	1.33
29	p	2630	LHG	O8-C23	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	608	CHL	CHC-C1C	4.29	1.47	1.38
24	p	601	CHL	CHC-C1C	4.29	1.47	1.38
24	2	606	CHL	O2A-CGA	4.28	1.45	1.33
24	G	607	CHL	O2A-CGA	4.28	1.45	1.33
24	1	601	CHL	CHD-C1D	4.28	1.46	1.38
24	4	607	CHL	O2A-CGA	4.28	1.45	1.33
24	Y	606	CHL	O2A-CGA	4.28	1.45	1.33
29	0	2630	LHG	O8-C23	4.28	1.45	1.33
24	p	607	CHL	CHD-C1D	4.28	1.46	1.38
24	4	606	CHL	O2A-CGA	4.28	1.45	1.33
24	3	605	CHL	O2A-CGA	4.27	1.45	1.33
24	6	606	CHL	CHC-C1C	4.27	1.47	1.38
24	0	606	CHL	CHD-C1D	4.27	1.46	1.38
24	1	607	CHL	O2A-CGA	4.27	1.45	1.33
24	g	605	CHL	CHC-C1C	4.27	1.47	1.38
24	3	606	CHL	CHD-C4C	4.27	1.49	1.39
24	5	601	CHL	CHC-C1C	4.27	1.47	1.38
36	S	2631	LMG	O8-C28	4.26	1.45	1.33
37	c	524	DGD	O1G-C1A	4.26	1.45	1.33
24	6	607	CHL	CHC-C1C	4.26	1.47	1.38
24	1	601	CHL	O2A-CGA	4.26	1.45	1.33
24	2	609	CHL	O2A-CGA	4.26	1.45	1.33
24	9	601	CHL	O2A-CGA	4.26	1.45	1.33
24	y	605	CHL	C2C-C3C	4.26	1.45	1.36
24	8	605	CHL	O2A-CGA	4.26	1.45	1.33
24	7	607	CHL	O2A-CGA	4.25	1.45	1.33
24	p	601	CHL	C2C-C3C	4.25	1.45	1.36
24	n	601	CHL	O2A-CGA	4.25	1.45	1.33
24	8	601	CHL	CHC-C1C	4.25	1.47	1.38
29	5	2630	LHG	O7-C7	4.25	1.46	1.34
24	2	601	CHL	CHD-C1D	4.25	1.46	1.38
24	G	606	CHL	CHC-C1C	4.25	1.47	1.38
24	9	605	CHL	O2A-CGA	4.24	1.45	1.33
24	2	605	CHL	O2A-CGA	4.24	1.45	1.33
24	N	608	CHL	O2A-CGA	4.24	1.45	1.33
36	s	2631	LMG	O8-C28	4.24	1.45	1.33
24	Y	605	CHL	C2C-C3C	4.24	1.45	1.36
24	n	605	CHL	C2C-C3C	4.23	1.45	1.36
24	n	605	CHL	CHD-C1D	4.23	1.46	1.38
24	6	609	CHL	CHC-C1C	4.23	1.47	1.38
29	N	2630	LHG	O8-C23	4.23	1.45	1.33
24	8	606	CHL	CHD-C4C	4.23	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	606	CHL	CHC-C1C	4.23	1.47	1.38
24	4	601	CHL	CHD-C1D	4.23	1.46	1.38
24	8	608	CHL	O2A-CGA	4.23	1.45	1.33
24	q	601	CHL	CHD-C1D	4.23	1.46	1.38
24	0	608	CHL	O2A-CGA	4.23	1.45	1.33
24	8	608	CHL	CHD-C1D	4.23	1.46	1.38
29	6	2630	LHG	O8-C23	4.23	1.45	1.33
24	N	601	CHL	O2A-CGA	4.23	1.45	1.33
24	6	608	CHL	O2A-CGA	4.23	1.45	1.33
24	G	605	CHL	CHC-C1C	4.22	1.47	1.38
24	0	607	CHL	O2A-CGA	4.22	1.45	1.33
24	1	606	CHL	CHC-C1C	4.22	1.47	1.38
37	C	524	DGD	O1G-C1A	4.22	1.45	1.33
24	2	609	CHL	CHC-C1C	4.22	1.47	1.38
24	G	607	CHL	CHC-C1C	4.22	1.47	1.38
24	6	607	CHL	CHD-C1D	4.22	1.46	1.38
24	G	608	CHL	CHD-C1D	4.22	1.46	1.38
24	0	609	CHL	CHD-C1D	4.22	1.46	1.38
29	8	2630	LHG	O8-C23	4.22	1.45	1.33
24	s	606	CHL	C2C-C3C	4.21	1.45	1.36
29	n	2630	LHG	O8-C23	4.21	1.45	1.33
24	9	606	CHL	O2A-CGA	4.21	1.45	1.33
24	2	608	CHL	CHD-C1D	4.20	1.46	1.38
24	1	601	CHL	CHC-C1C	4.20	1.47	1.38
24	3	608	CHL	O2A-CGA	4.20	1.45	1.33
24	N	605	CHL	CHD-C1D	4.20	1.46	1.38
29	2	2630	LHG	O8-C23	4.20	1.45	1.33
24	Y	601	CHL	O2A-CGA	4.20	1.45	1.33
24	g	607	CHL	CHC-C1C	4.20	1.47	1.38
24	S	606	CHL	C2C-C3C	4.19	1.45	1.36
37	C	523	DGD	O2G-C1B	4.19	1.46	1.34
36	a	413	LMG	O7-C10	4.19	1.46	1.34
24	5	607	CHL	O2A-CGA	4.19	1.45	1.33
24	9	609	CHL	O2A-CGA	4.19	1.45	1.33
36	S	2631	LMG	O7-C10	4.19	1.46	1.34
24	9	608	CHL	CHD-C1D	4.19	1.46	1.38
24	G	609	CHL	CHD-C1D	4.19	1.46	1.38
24	N	609	CHL	O2A-CGA	4.19	1.45	1.33
24	0	609	CHL	O2A-CGA	4.19	1.45	1.33
24	N	605	CHL	CHC-C1C	4.19	1.47	1.38
29	5	2630	LHG	O8-C23	4.18	1.45	1.33
24	r	608	CHL	C2C-C3C	4.18	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	411	LMG	O8-C28	4.18	1.45	1.33
29	3	2630	LHG	O8-C23	4.18	1.45	1.33
24	7	601	CHL	O2A-CGA	4.18	1.45	1.33
24	6	609	CHL	O2A-CGA	4.18	1.45	1.33
24	2	607	CHL	O2A-CGA	4.18	1.45	1.33
35	A	412	SQD	O48-C23	4.18	1.45	1.33
24	3	608	CHL	CHD-C1D	4.18	1.46	1.38
24	9	607	CHL	O2A-CGA	4.18	1.45	1.33
36	d	411	LMG	O7-C10	4.18	1.46	1.34
29	9	2630	LHG	O8-C23	4.17	1.45	1.33
24	1	607	CHL	CHD-C1D	4.17	1.46	1.38
24	p	607	CHL	O2A-CGA	4.17	1.45	1.33
36	s	2631	LMG	O7-C10	4.17	1.46	1.34
35	a	412	SQD	O48-C23	4.17	1.45	1.33
24	7	601	CHL	CHC-C1C	4.17	1.47	1.38
24	n	609	CHL	O2A-CGA	4.17	1.45	1.33
36	A	413	LMG	O7-C10	4.17	1.46	1.34
29	q	2630	LHG	O7-C7	4.16	1.46	1.34
37	c	523	DGD	O2G-C1B	4.16	1.46	1.34
29	4	2630	LHG	O7-C7	4.16	1.46	1.34
29	d	409	LHG	O8-C23	4.16	1.45	1.33
29	D	409	LHG	O8-C23	4.16	1.45	1.33
29	7	2630	LHG	O8-C23	4.16	1.45	1.33
24	1	606	CHL	CHD-C1D	4.15	1.46	1.38
24	p	601	CHL	CHD-C1D	4.15	1.46	1.38
24	q	606	CHL	CHD-C4C	4.15	1.48	1.39
24	R	607	CHL	CHC-C1C	4.15	1.47	1.38
24	R	608	CHL	C2C-C3C	4.15	1.45	1.36
24	p	608	CHL	O2A-CGA	4.15	1.45	1.33
24	0	608	CHL	CHD-C1D	4.15	1.46	1.38
36	d	411	LMG	O8-C28	4.15	1.45	1.33
24	0	605	CHL	CHD-C1D	4.15	1.46	1.38
29	l	101	LHG	O8-C23	4.15	1.45	1.33
24	R	606	CHL	O2A-CGA	4.15	1.45	1.33
24	1	601	CHL	C2C-C3C	4.15	1.45	1.36
24	p	608	CHL	CHD-C1D	4.14	1.46	1.38
24	N	606	CHL	CHC-C1C	4.14	1.46	1.38
29	L	101	LHG	O8-C23	4.14	1.45	1.33
24	g	609	CHL	CHD-C1D	4.14	1.46	1.38
24	5	608	CHL	O2A-CGA	4.14	1.45	1.33
36	D	411	LMG	O7-C10	4.14	1.46	1.34
24	3	601	CHL	CHD-C1D	4.14	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	606	CHL	CHD-C1D	4.14	1.46	1.38
24	7	601	CHL	C2C-C3C	4.14	1.45	1.36
37	C	518	DGD	O1G-C1A	4.14	1.45	1.33
24	q	606	CHL	CHC-C4B	4.13	1.48	1.39
24	n	605	CHL	CHC-C1C	4.13	1.46	1.38
24	S	606	CHL	CHD-C1D	4.13	1.46	1.38
29	1	2630	LHG	O8-C23	4.13	1.45	1.33
24	3	601	CHL	CHC-C1C	4.13	1.46	1.38
29	C	2630	LHG	O8-C23	4.13	1.45	1.33
29	q	2630	LHG	O8-C23	4.12	1.45	1.33
24	s	606	CHL	CHC-C1C	4.12	1.46	1.38
24	2	601	CHL	O2A-CGA	4.12	1.45	1.33
24	Y	606	CHL	CHC-C1C	4.12	1.46	1.38
24	s	606	CHL	CHD-C1D	4.12	1.46	1.38
29	D	410	LHG	O8-C23	4.12	1.45	1.33
24	0	607	CHL	CHC-C1C	4.12	1.46	1.38
24	y	608	CHL	O2A-CGA	4.12	1.45	1.33
35	B	623	SQD	O48-C23	4.12	1.45	1.33
24	4	606	CHL	CHC-C4B	4.12	1.48	1.39
24	6	607	CHL	C2C-C3C	4.12	1.45	1.36
24	r	606	CHL	O2A-CGA	4.11	1.45	1.33
29	d	410	LHG	O8-C23	4.11	1.45	1.33
24	0	607	CHL	C2C-C3C	4.11	1.45	1.36
35	B	623	SQD	O47-C7	4.11	1.45	1.34
24	g	608	CHL	CHD-C1D	4.11	1.46	1.38
24	n	609	CHL	CHD-C1D	4.11	1.46	1.38
24	y	606	CHL	CHC-C1C	4.11	1.46	1.38
24	r	607	CHL	CHC-C1C	4.11	1.46	1.38
24	R	608	CHL	CHC-C1C	4.11	1.46	1.38
37	c	518	DGD	O1G-C1A	4.11	1.45	1.33
24	p	606	CHL	CHD-C4C	4.10	1.48	1.39
29	p	2630	LHG	O7-C7	4.10	1.45	1.34
24	7	609	CHL	CHC-C1C	4.10	1.46	1.38
36	D	412	LMG	O8-C28	4.10	1.45	1.33
24	r	608	CHL	CHC-C1C	4.10	1.46	1.38
25	R	609	CLA	C4D-ND	-4.10	1.32	1.37
25	r	609	CLA	C4D-ND	-4.10	1.32	1.37
24	6	601	CHL	O2A-CGA	4.10	1.45	1.33
24	4	609	CHL	CHD-C4C	4.10	1.48	1.39
35	b	621	SQD	O47-C7	4.10	1.45	1.34
36	d	412	LMG	O8-C28	4.10	1.45	1.33
35	b	623	SQD	O48-C23	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	606	CHL	C2C-C3C	4.09	1.45	1.36
25	A	406	CLA	C4D-ND	-4.09	1.32	1.37
25	a	406	CLA	C4D-ND	-4.09	1.32	1.37
24	1	608	CHL	CHC-C1C	4.09	1.46	1.38
35	B	621	SQD	O47-C7	4.09	1.45	1.34
29	d	408	LHG	O8-C23	4.09	1.45	1.33
29	D	408	LHG	O8-C23	4.09	1.45	1.33
24	6	608	CHL	CHD-C1D	4.09	1.46	1.38
35	b	623	SQD	O47-C7	4.09	1.45	1.34
35	b	621	SQD	O48-C23	4.08	1.45	1.33
24	Y	608	CHL	O2A-CGA	4.08	1.45	1.33
24	n	607	CHL	O2A-CGA	4.08	1.45	1.33
24	G	601	CHL	CHC-C1C	4.08	1.46	1.38
29	c	2630	LHG	O8-C23	4.08	1.45	1.33
24	8	601	CHL	CHD-C1D	4.08	1.46	1.38
24	5	608	CHL	CHD-C1D	4.08	1.46	1.38
24	s	608	CHL	CHD-C1D	4.08	1.46	1.38
29	9	2630	LHG	O7-C7	4.08	1.45	1.34
24	Y	608	CHL	C2C-C3C	4.08	1.45	1.36
24	Y	607	CHL	C2C-C3C	4.07	1.45	1.36
24	7	608	CHL	CHC-C1C	4.07	1.46	1.38
35	B	621	SQD	O48-C23	4.07	1.45	1.33
24	7	607	CHL	C2C-C3C	4.07	1.45	1.36
24	R	606	CHL	CHC-C1C	4.07	1.46	1.38
24	S	606	CHL	CHC-C1C	4.07	1.46	1.38
24	Y	605	CHL	CHD-C1D	4.07	1.46	1.38
24	y	605	CHL	CHD-C1D	4.07	1.46	1.38
25	g	613	CLA	C4D-ND	-4.07	1.32	1.37
29	4	2630	LHG	O8-C23	4.07	1.45	1.33
24	y	607	CHL	C2C-C3C	4.07	1.45	1.36
24	y	608	CHL	C2C-C3C	4.07	1.45	1.36
35	a	412	SQD	O47-C7	4.06	1.45	1.34
24	9	605	CHL	CHD-C4C	4.06	1.48	1.39
24	n	601	CHL	CHC-C1C	4.06	1.46	1.38
24	6	606	CHL	CHD-C1D	4.06	1.46	1.38
24	7	607	CHL	CHD-C1D	4.06	1.46	1.38
24	9	601	CHL	CHC-C1C	4.06	1.46	1.38
24	R	608	CHL	O2A-CGA	4.05	1.45	1.33
35	d	413	SQD	O48-C23	4.05	1.45	1.33
24	N	601	CHL	CHC-C1C	4.05	1.46	1.38
29	2	2630	LHG	O7-C7	4.05	1.45	1.34
24	q	607	CHL	CHD-C4C	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	608	CHL	O2A-CGA	4.05	1.45	1.33
24	g	601	CHL	CHC-C1C	4.05	1.46	1.38
37	C	520	DGD	O1G-C1A	4.05	1.45	1.33
37	c	520	DGD	O1G-C1A	4.05	1.45	1.33
24	g	607	CHL	C2C-C3C	4.05	1.45	1.36
24	Y	606	CHL	C2C-C3C	4.05	1.45	1.36
24	1	601	CHL	CHD-C4C	4.05	1.48	1.39
24	2	605	CHL	CHD-C4C	4.05	1.48	1.39
35	A	412	SQD	O47-C7	4.04	1.45	1.34
35	D	413	SQD	O48-C23	4.04	1.45	1.33
24	g	601	CHL	O2A-CGA	4.04	1.45	1.33
29	d	410	LHG	O7-C7	4.04	1.45	1.34
24	r	606	CHL	CHC-C1C	4.04	1.46	1.38
24	g	607	CHL	CHD-C1D	4.04	1.46	1.38
24	5	609	CHL	CHC-C1C	4.04	1.46	1.38
29	D	410	LHG	O7-C7	4.03	1.45	1.34
25	G	613	CLA	C4D-ND	-4.03	1.32	1.37
24	N	609	CHL	CHD-C1D	4.03	1.46	1.38
24	S	608	CHL	CHD-C1D	4.03	1.46	1.38
36	D	412	LMG	O7-C10	4.03	1.45	1.34
24	0	601	CHL	O2A-CGA	4.03	1.45	1.33
29	s	2630	LHG	O7-C7	4.03	1.45	1.34
24	G	607	CHL	C2C-C3C	4.03	1.45	1.36
24	G	601	CHL	O2A-CGA	4.03	1.45	1.33
24	N	601	CHL	C2C-C3C	4.02	1.45	1.36
36	d	412	LMG	O7-C10	4.02	1.45	1.34
24	4	607	CHL	CHD-C4C	4.01	1.48	1.39
29	d	408	LHG	O7-C7	4.01	1.45	1.34
24	4	605	CHL	CHD-C4C	4.01	1.48	1.39
24	1	609	CHL	CHC-C1C	4.01	1.46	1.38
24	6	609	CHL	CHD-C1D	4.01	1.46	1.38
24	g	606	CHL	CHD-C1D	4.01	1.46	1.38
24	1	606	CHL	C2C-C3C	4.01	1.45	1.36
24	n	609	CHL	C2C-C3C	4.00	1.45	1.36
24	r	607	CHL	O2A-CGA	4.00	1.45	1.33
24	7	601	CHL	CHD-C4C	4.00	1.48	1.39
24	p	605	CHL	CHD-C4C	4.00	1.48	1.39
29	R	2630	LHG	O7-C7	4.00	1.45	1.34
36	h	102	LMG	O8-C28	4.00	1.45	1.33
24	7	606	CHL	C2C-C3C	4.00	1.45	1.36
24	R	607	CHL	O2A-CGA	4.00	1.45	1.33
24	G	606	CHL	CHD-C1D	4.00	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	521	LMG	O8-C28	4.00	1.45	1.33
24	7	606	CHL	CHC-C1C	4.00	1.46	1.38
29	S	2630	LHG	O7-C7	4.00	1.45	1.34
24	G	607	CHL	CHD-C1D	4.00	1.46	1.38
36	H	102	LMG	O8-C28	3.99	1.45	1.33
35	D	413	SQD	O47-C7	3.99	1.45	1.34
24	0	607	CHL	CHD-C1D	3.99	1.46	1.38
29	r	2630	LHG	O8-C23	3.99	1.45	1.33
29	D	408	LHG	O7-C7	3.99	1.45	1.34
35	d	413	SQD	O47-C7	3.98	1.45	1.34
24	2	601	CHL	CHC-C1C	3.98	1.46	1.38
25	5	612	CLA	C1D-ND	3.98	1.42	1.37
29	R	2630	LHG	O8-C23	3.98	1.45	1.33
36	c	521	LMG	O8-C28	3.98	1.45	1.33
24	y	608	CHL	CHC-C1C	3.98	1.46	1.38
29	r	2630	LHG	O7-C7	3.98	1.45	1.34
37	c	520	DGD	O2G-C1B	3.98	1.45	1.34
24	7	609	CHL	C2C-C3C	3.97	1.45	1.36
29	s	2630	LHG	O8-C23	3.97	1.45	1.33
36	h	102	LMG	O7-C10	3.97	1.45	1.34
24	g	609	CHL	C2C-C3C	3.97	1.45	1.36
36	H	102	LMG	O7-C10	3.97	1.45	1.34
36	b	622	LMG	O8-C28	3.97	1.44	1.33
24	N	608	CHL	C2C-C3C	3.97	1.45	1.36
25	B	612	CLA	C4D-ND	-3.97	1.32	1.37
25	b	612	CLA	C4D-ND	-3.97	1.32	1.37
24	N	607	CHL	O2A-CGA	3.97	1.44	1.33
24	q	605	CHL	CHD-C4C	3.96	1.48	1.39
29	8	2630	LHG	O7-C7	3.96	1.45	1.34
24	1	609	CHL	C2C-C3C	3.96	1.45	1.36
24	g	606	CHL	C2C-C3C	3.96	1.45	1.36
24	4	606	CHL	CHD-C4C	3.96	1.48	1.39
25	C	504	CLA	C4D-ND	-3.96	1.32	1.37
29	0	2630	LHG	O7-C7	3.96	1.45	1.34
24	q	609	CHL	CHC-C4B	3.96	1.48	1.39
24	1	607	CHL	C2C-C3C	3.96	1.45	1.36
24	y	601	CHL	CHD-C1D	3.95	1.46	1.38
24	9	609	CHL	CHD-C4C	3.95	1.48	1.39
36	b	622	LMG	O7-C10	3.95	1.45	1.34
24	1	608	CHL	C2C-C3C	3.95	1.45	1.36
24	G	609	CHL	C2C-C3C	3.95	1.45	1.36
25	C	508	CLA	C4D-ND	-3.95	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	2630	LHG	O8-C23	3.95	1.44	1.33
24	n	608	CHL	C2C-C3C	3.95	1.45	1.36
24	n	606	CHL	C2C-C3C	3.94	1.45	1.36
36	B	622	LMG	O8-C28	3.94	1.44	1.33
24	6	601	CHL	CHD-C1D	3.94	1.46	1.38
37	C	520	DGD	O2G-C1B	3.94	1.45	1.34
24	G	606	CHL	C2C-C3C	3.94	1.45	1.36
24	8	609	CHL	CHC-C1C	3.94	1.46	1.38
36	B	622	LMG	O7-C10	3.94	1.45	1.34
29	3	2630	LHG	O7-C7	3.94	1.45	1.34
24	Y	608	CHL	CHC-C1C	3.94	1.46	1.38
24	7	608	CHL	C2C-C3C	3.94	1.45	1.36
29	S	2630	LHG	O8-C23	3.93	1.44	1.33
25	C	502	CLA	C4D-ND	-3.93	1.32	1.37
24	N	608	CHL	CHC-C1C	3.93	1.46	1.38
24	8	605	CHL	CHC-C4B	3.93	1.48	1.39
29	g	2630	LHG	O7-C7	3.92	1.45	1.34
25	b	604	CLA	C4D-ND	-3.92	1.32	1.37
25	b	616	CLA	C4D-ND	-3.92	1.32	1.37
37	C	518	DGD	O2G-C1B	3.92	1.45	1.34
29	7	2630	LHG	O7-C7	3.92	1.45	1.34
24	0	601	CHL	CHD-C1D	3.92	1.46	1.38
24	n	605	CHL	O2A-CGA	3.92	1.44	1.33
24	s	601	CHL	CHD-C4C	3.92	1.48	1.39
24	4	609	CHL	CHC-C4B	3.92	1.48	1.39
25	c	502	CLA	C4D-ND	-3.92	1.32	1.37
29	G	2630	LHG	O7-C7	3.91	1.45	1.34
24	3	605	CHL	CHC-C4B	3.91	1.48	1.39
24	N	606	CHL	C2C-C3C	3.91	1.45	1.36
24	G	605	CHL	CHD-C4C	3.91	1.48	1.39
24	3	605	CHL	CHD-C4C	3.91	1.48	1.39
24	n	607	CHL	C2C-C3C	3.91	1.45	1.36
29	1	2630	LHG	O7-C7	3.91	1.45	1.34
24	G	601	CHL	CHD-C1D	3.91	1.46	1.38
25	c	508	CLA	C4D-ND	-3.91	1.32	1.37
24	5	607	CHL	CHD-C1D	3.90	1.46	1.38
24	g	601	CHL	CHD-C1D	3.90	1.46	1.38
29	6	2630	LHG	O7-C7	3.90	1.45	1.34
24	G	609	CHL	CHC-C1C	3.90	1.46	1.38
25	c	504	CLA	C4D-ND	-3.90	1.32	1.37
24	Y	601	CHL	CHD-C1D	3.89	1.45	1.38
29	n	2630	LHG	O7-C7	3.89	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	CHD-C4C	3.89	1.48	1.39
29	Y	2630	LHG	O8-C23	3.89	1.44	1.33
24	q	609	CHL	CHB-C1B	3.89	1.48	1.39
37	c	518	DGD	O2G-C1B	3.89	1.45	1.34
29	N	2630	LHG	O7-C7	3.89	1.45	1.34
25	0	611	CLA	C1D-ND	3.89	1.42	1.37
24	p	609	CHL	CHC-C1C	3.88	1.46	1.38
25	B	604	CLA	C4D-ND	-3.88	1.32	1.37
24	n	608	CHL	CHC-C1C	3.88	1.46	1.38
25	B	616	CLA	C4D-ND	-3.88	1.32	1.37
24	g	605	CHL	CHD-C4C	3.88	1.48	1.39
24	5	609	CHL	CHD-C4C	3.88	1.48	1.39
24	5	606	CHL	CHD-C4C	3.87	1.48	1.39
24	8	605	CHL	CHD-C4C	3.87	1.48	1.39
25	R	601	CLA	C1D-ND	3.87	1.42	1.37
36	a	413	LMG	O8-C28	3.87	1.44	1.33
36	A	413	LMG	O8-C28	3.87	1.44	1.33
24	4	608	CHL	CHD-C4C	3.87	1.48	1.39
25	d	402	CLA	C4D-ND	-3.87	1.32	1.37
25	d	403	CLA	C4D-ND	-3.87	1.32	1.37
25	r	601	CLA	C1D-ND	3.87	1.42	1.37
25	p	612	CLA	C1D-ND	3.87	1.42	1.37
24	N	601	CHL	CHD-C1D	3.86	1.45	1.38
24	2	607	CHL	CHD-C4C	3.86	1.48	1.39
24	N	605	CHL	O2A-CGA	3.86	1.44	1.33
25	D	403	CLA	C4D-ND	-3.86	1.32	1.37
25	B	609	CLA	C4D-ND	-3.86	1.32	1.37
24	N	607	CHL	C2C-C3C	3.86	1.45	1.36
24	5	605	CHL	CHD-C4C	3.86	1.48	1.39
24	R	607	CHL	C2C-C3C	3.86	1.45	1.36
29	C	2630	LHG	O7-C7	3.85	1.45	1.34
24	5	601	CHL	CHD-C4C	3.85	1.48	1.39
24	2	609	CHL	CHD-C4C	3.85	1.48	1.39
24	g	609	CHL	CHC-C1C	3.85	1.46	1.38
37	C	519	DGD	O1G-C1A	3.85	1.44	1.33
25	4	610	CLA	C1D-ND	3.85	1.42	1.37
24	q	608	CHL	CHD-C4C	3.85	1.48	1.39
24	n	601	CHL	CHD-C1D	3.84	1.45	1.38
25	q	610	CLA	C1D-ND	3.84	1.42	1.37
24	q	608	CHL	CHC-C4B	3.84	1.48	1.39
24	r	607	CHL	C2C-C3C	3.84	1.45	1.36
24	9	607	CHL	CHD-C4C	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	521	LMG	O7-C10	3.84	1.45	1.34
36	c	521	LMG	O7-C10	3.84	1.45	1.34
24	2	606	CHL	CHD-C4C	3.84	1.48	1.39
25	D	402	CLA	C4D-ND	-3.84	1.32	1.37
25	b	609	CLA	C4D-ND	-3.83	1.32	1.37
37	c	519	DGD	O1G-C1A	3.83	1.44	1.33
24	n	601	CHL	C2C-C3C	3.83	1.45	1.36
24	n	609	CHL	CHC-C1C	3.83	1.46	1.38
24	9	601	CHL	CHD-C4C	3.83	1.48	1.39
24	5	606	CHL	CHC-C4B	3.83	1.48	1.39
37	c	519	DGD	O2G-C1B	3.82	1.45	1.34
24	3	601	CHL	CHD-C4C	3.82	1.48	1.39
24	p	605	CHL	CHB-C1B	3.82	1.48	1.39
25	5	610	CLA	C1D-ND	3.82	1.42	1.37
25	5	614	CLA	C1D-ND	3.82	1.42	1.37
25	p	604	CLA	C1D-ND	3.82	1.42	1.37
25	3	612	CLA	C1D-ND	3.82	1.42	1.37
29	c	2630	LHG	O7-C7	3.82	1.45	1.34
24	6	605	CHL	CHD-C4C	3.82	1.47	1.39
25	B	615	CLA	C4D-ND	-3.81	1.32	1.37
37	C	519	DGD	O2G-C1B	3.81	1.45	1.34
24	q	601	CHL	CHD-C4C	3.81	1.47	1.39
25	C	503	CLA	C4D-ND	-3.81	1.32	1.37
24	y	609	CHL	C1B-NB	-3.81	1.33	1.37
24	p	605	CHL	CHC-C4B	3.81	1.48	1.39
24	3	609	CHL	CHC-C1C	3.81	1.46	1.38
24	N	609	CHL	C2C-C3C	3.81	1.44	1.36
37	C	523	DGD	O1G-C1A	3.81	1.44	1.33
37	c	523	DGD	O1G-C1A	3.81	1.44	1.33
29	L	101	LHG	O7-C7	3.81	1.45	1.34
24	G	601	CHL	C2C-C3C	3.80	1.44	1.36
25	6	611	CLA	C1D-ND	3.80	1.42	1.37
24	p	601	CHL	CHD-C4C	3.80	1.47	1.39
25	c	503	CLA	C4D-ND	-3.80	1.32	1.37
24	4	607	CHL	CHC-C4B	3.80	1.47	1.39
24	p	607	CHL	CHD-C4C	3.80	1.47	1.39
25	A	405	CLA	C4D-ND	-3.80	1.32	1.37
24	n	609	CHL	C4B-NB	-3.80	1.33	1.37
25	6	614	CLA	C1D-ND	3.79	1.42	1.37
24	4	609	CHL	CHB-C1B	3.79	1.47	1.39
24	8	609	CHL	CHD-C1D	3.79	1.45	1.38
25	s	613	CLA	C4D-ND	-3.79	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	601	CHL	OBD-CAD	3.79	1.29	1.22
25	p	613	CLA	C1D-ND	3.79	1.42	1.37
24	4	608	CHL	OBD-CAD	3.79	1.29	1.22
29	G	2630	LHG	O8-C23	3.79	1.44	1.33
24	Y	609	CHL	C1B-NB	-3.79	1.33	1.37
24	9	606	CHL	CHD-C4C	3.79	1.47	1.39
24	2	601	CHL	CHD-C4C	3.78	1.47	1.39
25	c	512	CLA	C4D-ND	-3.78	1.32	1.37
25	b	614	CLA	C4D-ND	-3.78	1.32	1.37
25	y	603	CLA	C4D-ND	-3.78	1.32	1.37
24	9	605	CHL	CHC-C4B	3.78	1.47	1.39
24	6	601	CHL	CHD-C4C	3.78	1.47	1.39
25	C	512	CLA	C4D-ND	-3.77	1.32	1.37
24	6	607	CHL	CHD-C4C	3.77	1.47	1.39
25	c	506	CLA	C4D-ND	-3.77	1.32	1.37
25	b	615	CLA	C4D-ND	-3.77	1.32	1.37
29	g	2630	LHG	O8-C23	3.77	1.44	1.33
25	Y	614	CLA	C4D-ND	-3.76	1.32	1.37
24	p	609	CHL	CHD-C4C	3.76	1.47	1.39
25	0	613	CLA	C1D-ND	3.76	1.42	1.37
24	g	601	CHL	C2C-C3C	3.76	1.44	1.36
29	l	101	LHG	O7-C7	3.76	1.44	1.34
25	8	614	CLA	C1D-ND	3.76	1.42	1.37
24	2	605	CHL	CHC-C4B	3.76	1.47	1.39
24	q	607	CHL	CHC-C4B	3.76	1.47	1.39
25	C	506	CLA	C4D-ND	-3.76	1.32	1.37
24	5	605	CHL	CHB-C1B	3.76	1.47	1.39
25	p	614	CLA	C1D-ND	3.76	1.42	1.37
24	q	608	CHL	OBD-CAD	3.76	1.29	1.22
25	B	606	CLA	C4D-ND	-3.75	1.32	1.37
25	b	606	CLA	C4D-ND	-3.75	1.32	1.37
25	c	513	CLA	C4D-ND	-3.75	1.32	1.37
24	1	609	CHL	CHD-C1D	3.75	1.45	1.38
24	p	606	CHL	CHC-C4B	3.75	1.47	1.39
24	8	601	CHL	CHD-C4C	3.75	1.47	1.39
24	3	609	CHL	CHD-C1D	3.75	1.45	1.38
25	7	614	CLA	C1D-ND	3.75	1.42	1.37
24	4	605	CHL	CHB-C1B	3.75	1.47	1.39
25	a	405	CLA	C4D-ND	-3.75	1.32	1.37
25	y	613	CLA	C4D-ND	-3.75	1.32	1.37
24	S	608	CHL	CHD-C4C	3.75	1.47	1.39
25	B	614	CLA	C4D-ND	-3.74	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	605	CHL	OBD-CAD	3.74	1.28	1.22
25	0	614	CLA	C1D-ND	3.74	1.42	1.37
24	8	605	CHL	CHB-C1B	3.74	1.47	1.39
25	4	602	CLA	C1D-ND	3.74	1.42	1.37
29	D	409	LHG	O7-C7	3.74	1.44	1.34
25	q	602	CLA	C1D-ND	3.74	1.42	1.37
24	3	605	CHL	CHB-C1B	3.73	1.47	1.39
24	4	605	CHL	CHC-C4B	3.73	1.47	1.39
24	q	608	CHL	CHB-C1B	3.73	1.47	1.39
24	q	605	CHL	OBD-CAD	3.73	1.28	1.22
24	r	606	CHL	CHD-C1D	3.73	1.45	1.38
25	A	410	CLA	C4D-ND	-3.73	1.32	1.37
25	a	410	CLA	C4D-ND	-3.73	1.32	1.37
24	s	608	CHL	CHD-C4C	3.73	1.47	1.39
25	A	407	CLA	C4D-ND	-3.73	1.32	1.37
25	Y	603	CLA	C4D-ND	-3.73	1.32	1.37
24	0	606	CHL	CHD-C4C	3.73	1.47	1.39
25	c	507	CLA	C4D-ND	-3.73	1.32	1.37
24	5	605	CHL	CHC-C4B	3.73	1.47	1.39
25	6	613	CLA	C1D-ND	3.73	1.42	1.37
24	G	608	CHL	OBD-CAD	3.73	1.28	1.22
24	y	601	CHL	C2C-C3C	3.73	1.44	1.36
25	B	611	CLA	C4D-ND	-3.73	1.32	1.37
24	4	608	CHL	CHC-C4B	3.72	1.47	1.39
24	2	605	CHL	OBD-CAD	3.72	1.28	1.22
25	S	613	CLA	C4D-ND	-3.72	1.32	1.37
24	R	606	CHL	CHD-C1D	3.72	1.45	1.38
24	p	605	CHL	OBD-CAD	3.72	1.28	1.22
25	B	603	CLA	C4D-ND	-3.72	1.32	1.37
25	Y	613	CLA	C4D-ND	-3.72	1.32	1.37
29	d	409	LHG	O7-C7	3.72	1.44	1.34
25	6	602	CLA	C1D-ND	3.71	1.42	1.37
24	6	606	CHL	OBD-CAD	3.71	1.28	1.22
25	b	603	CLA	C4D-ND	-3.71	1.32	1.37
25	r	602	CLA	C4D-ND	-3.71	1.32	1.37
24	2	607	CHL	OBD-CAD	3.71	1.28	1.22
24	n	605	CHL	CHD-C4C	3.71	1.47	1.39
25	C	507	CLA	C4D-ND	-3.71	1.32	1.37
24	9	606	CHL	CHB-C1B	3.71	1.47	1.39
24	N	605	CHL	CHD-C4C	3.71	1.47	1.39
24	s	607	CHL	CHD-C4C	3.71	1.47	1.39
24	g	609	CHL	C1B-NB	-3.70	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	614	CLA	C4D-ND	-3.70	1.32	1.37
24	q	606	CHL	CHB-C1B	3.70	1.47	1.39
24	N	609	CHL	CHC-C1C	3.70	1.46	1.38
29	y	2630	LHG	O7-C7	3.70	1.44	1.34
25	5	613	CLA	C1D-ND	3.70	1.42	1.37
24	R	608	CHL	CHD-C1D	3.70	1.45	1.38
24	0	605	CHL	CHD-C4C	3.70	1.47	1.39
24	0	608	CHL	CHD-C4C	3.70	1.47	1.39
24	9	608	CHL	CHD-C4C	3.70	1.47	1.39
24	4	601	CHL	CHD-C4C	3.70	1.47	1.39
24	5	605	CHL	OBD-CAD	3.70	1.28	1.22
25	R	602	CLA	C4D-ND	-3.70	1.32	1.37
25	b	617	CLA	C4D-ND	-3.69	1.32	1.37
24	N	609	CHL	C4B-NB	-3.69	1.33	1.37
24	9	607	CHL	OBD-CAD	3.69	1.28	1.22
24	q	605	CHL	CHC-C4B	3.69	1.47	1.39
24	0	607	CHL	OBD-CAD	3.69	1.28	1.22
24	2	608	CHL	CHD-C4C	3.69	1.47	1.39
24	2	605	CHL	CHB-C1B	3.69	1.47	1.39
25	3	611	CLA	C1D-ND	3.69	1.42	1.37
25	Y	611	CLA	C4D-ND	-3.69	1.32	1.37
24	y	607	CHL	CHD-C1D	3.69	1.45	1.38
25	C	501	CLA	C4D-ND	-3.68	1.32	1.37
25	6	604	CLA	C1D-ND	3.68	1.42	1.37
25	1	614	CLA	C1D-ND	3.68	1.42	1.37
24	g	605	CHL	OBD-CAD	3.68	1.28	1.22
25	b	611	CLA	C4D-ND	-3.68	1.32	1.37
25	N	603	CLA	C4D-ND	-3.68	1.32	1.37
25	5	604	CLA	C1D-ND	3.68	1.42	1.37
25	C	513	CLA	C4D-ND	-3.68	1.32	1.37
25	s	602	CLA	C4D-ND	-3.68	1.32	1.37
24	G	609	CHL	C1B-NB	-3.68	1.33	1.37
24	8	607	CHL	CHD-C1D	3.68	1.45	1.38
24	S	607	CHL	CHD-C4C	3.68	1.47	1.39
24	4	601	CHL	CHC-C4B	3.68	1.47	1.39
24	p	606	CHL	CHB-C1B	3.67	1.47	1.39
24	Y	601	CHL	C2C-C3C	3.67	1.44	1.36
25	a	407	CLA	C4D-ND	-3.67	1.32	1.37
24	p	608	CHL	CHD-C4C	3.67	1.47	1.39
24	q	607	CHL	OBD-CAD	3.67	1.28	1.22
25	c	501	CLA	C4D-ND	-3.67	1.32	1.37
25	9	610	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	601	CHL	OBD-CAD	3.67	1.28	1.22
24	4	606	CHL	CHB-C1B	3.67	1.47	1.39
25	8	612	CLA	C1D-ND	3.67	1.42	1.37
25	y	611	CLA	C4D-ND	-3.67	1.32	1.37
24	r	608	CHL	CHD-C1D	3.66	1.45	1.38
24	p	607	CHL	OBD-CAD	3.66	1.28	1.22
24	9	605	CHL	CHB-C1B	3.66	1.47	1.39
25	9	612	CLA	C1D-ND	3.66	1.42	1.37
24	q	605	CHL	CHB-C1B	3.66	1.47	1.39
25	B	617	CLA	C4D-ND	-3.66	1.32	1.37
25	3	604	CLA	C4D-ND	-3.66	1.32	1.37
25	0	602	CLA	C1D-ND	3.66	1.42	1.37
24	5	606	CHL	CHB-C1B	3.66	1.47	1.39
25	p	603	CLA	C1D-ND	3.66	1.42	1.37
24	g	608	CHL	OBD-CAD	3.65	1.28	1.22
24	s	607	CHL	CHC-C4B	3.65	1.47	1.39
24	0	606	CHL	OBD-CAD	3.65	1.28	1.22
25	g	602	CLA	C4D-ND	-3.65	1.32	1.37
25	2	604	CLA	C1D-ND	3.65	1.42	1.37
25	5	603	CLA	C1D-ND	3.65	1.42	1.37
25	R	610	CLA	C4D-ND	-3.65	1.32	1.37
24	G	605	CHL	OBD-CAD	3.65	1.28	1.22
25	4	614	CLA	C1D-ND	3.65	1.42	1.37
24	G	608	CHL	CHD-C4C	3.65	1.47	1.39
24	Y	607	CHL	CHD-C1D	3.65	1.45	1.38
24	Y	606	CHL	CHD-C1D	3.65	1.45	1.38
29	Y	2630	LHG	O7-C7	3.64	1.44	1.34
25	n	603	CLA	C4D-ND	-3.64	1.32	1.37
24	g	609	CHL	CHD-C4C	3.64	1.47	1.39
24	G	609	CHL	CHD-C4C	3.64	1.47	1.39
24	5	608	CHL	CHD-C4C	3.64	1.47	1.39
25	G	611	CLA	C1D-ND	3.64	1.42	1.37
24	4	605	CHL	OBD-CAD	3.64	1.28	1.22
25	c	505	CLA	C4D-ND	-3.64	1.32	1.37
24	Y	601	CHL	CHD-C4C	3.64	1.47	1.39
25	q	612	CLA	C1D-ND	3.64	1.42	1.37
24	6	605	CHL	OBD-CAD	3.64	1.28	1.22
25	N	613	CLA	C4D-ND	-3.64	1.32	1.37
24	N	606	CHL	CHD-C1D	3.64	1.45	1.38
24	8	606	CHL	CHC-C4B	3.64	1.47	1.39
25	3	614	CLA	C1D-ND	3.64	1.42	1.37
25	g	610	CLA	C4D-ND	-3.63	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	604	CLA	C1D-ND	3.63	1.42	1.37
25	8	610	CLA	C1D-ND	3.63	1.42	1.37
24	0	601	CHL	CHD-C4C	3.63	1.47	1.39
24	6	606	CHL	CHD-C4C	3.63	1.47	1.39
24	8	608	CHL	CHD-C4C	3.63	1.47	1.39
24	S	607	CHL	CHC-C4B	3.63	1.47	1.39
25	q	604	CLA	C1D-ND	3.62	1.42	1.37
25	C	505	CLA	C4D-ND	-3.62	1.32	1.37
25	n	602	CLA	C4D-ND	-3.62	1.32	1.37
25	c	509	CLA	C4D-ND	-3.62	1.32	1.37
24	3	608	CHL	CHD-C4C	3.62	1.47	1.39
24	3	606	CHL	CHC-C4B	3.62	1.47	1.39
25	g	611	CLA	C1D-ND	3.62	1.42	1.37
25	6	614	CLA	C4B-NB	3.62	1.42	1.37
24	4	608	CHL	CHB-C1B	3.62	1.47	1.39
25	b	608	CLA	C4D-ND	-3.62	1.32	1.37
24	g	606	CHL	CHD-C4C	3.62	1.47	1.39
24	y	601	CHL	CHD-C4C	3.62	1.47	1.39
24	3	607	CHL	OBD-CAD	3.61	1.28	1.22
24	5	607	CHL	CHC-C4B	3.61	1.47	1.39
25	S	602	CLA	C4D-ND	-3.61	1.32	1.37
37	C	524	DGD	O2G-C1B	3.61	1.44	1.34
24	4	609	CHL	OBD-CAD	3.61	1.28	1.22
25	7	603	CLA	C4D-ND	-3.61	1.32	1.37
25	4	604	CLA	C1D-ND	3.61	1.42	1.37
25	n	604	CLA	C4D-ND	-3.61	1.32	1.37
25	C	509	CLA	C4D-ND	-3.61	1.32	1.37
25	3	613	CLA	C1D-ND	3.61	1.42	1.37
25	y	612	CLA	C4D-ND	-3.61	1.32	1.37
25	G	610	CLA	C4D-ND	-3.61	1.32	1.37
25	R	613	CLA	C4D-ND	-3.61	1.32	1.37
25	r	613	CLA	C4D-ND	-3.61	1.32	1.37
25	3	610	CLA	C1D-ND	3.61	1.42	1.37
25	s	610	CLA	C4D-ND	-3.60	1.32	1.37
25	g	603	CLA	C4D-ND	-3.60	1.32	1.37
24	7	607	CHL	CHD-C4C	3.60	1.47	1.39
25	G	602	CLA	C4D-ND	-3.60	1.32	1.37
25	r	610	CLA	C4D-ND	-3.60	1.32	1.37
24	n	606	CHL	CHD-C1D	3.60	1.45	1.38
25	B	608	CLA	C4D-ND	-3.60	1.32	1.37
24	N	607	CHL	CHC-C4B	3.60	1.47	1.39
25	n	613	CLA	C4D-ND	-3.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	607	CHL	CHD-C1D	3.60	1.45	1.38
25	8	611	CLA	C1D-ND	3.60	1.42	1.37
24	n	609	CHL	CHD-C4C	3.60	1.47	1.39
24	q	606	CHL	OBD-CAD	3.60	1.28	1.22
25	8	613	CLA	C1D-ND	3.60	1.42	1.37
25	2	610	CLA	C1D-ND	3.60	1.42	1.37
24	N	608	CHL	CHD-C1D	3.60	1.45	1.38
24	y	606	CHL	CHD-C1D	3.59	1.45	1.38
24	Y	609	CHL	CHC-C1C	3.59	1.45	1.38
25	4	612	CLA	C1D-ND	3.59	1.42	1.37
25	N	611	CLA	C4D-ND	-3.59	1.32	1.37
24	8	607	CHL	OBD-CAD	3.59	1.28	1.22
24	2	606	CHL	CHB-C1B	3.59	1.47	1.39
24	3	601	CHL	OBD-CAD	3.59	1.28	1.22
25	p	602	CLA	C4B-NB	3.59	1.42	1.37
24	S	601	CHL	CHC-C4B	3.59	1.47	1.39
24	7	609	CHL	CHD-C1D	3.59	1.45	1.38
24	g	608	CHL	CHD-C4C	3.59	1.47	1.39
24	G	606	CHL	CHD-C4C	3.59	1.47	1.39
25	R	603	CLA	C4D-ND	-3.58	1.32	1.37
24	y	609	CHL	CHC-C1C	3.58	1.45	1.38
24	Y	601	CHL	C4B-NB	-3.58	1.33	1.37
25	S	610	CLA	C4D-ND	-3.58	1.32	1.37
37	c	524	DGD	O2G-C1B	3.58	1.44	1.34
24	s	601	CHL	CHC-C4B	3.58	1.47	1.39
25	b	607	CLA	C4D-ND	-3.58	1.32	1.37
24	7	608	CHL	CHD-C1D	3.58	1.45	1.38
25	N	602	CLA	C4D-ND	-3.58	1.32	1.37
24	8	605	CHL	OBD-CAD	3.58	1.28	1.22
24	0	609	CHL	CHD-C4C	3.58	1.47	1.39
24	4	607	CHL	OBD-CAD	3.58	1.28	1.22
25	q	614	CLA	C1D-ND	3.58	1.42	1.37
25	N	604	CLA	C4D-ND	-3.57	1.32	1.37
25	B	613	CLA	C4D-ND	-3.57	1.32	1.37
25	G	611	CLA	C4D-ND	-3.57	1.32	1.37
25	b	613	CLA	C4D-ND	-3.57	1.32	1.37
24	5	607	CHL	OBD-CAD	3.57	1.28	1.22
25	p	610	CLA	C1D-ND	3.57	1.42	1.37
24	0	607	CHL	CHD-C4C	3.57	1.47	1.39
25	4	613	CLA	C1D-ND	3.57	1.42	1.37
24	S	606	CHL	CHD-C4C	3.57	1.47	1.39
25	p	602	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	OBD-CAD	3.57	1.28	1.22
24	9	609	CHL	OBD-CAD	3.57	1.28	1.22
24	n	607	CHL	CHC-C4B	3.57	1.47	1.39
25	r	603	CLA	C4D-ND	-3.57	1.32	1.37
24	Y	609	CHL	C4B-NB	-3.57	1.33	1.37
24	2	609	CHL	OBD-CAD	3.57	1.28	1.22
24	7	605	CHL	CHD-C4C	3.56	1.47	1.39
25	0	614	CLA	C4B-NB	3.56	1.42	1.37
24	2	606	CHL	OBD-CAD	3.56	1.28	1.22
24	9	606	CHL	OBD-CAD	3.56	1.28	1.22
25	p	614	CLA	C4B-NB	3.56	1.42	1.37
24	0	605	CHL	OBD-CAD	3.56	1.28	1.22
24	3	605	CHL	OBD-CAD	3.56	1.28	1.22
24	7	607	CHL	CHC-C4B	3.56	1.47	1.39
24	1	607	CHL	CHD-C4C	3.56	1.47	1.39
24	6	609	CHL	CHD-C4C	3.56	1.47	1.39
25	G	604	CLA	C4D-ND	-3.56	1.32	1.37
25	S	611	CLA	C4D-ND	-3.56	1.32	1.37
25	4	612	CLA	C4B-NB	3.56	1.42	1.37
25	7	613	CLA	C1D-ND	3.56	1.42	1.37
25	B	610	CLA	C4D-ND	-3.56	1.32	1.37
25	5	602	CLA	C1D-ND	3.56	1.42	1.37
24	r	607	CHL	CHD-C1D	3.55	1.45	1.38
24	s	606	CHL	CHD-C4C	3.55	1.47	1.39
24	3	608	CHL	OBD-CAD	3.55	1.28	1.22
25	b	610	CLA	C4D-ND	-3.55	1.32	1.37
24	p	607	CHL	CHC-C4B	3.55	1.47	1.39
24	y	605	CHL	CHD-C4C	3.55	1.47	1.39
25	1	603	CLA	C4D-ND	-3.55	1.32	1.37
24	q	601	CHL	CHC-C4B	3.55	1.47	1.39
25	G	603	CLA	C4D-ND	-3.55	1.32	1.37
24	q	607	CHL	CHB-C1B	3.55	1.47	1.39
25	s	611	CLA	C4D-ND	-3.55	1.32	1.37
24	8	606	CHL	OBD-CAD	3.54	1.28	1.22
24	n	608	CHL	CHD-C1D	3.54	1.45	1.38
24	1	606	CHL	CHC-C4B	3.54	1.47	1.39
24	0	606	CHL	CHB-C1B	3.54	1.47	1.39
24	1	608	CHL	CHD-C1D	3.54	1.45	1.38
25	Y	612	CLA	C4D-ND	-3.54	1.32	1.37
25	9	602	CLA	C4D-ND	-3.54	1.32	1.37
24	7	606	CHL	CHD-C4C	3.54	1.47	1.39
24	s	607	CHL	CHB-C1B	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	607	CHL	CHD-C4C	3.54	1.47	1.39
25	2	612	CLA	C1D-ND	3.54	1.42	1.37
24	1	607	CHL	CHC-C4B	3.54	1.47	1.39
25	n	611	CLA	C4D-ND	-3.54	1.32	1.37
24	8	601	CHL	OBD-CAD	3.54	1.28	1.22
24	6	606	CHL	CHB-C1B	3.54	1.47	1.39
25	1	611	CLA	C4D-ND	-3.53	1.32	1.37
25	8	604	CLA	C4D-ND	-3.53	1.32	1.37
24	y	609	CHL	C4B-NB	-3.53	1.33	1.37
25	c	510	CLA	C4D-ND	-3.53	1.32	1.37
25	9	613	CLA	C4D-ND	-3.53	1.32	1.37
25	p	613	CLA	C4B-NB	3.53	1.42	1.37
24	G	601	CHL	CHD-C4C	3.53	1.47	1.39
24	3	606	CHL	CHB-C1B	3.53	1.47	1.39
24	Y	605	CHL	CHD-C4C	3.53	1.47	1.39
24	5	609	CHL	CHB-C1B	3.53	1.47	1.39
25	5	614	CLA	C4B-NB	3.53	1.42	1.37
24	0	601	CHL	OBD-CAD	3.53	1.28	1.22
25	n	614	CLA	C1D-ND	3.53	1.42	1.37
25	2	613	CLA	C4D-ND	-3.52	1.32	1.37
24	4	607	CHL	CHB-C1B	3.52	1.47	1.39
25	S	603	CLA	C1D-ND	3.52	1.42	1.37
24	6	608	CHL	CHD-C4C	3.52	1.47	1.39
25	S	614	CLA	C4D-ND	-3.52	1.32	1.37
25	n	614	CLA	C4D-ND	-3.52	1.32	1.37
24	8	606	CHL	CHB-C1B	3.52	1.47	1.39
25	S	609	CLA	C1D-ND	3.52	1.42	1.37
25	s	609	CLA	C1D-ND	3.52	1.42	1.37
24	1	605	CHL	CHD-C4C	3.52	1.47	1.39
25	g	604	CLA	C4D-ND	-3.52	1.32	1.37
24	0	609	CHL	C4B-NB	-3.52	1.33	1.37
24	y	601	CHL	C4B-NB	-3.52	1.33	1.37
25	r	603	CLA	C1D-ND	3.52	1.42	1.37
25	8	604	CLA	C1D-ND	3.52	1.42	1.37
24	N	609	CHL	C1B-NB	-3.52	1.33	1.37
24	0	609	CHL	OBD-CAD	3.52	1.28	1.22
24	8	609	CHL	OBD-CAD	3.52	1.28	1.22
24	q	609	CHL	MG-NA	-3.52	1.97	2.06
24	p	608	CHL	OBD-CAD	3.52	1.28	1.22
24	R	607	CHL	CHD-C1D	3.51	1.45	1.38
25	6	604	CLA	C4B-NB	3.51	1.42	1.37
24	1	606	CHL	CHD-C4C	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	603	CLA	C1D-ND	3.51	1.42	1.37
25	B	607	CLA	C4D-ND	-3.51	1.32	1.37
24	g	601	CHL	CHD-C4C	3.51	1.47	1.39
24	n	609	CHL	C1B-NB	-3.51	1.33	1.37
25	5	602	CLA	C4B-NB	3.51	1.42	1.37
24	n	607	CHL	CHD-C1D	3.51	1.45	1.38
25	s	614	CLA	C4D-ND	-3.51	1.32	1.37
25	7	611	CLA	C4D-ND	-3.51	1.32	1.37
25	S	604	CLA	C4D-ND	-3.50	1.32	1.37
24	p	609	CHL	OBD-CAD	3.50	1.28	1.22
24	S	607	CHL	CHB-C1B	3.50	1.47	1.39
25	9	614	CLA	C1D-ND	3.50	1.42	1.37
24	3	606	CHL	OBD-CAD	3.50	1.28	1.22
24	4	601	CHL	OBD-CAD	3.50	1.28	1.22
25	p	611	CLA	C1D-ND	3.50	1.42	1.37
24	6	609	CHL	OBD-CAD	3.50	1.28	1.22
25	2	614	CLA	C1D-ND	3.50	1.42	1.37
25	R	603	CLA	C1D-ND	3.49	1.42	1.37
24	4	609	CHL	MG-NA	-3.49	1.98	2.06
24	2	607	CHL	CHC-C4B	3.49	1.47	1.39
24	7	607	CHL	OBD-CAD	3.49	1.28	1.22
25	q	613	CLA	C1D-ND	3.49	1.42	1.37
24	5	608	CHL	CHC-C4B	3.49	1.47	1.39
25	g	612	CLA	C4D-ND	-3.49	1.32	1.37
25	s	604	CLA	C4D-ND	-3.49	1.32	1.37
24	1	607	CHL	OBD-CAD	3.49	1.28	1.22
25	b	605	CLA	C4D-ND	-3.49	1.32	1.37
24	5	609	CHL	OBD-CAD	3.49	1.28	1.22
24	3	608	CHL	CHC-C4B	3.49	1.47	1.39
25	B	605	CLA	C4D-ND	-3.48	1.32	1.37
24	5	608	CHL	OBD-CAD	3.48	1.28	1.22
24	8	608	CHL	OBD-CAD	3.48	1.28	1.22
24	G	605	CHL	CHB-C1B	3.48	1.47	1.39
24	2	606	CHL	CHC-C4B	3.48	1.47	1.39
24	S	607	CHL	OBD-CAD	3.48	1.28	1.22
25	2	602	CLA	C4D-ND	-3.48	1.32	1.37
25	7	610	CLA	C4D-ND	-3.48	1.32	1.37
25	1	610	CLA	C4D-ND	-3.48	1.32	1.37
25	N	614	CLA	C4D-ND	-3.48	1.32	1.37
24	7	606	CHL	CHC-C4B	3.48	1.47	1.39
24	N	601	CHL	CHD-C4C	3.48	1.47	1.39
24	0	601	CHL	CHC-C4B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	606	CHL	OBD-CAD	3.48	1.28	1.22
24	6	608	CHL	CHC-C4B	3.47	1.47	1.39
25	s	609	CLA	C4B-NB	3.47	1.42	1.37
24	9	607	CHL	CHC-C4B	3.47	1.47	1.39
25	q	612	CLA	C4B-NB	3.47	1.42	1.37
25	y	610	CLA	C4D-ND	-3.47	1.32	1.37
25	S	612	CLA	C4D-ND	-3.46	1.32	1.37
24	R	607	CHL	C4B-NB	-3.46	1.33	1.37
24	r	607	CHL	C4B-NB	-3.46	1.33	1.37
25	c	511	CLA	C4D-ND	-3.46	1.32	1.37
24	3	607	CHL	CHC-C4B	3.46	1.47	1.39
25	p	611	CLA	C4B-NB	3.46	1.42	1.37
24	1	609	CHL	CHD-C4C	3.46	1.47	1.39
25	S	614	CLA	C1D-ND	3.46	1.42	1.37
24	N	607	CHL	CHD-C1D	3.46	1.45	1.38
24	n	601	CHL	CHD-C4C	3.46	1.47	1.39
24	1	601	CHL	OBD-CAD	3.46	1.28	1.22
25	C	511	CLA	C4D-ND	-3.46	1.32	1.37
25	g	614	CLA	C4D-ND	-3.46	1.32	1.37
24	1	608	CHL	CHC-C4B	3.46	1.47	1.39
24	s	607	CHL	OBD-CAD	3.46	1.28	1.22
24	6	605	CHL	CHC-C4B	3.46	1.47	1.39
24	9	606	CHL	CHC-C4B	3.46	1.47	1.39
25	s	603	CLA	C1D-ND	3.45	1.42	1.37
25	6	612	CLA	C1D-ND	3.45	1.42	1.37
24	8	608	CHL	CHC-C4B	3.45	1.47	1.39
24	n	606	CHL	CHC-C4B	3.45	1.47	1.39
25	3	614	CLA	C4B-NB	3.45	1.42	1.37
25	S	605	CLA	C4D-ND	-3.45	1.32	1.37
25	3	604	CLA	C4B-NB	3.45	1.42	1.37
24	7	601	CHL	OBD-CAD	3.45	1.28	1.22
25	C	510	CLA	C4D-ND	-3.45	1.32	1.37
25	G	612	CLA	C4D-ND	-3.45	1.33	1.37
25	Y	602	CLA	C4D-ND	-3.45	1.33	1.37
24	1	605	CHL	CHB-C1B	3.45	1.47	1.39
25	5	610	CLA	C4B-NB	3.45	1.42	1.37
24	7	605	CHL	OBD-CAD	3.45	1.28	1.22
24	R	606	CHL	CHD-C4C	3.45	1.47	1.39
25	3	604	CLA	C1D-ND	3.45	1.42	1.37
25	q	611	CLA	C1D-ND	3.45	1.42	1.37
24	0	606	CHL	CHC-C4B	3.45	1.47	1.39
24	y	607	CHL	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	611	CLA	C4D-ND	-3.44	1.33	1.37
25	N	614	CLA	C1D-ND	3.44	1.42	1.37
24	7	606	CHL	CHB-C1B	3.44	1.47	1.39
25	0	612	CLA	C1D-ND	3.44	1.42	1.37
24	0	605	CHL	CHC-C4B	3.44	1.47	1.39
25	4	604	CLA	C4B-NB	3.44	1.42	1.37
25	y	602	CLA	C4D-ND	-3.44	1.33	1.37
24	S	606	CHL	OBD-CAD	3.44	1.28	1.22
24	8	607	CHL	CHC-C4B	3.44	1.47	1.39
25	p	610	CLA	C4B-NB	3.44	1.42	1.37
25	5	611	CLA	C4D-ND	-3.44	1.33	1.37
24	p	608	CHL	CHC-C4B	3.44	1.47	1.39
24	N	606	CHL	OBD-CAD	3.44	1.28	1.22
25	S	609	CLA	C4B-NB	3.44	1.42	1.37
25	p	603	CLA	C4B-NB	3.44	1.42	1.37
24	1	605	CHL	OBD-CAD	3.44	1.28	1.22
25	Y	610	CLA	C4D-ND	-3.43	1.33	1.37
24	Y	607	CHL	CHC-C4B	3.43	1.47	1.39
25	8	603	CLA	C1D-ND	3.43	1.42	1.37
24	7	605	CHL	CHB-C1B	3.43	1.47	1.39
24	p	609	CHL	CHB-C1B	3.43	1.47	1.39
24	g	607	CHL	CHD-C4C	3.43	1.47	1.39
25	9	612	CLA	C4B-NB	3.42	1.42	1.37
25	s	605	CLA	C4D-ND	-3.42	1.33	1.37
25	s	614	CLA	C1D-ND	3.42	1.42	1.37
24	S	608	CHL	OBD-CAD	3.42	1.28	1.22
24	2	607	CHL	CHB-C1B	3.42	1.47	1.39
24	3	609	CHL	OBD-CAD	3.42	1.28	1.22
24	6	607	CHL	OBD-CAD	3.42	1.28	1.22
24	s	608	CHL	OBD-CAD	3.42	1.28	1.22
25	1	613	CLA	C1D-ND	3.42	1.42	1.37
24	g	605	CHL	CHB-C1B	3.41	1.47	1.39
24	7	609	CHL	CHD-C4C	3.41	1.47	1.39
25	s	612	CLA	C4D-ND	-3.41	1.33	1.37
25	1	604	CLA	C4D-ND	-3.41	1.33	1.37
25	1	604	CLA	C1D-ND	3.41	1.42	1.37
24	1	608	CHL	OBD-CAD	3.41	1.28	1.22
25	G	614	CLA	C4D-ND	-3.41	1.33	1.37
25	3	602	CLA	C4D-ND	-3.41	1.33	1.37
25	5	603	CLA	C4B-NB	3.40	1.42	1.37
25	8	610	CLA	C4B-NB	3.40	1.42	1.37
25	8	614	CLA	C4B-NB	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	604	CLA	C4B-NB	3.40	1.42	1.37
24	N	609	CHL	CHD-C4C	3.40	1.47	1.39
24	r	607	CHL	C1B-NB	-3.40	1.33	1.37
25	5	611	CLA	C4B-NB	3.40	1.42	1.37
24	r	606	CHL	CHD-C4C	3.40	1.47	1.39
25	b	602	CLA	C4D-ND	-3.40	1.33	1.37
25	5	613	CLA	C4B-NB	3.40	1.42	1.37
25	r	611	CLA	C4D-ND	-3.40	1.33	1.37
25	3	611	CLA	C4B-NB	3.40	1.42	1.37
24	2	608	CHL	CHC-C4B	3.39	1.47	1.39
24	9	607	CHL	CHB-C1B	3.39	1.47	1.39
25	R	611	CLA	C4D-ND	-3.39	1.33	1.37
24	0	608	CHL	CHC-C4B	3.39	1.47	1.39
24	6	601	CHL	OBD-CAD	3.39	1.28	1.22
24	y	608	CHL	CHC-C4B	3.39	1.47	1.39
25	c	511	CLA	C1D-ND	3.39	1.42	1.37
25	C	511	CLA	C1D-ND	3.39	1.41	1.37
24	1	606	CHL	OBD-CAD	3.39	1.28	1.22
24	s	601	CHL	CHB-C1B	3.39	1.47	1.39
24	R	607	CHL	C1B-NB	-3.38	1.33	1.37
24	G	608	CHL	CHC-C4B	3.38	1.47	1.39
25	1	603	CLA	C1D-ND	3.38	1.41	1.37
25	3	603	CLA	C1D-ND	3.38	1.41	1.37
24	n	606	CHL	OBD-CAD	3.38	1.28	1.22
24	g	607	CHL	OBD-CAD	3.38	1.28	1.22
24	6	607	CHL	CHC-C4B	3.38	1.47	1.39
24	S	601	CHL	CHB-C1B	3.38	1.47	1.39
25	S	602	CLA	C1D-ND	3.38	1.41	1.37
24	9	608	CHL	CHC-C4B	3.38	1.47	1.39
25	R	613	CLA	C1D-ND	3.38	1.41	1.37
25	9	614	CLA	C4B-NB	3.38	1.41	1.37
25	2	611	CLA	C4D-ND	-3.38	1.33	1.37
24	s	606	CHL	CHB-C1B	3.38	1.47	1.39
25	7	604	CLA	C4D-ND	-3.38	1.33	1.37
25	s	605	CLA	C4B-NB	3.38	1.41	1.37
25	r	604	CLA	C4D-ND	-3.38	1.33	1.37
25	7	614	CLA	C4B-NB	3.37	1.41	1.37
25	C	503	CLA	C1D-ND	3.37	1.41	1.37
24	6	606	CHL	CHC-C4B	3.37	1.47	1.39
24	G	607	CHL	OBD-CAD	3.37	1.28	1.22
25	5	611	CLA	C1D-ND	3.37	1.41	1.37
25	4	611	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	603	CLA	C4D-ND	-3.37	1.33	1.37
24	N	606	CHL	CHC-C4B	3.37	1.47	1.39
25	9	602	CLA	C1D-ND	3.37	1.41	1.37
25	B	602	CLA	C4D-ND	-3.37	1.33	1.37
25	8	602	CLA	C4D-ND	-3.37	1.33	1.37
24	S	608	CHL	CHC-C4B	3.37	1.47	1.39
25	n	610	CLA	C1D-ND	3.37	1.41	1.37
25	7	603	CLA	C1D-ND	3.37	1.41	1.37
25	3	603	CLA	C4D-ND	-3.37	1.33	1.37
25	q	604	CLA	C4B-NB	3.37	1.41	1.37
25	g	604	CLA	C1D-ND	3.37	1.41	1.37
24	Y	608	CHL	CHD-C1D	3.37	1.44	1.38
24	y	608	CHL	CHD-C1D	3.37	1.44	1.38
25	N	604	CLA	C1D-ND	3.36	1.41	1.37
25	S	605	CLA	C4B-NB	3.36	1.41	1.37
24	N	605	CHL	OBD-CAD	3.36	1.28	1.22
24	8	607	CHL	CHD-C4C	3.36	1.46	1.39
24	s	608	CHL	CHC-C4B	3.36	1.46	1.39
25	b	608	CLA	C1D-ND	3.36	1.41	1.37
24	S	606	CHL	CHB-C1B	3.36	1.46	1.39
24	n	605	CHL	OBD-CAD	3.36	1.28	1.22
24	Y	608	CHL	CHC-C4B	3.36	1.46	1.39
24	g	605	CHL	CHC-C4B	3.36	1.46	1.39
24	s	608	CHL	CHB-C1B	3.36	1.46	1.39
25	p	612	CLA	C4B-NB	3.36	1.41	1.37
24	g	607	CHL	CHC-C4B	3.35	1.46	1.39
25	n	612	CLA	C1D-ND	3.35	1.41	1.37
24	N	608	CHL	CHD-C4C	3.35	1.46	1.39
24	G	607	CHL	CHD-C4C	3.35	1.46	1.39
24	1	606	CHL	CHB-C1B	3.35	1.46	1.39
25	8	603	CLA	C4D-ND	-3.35	1.33	1.37
24	g	606	CHL	CHC-C4B	3.35	1.46	1.39
25	4	602	CLA	C4D-ND	-3.35	1.33	1.37
25	2	611	CLA	C1D-ND	3.35	1.41	1.37
25	B	608	CLA	C1D-ND	3.34	1.41	1.37
25	N	610	CLA	C1D-ND	3.34	1.41	1.37
25	N	613	CLA	C1D-ND	3.34	1.41	1.37
25	r	616	CLA	C1D-ND	3.34	1.41	1.37
24	G	608	CHL	CHB-C1B	3.34	1.46	1.39
24	G	605	CHL	CHC-C4B	3.34	1.46	1.39
25	3	613	CLA	C4B-NB	3.34	1.41	1.37
25	g	610	CLA	C1D-ND	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	604	CLA	C4D-ND	-3.34	1.33	1.37
25	s	602	CLA	C1D-ND	3.34	1.41	1.37
25	Y	604	CLA	C4D-ND	-3.34	1.33	1.37
25	p	611	CLA	C4D-ND	-3.34	1.33	1.37
24	1	605	CHL	CHC-C4B	3.34	1.46	1.39
25	c	503	CLA	C1D-ND	3.34	1.41	1.37
25	2	614	CLA	C4B-NB	3.34	1.41	1.37
25	4	603	CLA	C1D-ND	3.34	1.41	1.37
25	R	616	CLA	C1D-ND	3.34	1.41	1.37
24	r	606	CHL	C1B-NB	-3.33	1.33	1.37
25	S	603	CLA	C4D-ND	-3.33	1.33	1.37
24	R	606	CHL	C1B-NB	-3.33	1.33	1.37
25	c	502	CLA	C1D-ND	3.33	1.41	1.37
25	5	612	CLA	C4B-NB	3.33	1.41	1.37
25	9	603	CLA	C1D-ND	3.33	1.41	1.37
24	G	606	CHL	CHC-C4B	3.33	1.46	1.39
24	5	607	CHL	CHB-C1B	3.33	1.46	1.39
25	R	604	CLA	C4D-ND	-3.33	1.33	1.37
24	G	607	CHL	CHC-C4B	3.33	1.46	1.39
24	q	609	CHL	OBD-CAD	3.33	1.28	1.22
25	n	604	CLA	C1D-ND	3.33	1.41	1.37
24	7	606	CHL	OBD-CAD	3.33	1.28	1.22
25	8	613	CLA	C4B-NB	3.33	1.41	1.37
25	G	610	CLA	C1D-ND	3.33	1.41	1.37
25	8	604	CLA	C4B-NB	3.33	1.41	1.37
25	3	610	CLA	C4B-NB	3.32	1.41	1.37
24	6	605	CHL	CHB-C1B	3.32	1.46	1.39
24	g	608	CHL	CHC-C4B	3.32	1.46	1.39
25	6	604	CLA	C4D-ND	-3.32	1.33	1.37
24	4	601	CHL	CHB-C1B	3.32	1.46	1.39
24	G	606	CHL	CHB-C1B	3.32	1.46	1.39
25	6	613	CLA	C4B-NB	3.32	1.41	1.37
25	6	611	CLA	C4D-ND	-3.32	1.33	1.37
25	2	613	CLA	C4B-NB	3.32	1.41	1.37
24	S	608	CHL	CHB-C1B	3.32	1.46	1.39
24	y	605	CHL	CHC-C4B	3.32	1.46	1.39
25	1	613	CLA	C4D-ND	-3.32	1.33	1.37
24	n	608	CHL	CHD-C4C	3.32	1.46	1.39
24	R	608	CHL	CHD-C4C	3.32	1.46	1.39
24	r	608	CHL	CHD-C4C	3.32	1.46	1.39
24	y	601	CHL	CHC-C4B	3.32	1.46	1.39
25	n	613	CLA	C1D-ND	3.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	612	CLA	C4B-NB	3.32	1.41	1.37
25	N	612	CLA	C1D-ND	3.32	1.41	1.37
25	7	612	CLA	C1D-ND	3.31	1.41	1.37
25	q	602	CLA	C4B-NB	3.31	1.41	1.37
25	1	602	CLA	C4D-ND	-3.31	1.33	1.37
25	0	611	CLA	C4D-ND	-3.31	1.33	1.37
25	S	612	CLA	C1D-ND	3.31	1.41	1.37
25	9	611	CLA	C1D-ND	3.31	1.41	1.37
25	r	613	CLA	C1D-ND	3.31	1.41	1.37
24	9	608	CHL	OBD-CAD	3.31	1.28	1.22
24	7	605	CHL	CHC-C4B	3.30	1.46	1.39
24	Y	606	CHL	C4B-NB	-3.30	1.33	1.37
25	1	611	CLA	C1D-ND	3.30	1.41	1.37
25	2	603	CLA	C1D-ND	3.30	1.41	1.37
25	7	602	CLA	C4B-NB	3.30	1.41	1.37
24	Y	601	CHL	CHC-C4B	3.30	1.46	1.39
25	2	610	CLA	C4D-ND	-3.30	1.33	1.37
25	y	604	CLA	C4D-ND	-3.30	1.33	1.37
25	9	613	CLA	C1D-ND	3.30	1.41	1.37
24	g	601	CHL	OBD-CAD	3.30	1.28	1.22
33	a	409	PHO	C4D-ND	-3.30	1.34	1.38
24	g	606	CHL	CHB-C1B	3.30	1.46	1.39
25	C	502	CLA	C1D-ND	3.30	1.41	1.37
25	1	612	CLA	C1D-ND	3.30	1.41	1.37
24	3	607	CHL	CHD-C4C	3.30	1.46	1.39
24	0	607	CHL	CHC-C4B	3.30	1.46	1.39
25	0	604	CLA	C4B-NB	3.30	1.41	1.37
24	G	601	CHL	OBD-CAD	3.29	1.28	1.22
25	2	603	CLA	C4D-ND	-3.29	1.33	1.37
24	N	601	CHL	OBD-CAD	3.29	1.28	1.22
25	5	613	CLA	C4D-ND	-3.29	1.33	1.37
33	A	409	PHO	C4D-ND	-3.29	1.34	1.38
25	9	613	CLA	C4B-NB	3.29	1.41	1.37
24	g	608	CHL	CHB-C1B	3.29	1.46	1.39
25	7	612	CLA	C4D-ND	-3.29	1.33	1.37
25	r	601	CLA	C4D-ND	-3.29	1.33	1.37
24	p	605	CHL	C1D-C2D	3.29	1.51	1.45
24	Y	605	CHL	OBD-CAD	3.29	1.28	1.22
24	y	605	CHL	OBD-CAD	3.29	1.28	1.22
25	7	610	CLA	C1D-ND	3.29	1.41	1.37
25	b	602	CLA	C1D-ND	3.29	1.41	1.37
24	q	609	CHL	C1D-C2D	3.28	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	607	CHL	C1B-NB	-3.28	1.33	1.37
25	8	611	CLA	C4B-NB	3.28	1.41	1.37
24	9	609	CHL	CHB-C1B	3.28	1.46	1.39
24	N	605	CHL	C1B-NB	-3.28	1.33	1.37
24	Y	605	CHL	CHC-C4B	3.28	1.46	1.39
24	6	601	CHL	CHC-C4B	3.28	1.46	1.39
24	y	606	CHL	C1B-NB	-3.28	1.33	1.37
25	s	603	CLA	C4D-ND	-3.28	1.33	1.37
24	7	607	CHL	CHB-C1B	3.28	1.46	1.39
24	g	609	CHL	CHB-C1B	3.28	1.46	1.39
25	r	616	CLA	C4B-NB	3.28	1.41	1.37
24	G	609	CHL	C4B-NB	-3.28	1.33	1.37
24	N	606	CHL	C1B-NB	-3.28	1.33	1.37
24	p	601	CHL	CHC-C4B	3.28	1.46	1.39
25	C	508	CLA	CMC-C2C	-3.27	1.43	1.50
24	n	605	CHL	C4B-NB	-3.27	1.33	1.37
25	G	604	CLA	C1D-ND	3.27	1.41	1.37
24	0	609	CHL	CHB-C1B	3.27	1.46	1.39
25	4	602	CLA	C4B-NB	3.27	1.41	1.37
24	n	601	CHL	OBD-CAD	3.27	1.28	1.22
25	r	612	CLA	C4D-ND	-3.27	1.33	1.37
24	R	608	CHL	OBD-CAD	3.27	1.28	1.22
24	7	608	CHL	OBD-CAD	3.27	1.28	1.22
25	7	611	CLA	C1D-ND	3.27	1.41	1.37
25	4	613	CLA	C4D-ND	-3.27	1.33	1.37
24	3	601	CHL	CHB-C1B	3.27	1.46	1.39
25	1	614	CLA	C4B-NB	3.27	1.41	1.37
24	0	605	CHL	CHB-C1B	3.27	1.46	1.39
25	4	611	CLA	C4D-ND	-3.27	1.33	1.37
25	7	602	CLA	C4D-ND	-3.27	1.33	1.37
24	N	608	CHL	CHB-C1B	3.27	1.46	1.39
24	r	608	CHL	CHB-C1B	3.27	1.46	1.39
24	q	608	CHL	MG-NA	-3.27	1.98	2.06
25	n	612	CLA	C4D-ND	-3.27	1.33	1.37
24	N	601	CHL	C4B-NB	-3.26	1.33	1.37
24	G	609	CHL	CHB-C1B	3.26	1.46	1.39
24	q	601	CHL	OBD-CAD	3.26	1.28	1.22
25	2	603	CLA	C4B-NB	3.26	1.41	1.37
25	G	614	CLA	C1D-ND	3.26	1.41	1.37
25	8	612	CLA	C4B-NB	3.26	1.41	1.37
24	0	609	CHL	CHC-C4B	3.26	1.46	1.39
25	9	603	CLA	C4B-NB	3.26	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	614	CLA	C4D-ND	-3.26	1.33	1.37
25	q	613	CLA	C4D-ND	-3.26	1.33	1.37
25	2	614	CLA	C4D-ND	-3.26	1.33	1.37
24	g	609	CHL	C4B-NB	-3.26	1.33	1.37
25	s	612	CLA	C1D-ND	3.26	1.41	1.37
24	Y	606	CHL	C1B-NB	-3.26	1.33	1.37
25	2	613	CLA	C1D-ND	3.25	1.41	1.37
25	R	601	CLA	C4D-ND	-3.25	1.33	1.37
24	4	609	CHL	C1B-NB	-3.25	1.33	1.37
25	7	604	CLA	C1D-ND	3.25	1.41	1.37
25	6	613	CLA	C4D-ND	-3.25	1.33	1.37
25	N	612	CLA	C4D-ND	-3.25	1.33	1.37
25	1	602	CLA	C4B-NB	3.25	1.41	1.37
25	0	604	CLA	C1D-ND	3.25	1.41	1.37
24	r	608	CHL	OBD-CAD	3.25	1.28	1.22
24	5	601	CHL	CHC-C4B	3.25	1.46	1.39
24	Y	606	CHL	CHC-C4B	3.25	1.46	1.39
25	n	612	CLA	C4B-NB	3.25	1.41	1.37
24	5	606	CHL	OBD-CAD	3.24	1.28	1.22
24	0	609	CHL	C1B-NB	-3.24	1.33	1.37
24	1	609	CHL	CHB-C1B	3.24	1.46	1.39
25	1	612	CLA	C4D-ND	-3.24	1.33	1.37
25	B	602	CLA	C1D-ND	3.24	1.41	1.37
25	q	611	CLA	C4D-ND	-3.24	1.33	1.37
24	y	609	CHL	CHD-C1D	3.24	1.44	1.38
25	B	612	CLA	CMC-C2C	-3.24	1.43	1.50
25	b	612	CLA	CMC-C2C	-3.24	1.43	1.50
25	9	611	CLA	C4D-ND	-3.24	1.33	1.37
25	3	602	CLA	C4B-NB	3.24	1.41	1.37
24	9	608	CHL	CHB-C1B	3.24	1.46	1.39
24	y	606	CHL	C4B-NB	-3.24	1.33	1.37
25	0	612	CLA	C4B-NB	3.24	1.41	1.37
24	S	606	CHL	CHC-C4B	3.24	1.46	1.39
25	7	613	CLA	C4D-ND	-3.23	1.33	1.37
24	Y	609	CHL	CHD-C1D	3.23	1.44	1.38
24	3	606	CHL	MG-NA	-3.23	1.98	2.06
25	g	614	CLA	C1D-ND	3.23	1.41	1.37
25	c	509	CLA	C1D-ND	3.23	1.41	1.37
24	6	609	CHL	CHC-C4B	3.23	1.46	1.39
24	0	601	CHL	CHB-C1B	3.23	1.46	1.39
25	c	508	CLA	CMC-C2C	-3.23	1.44	1.50
24	6	608	CHL	CHB-C1B	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	606	CHL	OBD-CAD	3.23	1.28	1.22
24	y	606	CHL	CHC-C4B	3.23	1.46	1.39
25	3	612	CLA	C4B-NB	3.23	1.41	1.37
24	2	608	CHL	CHB-C1B	3.23	1.46	1.39
24	7	609	CHL	CHC-C4B	3.23	1.46	1.39
25	6	612	CLA	C4B-NB	3.23	1.41	1.37
24	N	608	CHL	CHC-C4B	3.23	1.46	1.39
24	n	601	CHL	C1B-NB	-3.23	1.33	1.37
25	8	611	CLA	C4D-ND	-3.23	1.33	1.37
24	p	607	CHL	CHB-C1B	3.23	1.46	1.39
28	7	1623	NEX	C7-C8	-3.23	1.26	1.32
25	2	604	CLA	C4B-NB	3.22	1.41	1.37
25	R	616	CLA	C4B-NB	3.22	1.41	1.37
25	9	604	CLA	C4B-NB	3.22	1.41	1.37
25	p	613	CLA	C4D-ND	-3.22	1.33	1.37
24	p	608	CHL	CHB-C1B	3.22	1.46	1.39
25	0	610	CLA	C4B-NB	3.22	1.41	1.37
24	1	607	CHL	CHB-C1B	3.22	1.46	1.39
24	0	608	CHL	CHB-C1B	3.22	1.46	1.39
24	n	608	CHL	CHB-C1B	3.22	1.46	1.39
25	4	604	CLA	C4D-ND	-3.22	1.33	1.37
24	G	601	CHL	C1B-NB	-3.22	1.33	1.37
24	R	608	CHL	CHB-C1B	3.22	1.46	1.39
25	R	602	CLA	C1D-ND	3.22	1.41	1.37
25	8	602	CLA	C4B-NB	3.22	1.41	1.37
25	b	617	CLA	C1D-ND	3.22	1.41	1.37
24	N	606	CHL	CHD-C4C	3.22	1.46	1.39
25	5	604	CLA	C4B-NB	3.22	1.41	1.37
24	y	607	CHL	C1B-NB	-3.22	1.33	1.37
24	7	608	CHL	CHB-C1B	3.21	1.46	1.39
24	G	609	CHL	MG-NA	-3.21	1.98	2.06
24	7	608	CHL	CHC-C4B	3.21	1.46	1.39
24	8	609	CHL	CHC-C4B	3.21	1.46	1.39
24	n	607	CHL	CHD-C4C	3.21	1.46	1.39
25	6	603	CLA	C4D-ND	-3.21	1.33	1.37
25	R	612	CLA	C4D-ND	-3.21	1.33	1.37
25	0	602	CLA	C4D-ND	-3.21	1.33	1.37
24	s	601	CHL	OBD-CAD	3.21	1.28	1.22
24	Y	607	CHL	CHD-C4C	3.21	1.46	1.39
24	6	607	CHL	CHB-C1B	3.20	1.46	1.39
24	r	608	CHL	C1B-NB	-3.20	1.33	1.37
24	y	608	CHL	CHB-C1B	3.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	606	CHL	CHD-C4C	3.20	1.46	1.39
25	4	610	CLA	C4D-ND	-3.20	1.33	1.37
24	7	609	CHL	CHB-C1B	3.20	1.46	1.39
25	q	602	CLA	C4D-ND	-3.20	1.33	1.37
25	R	604	CLA	C4B-NB	3.20	1.41	1.37
25	r	611	CLA	C4B-NB	3.20	1.41	1.37
24	n	605	CHL	C1B-NB	-3.20	1.33	1.37
24	N	607	CHL	CHD-C4C	3.20	1.46	1.39
24	R	607	CHL	CHD-C4C	3.20	1.46	1.39
24	N	607	CHL	C1B-NB	-3.20	1.33	1.37
25	9	604	CLA	C4D-ND	-3.19	1.33	1.37
25	R	616	CLA	C4D-ND	-3.19	1.33	1.37
25	2	610	CLA	C4B-NB	3.19	1.41	1.37
25	6	610	CLA	C4B-NB	3.19	1.41	1.37
25	N	612	CLA	C4B-NB	3.19	1.41	1.37
25	Y	614	CLA	C1D-ND	3.19	1.41	1.37
24	s	606	CHL	CHC-C4B	3.19	1.46	1.39
25	1	610	CLA	C1D-ND	3.19	1.41	1.37
24	8	606	CHL	MG-NA	-3.19	1.98	2.06
24	9	601	CHL	C4B-NB	-3.19	1.33	1.37
25	q	613	CLA	C4B-NB	3.19	1.41	1.37
25	S	604	CLA	C1D-ND	3.19	1.41	1.37
24	n	606	CHL	C1B-NB	-3.19	1.33	1.37
25	s	604	CLA	C1D-ND	3.19	1.41	1.37
25	3	611	CLA	C4D-ND	-3.19	1.33	1.37
24	Y	608	CHL	CHB-C1B	3.19	1.46	1.39
24	1	608	CHL	CHB-C1B	3.19	1.46	1.39
25	0	610	CLA	C1D-ND	3.19	1.41	1.37
25	r	604	CLA	C1D-ND	3.19	1.41	1.37
25	r	604	CLA	C4B-NB	3.19	1.41	1.37
24	1	609	CHL	CHC-C4B	3.19	1.46	1.39
25	C	509	CLA	C1D-ND	3.19	1.41	1.37
25	r	602	CLA	C1D-ND	3.19	1.41	1.37
25	6	602	CLA	C4D-ND	-3.18	1.33	1.37
25	8	613	CLA	C4D-ND	-3.18	1.33	1.37
25	n	613	CLA	C4B-NB	3.18	1.41	1.37
24	r	607	CHL	CHD-C4C	3.18	1.46	1.39
25	B	617	CLA	C1D-ND	3.18	1.41	1.37
25	r	616	CLA	C4D-ND	-3.18	1.33	1.37
25	3	602	CLA	C1D-ND	3.18	1.41	1.37
24	S	601	CHL	OBD-CAD	3.18	1.28	1.22
25	0	610	CLA	C4D-ND	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	CHC-C4B	3.18	1.46	1.39
25	S	612	CLA	C4B-NB	3.18	1.41	1.37
25	c	502	CLA	CMB-C2B	-3.18	1.44	1.50
24	Y	601	CHL	OBD-CAD	3.18	1.28	1.22
25	0	603	CLA	C4D-ND	-3.18	1.33	1.37
25	9	610	CLA	C4D-ND	-3.18	1.33	1.37
25	8	602	CLA	C1D-ND	3.17	1.41	1.37
33	A	408	PHO	C4D-ND	-3.17	1.34	1.38
33	a	408	PHO	C4D-ND	-3.17	1.34	1.38
25	2	604	CLA	C4D-ND	-3.17	1.33	1.37
24	5	608	CHL	CHB-C1B	3.17	1.46	1.39
24	8	601	CHL	CHB-C1B	3.17	1.46	1.39
25	n	610	CLA	C4D-ND	-3.17	1.33	1.37
24	2	608	CHL	OBD-CAD	3.17	1.27	1.22
24	2	609	CHL	CHB-C1B	3.17	1.46	1.39
25	c	506	CLA	C4B-NB	3.16	1.41	1.37
35	b	621	SQD	C6-S	-3.16	1.65	1.77
24	g	601	CHL	C1B-NB	-3.16	1.33	1.37
25	p	610	CLA	C4D-ND	-3.16	1.33	1.37
25	6	603	CLA	C1D-ND	3.16	1.41	1.37
25	q	603	CLA	C4B-NB	3.16	1.41	1.37
28	s	1623	NEX	C7-C8	-3.16	1.26	1.32
25	n	611	CLA	C1D-ND	3.16	1.41	1.37
24	y	607	CHL	CHD-C4C	3.16	1.46	1.39
24	n	608	CHL	OBD-CAD	3.16	1.27	1.22
24	N	608	CHL	OBD-CAD	3.16	1.27	1.22
24	y	601	CHL	OBD-CAD	3.16	1.27	1.22
24	n	607	CHL	C1B-NB	-3.16	1.33	1.37
35	B	621	SQD	C6-S	-3.15	1.65	1.77
25	s	613	CLA	C1D-ND	3.15	1.41	1.37
24	8	609	CHL	CHD-C4C	3.15	1.46	1.39
24	9	609	CHL	C1D-C2D	3.15	1.51	1.45
24	g	609	CHL	MG-NA	-3.15	1.98	2.06
25	S	605	CLA	C1D-ND	3.15	1.41	1.37
24	q	605	CHL	C1D-C2D	3.15	1.51	1.45
25	3	613	CLA	C4D-ND	-3.15	1.33	1.37
24	R	606	CHL	C2C-C3C	3.15	1.43	1.36
24	0	608	CHL	OBD-CAD	3.15	1.27	1.22
25	C	502	CLA	CMB-C2B	-3.15	1.44	1.50
25	R	612	CLA	C1D-ND	3.15	1.41	1.37
25	r	612	CLA	C1D-ND	3.15	1.41	1.37
25	s	611	CLA	C1D-ND	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	607	CHL	MG-NA	-3.15	1.98	2.06
24	g	607	CHL	CHB-C1B	3.14	1.46	1.39
24	Y	607	CHL	C4B-NB	-3.14	1.33	1.37
24	7	606	CHL	C1B-NB	-3.14	1.33	1.37
25	4	614	CLA	C4B-NB	3.14	1.41	1.37
25	R	611	CLA	C4B-NB	3.14	1.41	1.37
25	7	603	CLA	C4B-NB	3.14	1.41	1.37
25	9	610	CLA	C4B-NB	3.14	1.41	1.37
24	S	607	CHL	MG-NA	-3.14	1.98	2.06
25	0	603	CLA	C1D-ND	3.14	1.41	1.37
24	1	609	CHL	OBD-CAD	3.14	1.27	1.22
24	0	607	CHL	CHB-C1B	3.14	1.46	1.39
25	3	610	CLA	C4D-ND	-3.14	1.33	1.37
25	8	612	CLA	C4D-ND	-3.14	1.33	1.37
25	q	610	CLA	C4D-ND	-3.14	1.33	1.37
25	N	611	CLA	C1D-ND	3.14	1.41	1.37
25	N	613	CLA	C4B-NB	3.14	1.41	1.37
24	G	608	CHL	C1B-NB	-3.13	1.33	1.37
25	R	604	CLA	C1D-ND	3.13	1.41	1.37
24	y	606	CHL	CHD-C4C	3.13	1.46	1.39
24	y	608	CHL	OBD-CAD	3.13	1.27	1.22
25	2	611	CLA	C4B-NB	3.13	1.41	1.37
25	6	602	CLA	C4B-NB	3.13	1.41	1.37
25	r	610	CLA	C1D-ND	3.13	1.41	1.37
24	q	607	CHL	MG-NA	-3.13	1.98	2.06
25	C	512	CLA	C1D-ND	3.13	1.41	1.37
24	1	601	CHL	CHC-C4B	3.13	1.46	1.39
35	d	413	SQD	C6-S	-3.13	1.65	1.77
24	N	605	CHL	C4B-NB	-3.13	1.33	1.37
25	s	605	CLA	C1D-ND	3.13	1.41	1.37
25	y	614	CLA	C1D-ND	3.13	1.41	1.37
24	5	605	CHL	C1D-C2D	3.13	1.51	1.45
25	C	506	CLA	C4B-NB	3.13	1.41	1.37
25	S	611	CLA	C1D-ND	3.13	1.41	1.37
25	r	609	CLA	C4B-NB	3.13	1.41	1.37
24	r	606	CHL	C2C-C3C	3.13	1.43	1.36
24	G	601	CHL	CHC-C4B	3.13	1.46	1.39
24	7	609	CHL	OBD-CAD	3.13	1.27	1.22
24	n	601	CHL	C4B-NB	-3.13	1.33	1.37
25	0	613	CLA	C4B-NB	3.12	1.41	1.37
24	Y	606	CHL	CHD-C4C	3.12	1.46	1.39
25	0	614	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	610	CLA	C4D-ND	-3.12	1.33	1.37
25	3	612	CLA	C4D-ND	-3.12	1.33	1.37
24	y	607	CHL	C4B-NB	-3.12	1.33	1.37
24	Y	608	CHL	CHD-C4C	3.12	1.46	1.39
25	6	610	CLA	C4D-ND	-3.12	1.33	1.37
25	p	603	CLA	C4D-ND	-3.12	1.33	1.37
25	S	613	CLA	C1D-ND	3.12	1.41	1.37
24	Y	608	CHL	OBD-CAD	3.12	1.27	1.22
33	a	408	PHO	CMC-C2C	-3.12	1.45	1.50
24	5	609	CHL	CHC-C4B	3.12	1.46	1.39
25	7	612	CLA	C4B-NB	3.12	1.41	1.37
24	4	607	CHL	MG-NA	-3.11	1.98	2.06
25	4	613	CLA	C4B-NB	3.11	1.41	1.37
25	q	614	CLA	C4B-NB	3.11	1.41	1.37
24	2	601	CHL	OBD-CAD	3.11	1.27	1.22
25	N	610	CLA	C4D-ND	-3.11	1.33	1.37
24	y	608	CHL	CHD-C4C	3.11	1.46	1.39
25	5	602	CLA	C4D-ND	-3.11	1.33	1.37
25	q	604	CLA	C4D-ND	-3.11	1.33	1.37
24	6	609	CHL	CHB-C1B	3.11	1.46	1.39
24	G	607	CHL	CHB-C1B	3.11	1.46	1.39
25	7	614	CLA	C4D-ND	-3.11	1.33	1.37
35	D	413	SQD	C6-S	-3.11	1.65	1.77
24	7	601	CHL	CHC-C4B	3.10	1.46	1.39
25	b	613	CLA	C1D-ND	3.10	1.41	1.37
25	y	604	CLA	CMB-C2B	-3.10	1.44	1.50
24	g	601	CHL	CHC-C4B	3.10	1.46	1.39
24	6	609	CHL	C4B-NB	-3.10	1.34	1.37
25	6	610	CLA	C1D-ND	3.10	1.41	1.37
24	8	601	CHL	CHC-C4B	3.10	1.46	1.39
24	4	605	CHL	C1D-C2D	3.10	1.51	1.45
25	6	614	CLA	C4D-ND	-3.10	1.33	1.37
24	8	605	CHL	MG-NA	-3.10	1.98	2.06
24	3	609	CHL	CHD-C4C	3.10	1.46	1.39
25	4	603	CLA	C4D-ND	-3.10	1.33	1.37
24	N	601	CHL	C1B-NB	-3.10	1.34	1.37
24	R	606	CHL	CHC-C4B	3.10	1.46	1.39
24	1	606	CHL	C1B-NB	-3.10	1.34	1.37
24	6	601	CHL	CHB-C1B	3.10	1.46	1.39
24	2	601	CHL	C1B-NB	-3.10	1.34	1.37
24	R	608	CHL	C1B-NB	-3.10	1.34	1.37
25	R	609	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	602	CLA	C4B-NB	3.10	1.41	1.37
25	S	613	CLA	C4B-NB	3.09	1.41	1.37
25	s	613	CLA	C4B-NB	3.09	1.41	1.37
24	r	606	CHL	CHC-C4B	3.09	1.46	1.39
25	g	613	CLA	C1D-ND	3.09	1.41	1.37
25	p	604	CLA	C4D-ND	-3.09	1.33	1.37
24	q	601	CHL	CHB-C1B	3.09	1.46	1.39
24	n	609	CHL	MG-NA	-3.09	1.98	2.06
24	y	601	CHL	C1B-NB	-3.09	1.34	1.37
25	B	616	CLA	C1D-ND	3.09	1.41	1.37
24	3	609	CHL	CHC-C4B	3.09	1.46	1.39
24	N	605	CHL	MG-NA	-3.09	1.98	2.06
25	1	603	CLA	C4B-NB	3.09	1.41	1.37
24	p	609	CHL	CHC-C4B	3.09	1.46	1.39
25	Y	604	CLA	C4B-NB	3.09	1.41	1.37
40	f	101	HEM	CAC-C3C	3.09	1.55	1.47
25	5	603	CLA	C4D-ND	-3.09	1.33	1.37
24	n	605	CHL	CHC-C4B	3.09	1.46	1.39
25	N	614	CLA	C4B-NB	3.09	1.41	1.37
24	9	601	CHL	C1B-NB	-3.09	1.34	1.37
25	Y	610	CLA	C1D-ND	3.09	1.41	1.37
24	G	606	CHL	OBD-CAD	3.09	1.27	1.22
25	9	611	CLA	C4B-NB	3.08	1.41	1.37
24	N	605	CHL	CHC-C4B	3.08	1.46	1.39
24	2	609	CHL	C1D-C2D	3.08	1.51	1.45
25	Y	604	CLA	CMB-C2B	-3.08	1.44	1.50
24	3	607	CHL	C1B-NB	-3.08	1.34	1.37
25	4	610	CLA	C4B-NB	3.08	1.41	1.37
24	7	608	CHL	CHD-C4C	3.08	1.46	1.39
24	6	609	CHL	C1B-NB	-3.08	1.34	1.37
25	s	612	CLA	C4B-NB	3.08	1.41	1.37
33	A	408	PHO	CMC-C2C	-3.08	1.45	1.50
24	Y	609	CHL	CHD-C4C	3.08	1.46	1.39
25	q	614	CLA	C4D-ND	-3.08	1.33	1.37
25	S	610	CLA	C1D-ND	3.08	1.41	1.37
25	1	614	CLA	C4D-ND	-3.08	1.33	1.37
24	9	601	CHL	OBD-CAD	3.08	1.27	1.22
25	5	610	CLA	C4D-ND	-3.08	1.33	1.37
24	1	608	CHL	CHD-C4C	3.08	1.46	1.39
25	R	609	CLA	C1D-ND	3.07	1.41	1.37
25	r	609	CLA	C1D-ND	3.07	1.41	1.37
25	B	607	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	611	CLA	C4B-NB	3.07	1.41	1.37
25	n	604	CLA	C4B-NB	3.07	1.41	1.37
24	8	608	CHL	CHB-C1B	3.07	1.46	1.39
25	6	612	CLA	C4D-ND	-3.07	1.33	1.37
24	3	605	CHL	MG-NA	-3.07	1.99	2.06
25	4	614	CLA	C4D-ND	-3.07	1.33	1.37
24	n	607	CHL	OBD-CAD	3.07	1.27	1.22
25	4	603	CLA	C4B-NB	3.06	1.41	1.37
25	R	610	CLA	C1D-ND	3.06	1.41	1.37
24	g	601	CHL	C4B-NB	-3.06	1.34	1.37
24	y	607	CHL	OBD-CAD	3.06	1.27	1.22
24	N	607	CHL	OBD-CAD	3.06	1.27	1.22
25	1	611	CLA	C4B-NB	3.06	1.41	1.37
39	d	405	PL9	C53-C6	-3.06	1.44	1.50
39	D	405	PL9	C53-C6	-3.06	1.44	1.50
28	N	1623	NEX	C7-C8	-3.05	1.26	1.32
24	y	608	CHL	C1B-NB	-3.05	1.34	1.37
24	2	609	CHL	CHC-C4B	3.05	1.46	1.39
24	Y	607	CHL	OBD-CAD	3.05	1.27	1.22
25	s	610	CLA	C1D-ND	3.05	1.41	1.37
24	N	609	CHL	MG-NA	-3.05	1.99	2.06
24	S	607	CHL	C1B-NB	-3.05	1.34	1.37
25	b	611	CLA	C1D-ND	3.05	1.41	1.37
25	d	403	CLA	C1D-ND	3.05	1.41	1.37
24	R	607	CHL	CHC-C4B	3.05	1.46	1.39
25	B	607	CLA	C1D-ND	3.05	1.41	1.37
24	3	608	CHL	CHB-C1B	3.05	1.46	1.39
24	r	607	CHL	CHC-C4B	3.05	1.46	1.39
25	n	614	CLA	C4B-NB	3.05	1.41	1.37
24	g	608	CHL	C1B-NB	-3.04	1.34	1.37
24	0	601	CHL	MG-NA	-3.04	1.99	2.06
25	c	512	CLA	C1D-ND	3.04	1.41	1.37
24	8	607	CHL	C1B-NB	-3.04	1.34	1.37
25	G	613	CLA	C1D-ND	3.04	1.41	1.37
24	y	609	CHL	CHD-C4C	3.04	1.46	1.39
24	s	607	CHL	C1B-NB	-3.04	1.34	1.37
25	B	613	CLA	C1D-ND	3.04	1.41	1.37
33	A	408	PHO	C1D-C2D	3.04	1.43	1.39
24	n	605	CHL	MG-NA	-3.04	1.99	2.06
25	B	611	CLA	C1D-ND	3.04	1.41	1.37
25	y	604	CLA	C4B-NB	3.04	1.41	1.37
24	G	601	CHL	C4B-NB	-3.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	606	CHL	C4B-NB	-3.03	1.34	1.37
25	S	602	CLA	C4B-NB	3.03	1.41	1.37
25	0	612	CLA	C4D-ND	-3.03	1.33	1.37
39	D	405	PL9	C41-C39	-3.03	1.45	1.51
25	7	611	CLA	C4B-NB	3.03	1.41	1.37
24	R	607	CHL	MG-NA	-3.03	1.99	2.06
25	b	607	CLA	C4B-NB	3.03	1.41	1.37
24	1	607	CHL	MG-NA	-3.03	1.99	2.06
25	q	610	CLA	C4B-NB	3.03	1.41	1.37
24	q	601	CHL	C4B-NB	-3.02	1.34	1.37
24	8	606	CHL	C4B-NB	-3.02	1.34	1.37
39	d	405	PL9	C41-C39	-3.02	1.45	1.51
24	R	606	CHL	C4B-NB	-3.02	1.34	1.37
25	y	610	CLA	C1D-ND	3.02	1.41	1.37
24	4	609	CHL	C3D-C2D	3.02	1.47	1.39
25	9	610	CLA	C3B-C4B	3.02	1.49	1.42
25	6	611	CLA	C4B-NB	3.02	1.41	1.37
24	r	607	CHL	MG-NA	-3.02	1.99	2.06
24	Y	601	CHL	C1B-NB	-3.02	1.34	1.37
24	9	609	CHL	C4B-NB	-3.02	1.34	1.37
25	1	602	CLA	C1D-ND	3.02	1.41	1.37
25	B	605	CLA	C4B-NB	3.02	1.41	1.37
40	F	101	HEM	CAC-C3C	3.01	1.55	1.47
25	q	603	CLA	C4D-ND	-3.01	1.33	1.37
25	8	614	CLA	C4D-ND	-3.01	1.33	1.37
24	Y	608	CHL	C1B-NB	-3.01	1.34	1.37
24	g	606	CHL	OBD-CAD	3.01	1.27	1.22
25	1	612	CLA	C4B-NB	3.01	1.41	1.37
24	3	605	CHL	C1D-C2D	3.01	1.51	1.45
25	N	604	CLA	C4B-NB	3.01	1.41	1.37
25	y	602	CLA	C1D-ND	3.01	1.41	1.37
25	c	507	CLA	C1D-ND	3.00	1.41	1.37
24	8	605	CHL	C1D-C2D	3.00	1.51	1.45
28	4	1623	NEX	C7-C8	-3.00	1.27	1.32
33	a	408	PHO	C1D-C2D	3.00	1.42	1.39
25	C	507	CLA	C1D-ND	3.00	1.41	1.37
24	8	609	CHL	CHB-C1B	3.00	1.46	1.39
25	b	616	CLA	C1D-ND	3.00	1.41	1.37
24	R	608	CHL	CHC-C4B	2.99	1.46	1.39
25	p	602	CLA	C4D-ND	-2.99	1.33	1.37
24	1	601	CHL	C1D-C2D	2.99	1.51	1.45
25	R	602	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	606	CHL	CHB-C1B	2.99	1.46	1.39
24	5	609	CHL	C1D-C2D	2.99	1.51	1.45
25	6	603	CLA	C4B-NB	2.99	1.41	1.37
24	G	609	CHL	OBD-CAD	2.99	1.27	1.22
25	0	611	CLA	C3B-C4B	2.99	1.49	1.42
25	g	614	CLA	C4B-NB	2.99	1.41	1.37
24	R	608	CHL	MG-NA	-2.99	1.99	2.06
25	G	602	CLA	C1D-ND	2.99	1.41	1.37
25	Y	602	CLA	C1D-ND	2.99	1.41	1.37
24	q	609	CHL	C3D-C2D	2.99	1.47	1.39
24	3	601	CHL	CHC-C4B	2.99	1.46	1.39
24	p	609	CHL	C1D-C2D	2.99	1.51	1.45
25	3	603	CLA	C4B-NB	2.99	1.41	1.37
25	2	610	CLA	C3B-C4B	2.99	1.49	1.42
25	g	611	CLA	C4B-NB	2.99	1.41	1.37
25	s	602	CLA	C4B-NB	2.99	1.41	1.37
25	y	613	CLA	C4B-NB	2.99	1.41	1.37
25	R	611	CLA	C1D-ND	2.98	1.41	1.37
24	r	608	CHL	CHC-C4B	2.98	1.46	1.39
24	4	609	CHL	C1D-C2D	2.98	1.51	1.45
25	b	605	CLA	C1D-ND	2.98	1.41	1.37
25	g	604	CLA	C4B-NB	2.98	1.41	1.37
25	D	403	CLA	C1D-ND	2.98	1.41	1.37
25	a	405	CLA	C1D-ND	2.98	1.41	1.37
25	G	604	CLA	C4B-NB	2.98	1.41	1.37
25	7	602	CLA	C1D-ND	2.98	1.41	1.37
24	2	601	CHL	CHC-C4B	2.98	1.46	1.39
24	7	609	CHL	C4B-NB	-2.98	1.34	1.37
24	5	601	CHL	CHB-C1B	2.98	1.46	1.39
24	7	601	CHL	C1D-C2D	2.98	1.51	1.45
25	C	504	CLA	C4B-NB	2.98	1.41	1.37
25	c	504	CLA	C4B-NB	2.98	1.41	1.37
25	c	504	CLA	C1D-ND	2.98	1.41	1.37
25	5	604	CLA	C4D-ND	-2.98	1.33	1.37
24	y	606	CHL	CHB-C1B	2.97	1.46	1.39
24	Y	606	CHL	CHB-C1B	2.97	1.46	1.39
24	3	606	CHL	C4B-NB	-2.97	1.34	1.37
40	f	101	HEM	CAB-C3B	2.97	1.55	1.47
25	G	612	CLA	C1D-ND	2.97	1.41	1.37
39	D	405	PL9	C21-C19	-2.97	1.45	1.51
25	r	602	CLA	C4B-NB	2.97	1.41	1.37
24	7	607	CHL	MG-NA	-2.97	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	606	CHL	MG-NA	-2.97	1.99	2.06
24	n	606	CHL	CHB-C1B	2.97	1.46	1.39
25	A	405	CLA	C1D-ND	2.97	1.41	1.37
25	r	612	CLA	C4B-NB	2.97	1.41	1.37
24	r	608	CHL	MG-NA	-2.97	1.99	2.06
24	p	601	CHL	CHB-C1B	2.97	1.46	1.39
25	0	603	CLA	C4B-NB	2.96	1.41	1.37
39	d	405	PL9	C21-C19	-2.96	1.45	1.51
25	A	410	CLA	C1D-ND	2.96	1.41	1.37
25	G	612	CLA	C4B-NB	2.96	1.41	1.37
25	g	612	CLA	C4B-NB	2.96	1.41	1.37
39	D	405	PL9	C52-C5	-2.96	1.44	1.50
28	0	1623	NEX	C7-C8	-2.96	1.27	1.32
24	1	606	CHL	MG-NA	-2.96	1.99	2.06
25	3	614	CLA	C4D-ND	-2.96	1.33	1.37
25	B	606	CLA	C1D-ND	2.96	1.41	1.37
24	q	609	CHL	C4B-NB	-2.96	1.34	1.37
24	6	608	CHL	OBD-CAD	2.96	1.27	1.22
33	a	409	PHO	CMC-C2C	-2.96	1.45	1.50
24	9	609	CHL	CHC-C4B	2.96	1.46	1.39
25	2	602	CLA	C1D-ND	2.96	1.41	1.37
25	b	605	CLA	C4B-NB	2.96	1.41	1.37
24	3	606	CHL	C1D-C2D	2.96	1.51	1.45
25	N	603	CLA	C1D-ND	2.95	1.41	1.37
25	q	602	CLA	C3B-C4B	2.95	1.49	1.42
25	S	603	CLA	C4B-NB	2.95	1.41	1.37
24	n	601	CHL	CHC-C4B	2.95	1.46	1.39
25	C	504	CLA	C1D-ND	2.95	1.41	1.37
25	6	611	CLA	C3B-C4B	2.95	1.49	1.42
24	n	607	CHL	MG-NA	-2.95	1.99	2.06
25	0	611	CLA	C4B-NB	2.95	1.41	1.37
28	q	1623	NEX	C7-C8	-2.95	1.27	1.32
24	1	601	CHL	C4B-NB	-2.95	1.34	1.37
24	8	606	CHL	C1D-C2D	2.95	1.51	1.45
24	9	601	CHL	CHC-C4B	2.95	1.46	1.39
24	q	608	CHL	C1B-NB	-2.94	1.34	1.37
39	d	405	PL9	C52-C5	-2.94	1.44	1.50
25	B	605	CLA	C1D-ND	2.94	1.41	1.37
24	q	606	CHL	C3D-C2D	2.94	1.47	1.39
25	S	609	CLA	C4D-ND	-2.94	1.33	1.37
24	g	609	CHL	OBD-CAD	2.94	1.27	1.22
25	a	410	CLA	C1D-ND	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	611	CLA	C4B-NB	2.94	1.41	1.37
40	F	101	HEM	CAB-C3B	2.94	1.55	1.47
24	r	607	CHL	OBD-CAD	2.94	1.27	1.22
25	c	506	CLA	C1D-ND	2.94	1.41	1.37
25	2	602	CLA	C4B-NB	2.94	1.41	1.37
24	g	608	CHL	MG-NA	-2.93	1.99	2.06
25	G	613	CLA	C4B-NB	2.93	1.41	1.37
25	8	603	CLA	C4B-NB	2.93	1.41	1.37
25	b	607	CLA	C1D-ND	2.93	1.41	1.37
24	3	609	CHL	CHB-C1B	2.93	1.46	1.39
25	c	510	CLA	C1D-ND	2.93	1.41	1.37
25	n	603	CLA	C1D-ND	2.93	1.41	1.37
25	4	610	CLA	C3B-C4B	2.93	1.49	1.42
25	s	603	CLA	C4B-NB	2.93	1.41	1.37
25	C	505	CLA	CMD-C2D	-2.93	1.44	1.50
25	5	611	CLA	C3B-C4B	2.93	1.49	1.42
24	q	608	CHL	C3D-C2D	2.93	1.47	1.39
25	5	612	CLA	C4D-ND	-2.93	1.33	1.37
33	A	409	PHO	CMC-C2C	-2.93	1.45	1.50
24	7	601	CHL	C4B-NB	-2.93	1.34	1.37
25	b	606	CLA	C1D-ND	2.93	1.41	1.37
25	n	604	CLA	CMB-C2B	-2.93	1.44	1.50
25	c	505	CLA	CMD-C2D	-2.93	1.44	1.50
33	A	408	PHO	C4D-CHA	2.93	1.44	1.39
24	s	608	CHL	C1B-NB	-2.93	1.34	1.37
28	2	1623	NEX	C7-C8	-2.93	1.27	1.32
24	N	601	CHL	CHB-C1B	2.93	1.46	1.39
25	N	610	CLA	C4B-NB	2.93	1.41	1.37
24	1	609	CHL	C4B-NB	-2.93	1.34	1.37
25	N	604	CLA	CMB-C2B	-2.92	1.44	1.50
24	n	609	CHL	OBD-CAD	2.92	1.27	1.22
24	N	607	CHL	C4B-NB	-2.92	1.34	1.37
25	7	613	CLA	C4B-NB	2.92	1.41	1.37
25	r	613	CLA	C4B-NB	2.92	1.41	1.37
33	a	409	PHO	CMD-C2D	-2.92	1.45	1.51
24	g	607	CHL	C4B-NB	-2.92	1.34	1.37
25	q	611	CLA	C4B-NB	2.92	1.41	1.37
25	s	614	CLA	C4B-NB	2.92	1.41	1.37
24	G	608	CHL	MG-NA	-2.92	1.99	2.06
24	N	609	CHL	CHC-C4B	2.92	1.46	1.39
24	4	607	CHL	C1D-C2D	2.92	1.51	1.45
25	C	513	CLA	C1D-ND	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	606	CHL	C1D-C2D	2.92	1.51	1.45
25	r	611	CLA	C1D-ND	2.91	1.41	1.37
24	p	605	CHL	MG-NA	-2.91	1.99	2.06
25	p	602	CLA	C3B-C4B	2.91	1.49	1.42
24	7	606	CHL	C4B-NB	-2.91	1.34	1.37
24	Y	606	CHL	OBD-CAD	2.91	1.27	1.22
25	d	402	CLA	C4B-NB	2.91	1.41	1.37
24	p	606	CHL	C1D-C2D	2.91	1.51	1.45
25	s	609	CLA	C4D-ND	-2.91	1.33	1.37
25	c	513	CLA	C1D-ND	2.91	1.41	1.37
24	7	601	CHL	CHB-C1B	2.91	1.45	1.39
25	R	613	CLA	C4B-NB	2.91	1.41	1.37
25	R	612	CLA	C4B-NB	2.91	1.41	1.37
33	a	409	PHO	C4D-CHA	2.91	1.44	1.39
25	Y	613	CLA	C4B-NB	2.90	1.41	1.37
24	8	607	CHL	MG-NA	-2.90	1.99	2.06
25	S	604	CLA	C4B-NB	2.90	1.41	1.37
24	y	609	CHL	C1C-NC	-2.90	1.33	1.37
25	r	610	CLA	C4B-NB	2.90	1.41	1.37
24	1	608	CHL	C3B-C4B	2.90	1.49	1.42
25	g	603	CLA	C4B-NB	2.90	1.41	1.37
25	D	402	CLA	CMD-C2D	-2.90	1.44	1.50
25	d	402	CLA	CMD-C2D	-2.90	1.44	1.50
25	5	602	CLA	C3B-C4B	2.90	1.49	1.42
28	Y	1623	NEX	C7-C8	-2.90	1.27	1.32
24	0	606	CHL	MG-NA	-2.90	1.99	2.06
25	y	613	CLA	C1D-ND	2.90	1.41	1.37
24	y	606	CHL	OBD-CAD	2.90	1.27	1.22
33	A	409	PHO	C4D-CHA	2.90	1.44	1.39
24	R	607	CHL	OBD-CAD	2.90	1.27	1.22
25	p	611	CLA	C3B-C4B	2.90	1.49	1.42
24	S	608	CHL	C1B-NB	-2.89	1.34	1.37
24	N	601	CHL	CHC-C4B	2.89	1.45	1.39
33	A	409	PHO	CMD-C2D	-2.89	1.45	1.51
25	R	610	CLA	C4B-NB	2.89	1.41	1.37
24	g	601	CHL	CHB-C1B	2.89	1.45	1.39
33	a	408	PHO	C4D-CHA	2.89	1.44	1.39
25	Y	613	CLA	C1D-ND	2.89	1.41	1.37
24	1	601	CHL	CHB-C1B	2.89	1.45	1.39
24	5	601	CHL	C1D-C2D	2.89	1.51	1.45
24	3	608	CHL	C1B-NB	-2.89	1.34	1.37
25	7	610	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	609	CHL	C1C-NC	-2.88	1.33	1.37
24	q	609	CHL	C1B-NB	-2.88	1.34	1.37
25	n	610	CLA	C4B-NB	2.88	1.41	1.37
24	G	601	CHL	CHB-C1B	2.88	1.45	1.39
24	1	609	CHL	C1B-NB	-2.88	1.34	1.37
25	4	614	CLA	C3B-C4B	2.88	1.49	1.42
25	g	612	CLA	C1D-ND	2.88	1.41	1.37
25	1	613	CLA	C4B-NB	2.88	1.41	1.37
25	4	604	CLA	C3B-C4B	2.88	1.49	1.42
33	A	408	PHO	CMB-C2B	-2.88	1.45	1.51
24	n	607	CHL	C4B-NB	-2.88	1.34	1.37
25	g	602	CLA	C1D-ND	2.88	1.41	1.37
24	s	608	CHL	C4B-NB	-2.88	1.34	1.37
25	D	402	CLA	C4B-NB	2.88	1.41	1.37
25	G	603	CLA	C4B-NB	2.88	1.41	1.37
24	N	607	CHL	MG-NA	-2.88	1.99	2.06
25	3	602	CLA	C3B-C4B	2.88	1.49	1.42
39	D	405	PL9	C46-C44	-2.88	1.45	1.51
24	0	601	CHL	C1B-NB	-2.87	1.34	1.37
25	p	612	CLA	C4D-ND	-2.87	1.33	1.37
25	p	614	CLA	C4D-ND	-2.87	1.33	1.37
28	1	1623	NEX	C7-C8	-2.87	1.27	1.32
24	G	607	CHL	C4B-NB	-2.87	1.34	1.37
24	2	605	CHL	C1D-C2D	2.87	1.51	1.45
24	4	601	CHL	C3B-C4B	2.87	1.49	1.42
28	y	1623	NEX	C7-C8	-2.87	1.27	1.32
25	7	604	CLA	C4B-NB	2.87	1.41	1.37
24	y	609	CHL	MG-NA	-2.87	1.99	2.06
25	6	614	CLA	C3B-C4B	2.86	1.49	1.42
24	p	606	CHL	C3B-C4B	2.86	1.49	1.42
25	N	602	CLA	C1D-ND	2.86	1.41	1.37
25	Y	611	CLA	C4B-NB	2.86	1.41	1.37
24	N	609	CHL	OBD-CAD	2.86	1.27	1.22
24	p	609	CHL	C4C-C3C	2.86	1.50	1.45
25	G	614	CLA	C4B-NB	2.86	1.41	1.37
25	n	602	CLA	C1D-ND	2.86	1.41	1.37
28	g	1623	NEX	C7-C8	-2.86	1.27	1.32
24	9	609	CHL	C1B-NB	-2.86	1.34	1.37
24	7	609	CHL	C1B-NB	-2.86	1.34	1.37
24	2	607	CHL	MG-NA	-2.86	1.99	2.06
24	q	607	CHL	C1D-C2D	2.86	1.51	1.45
25	S	614	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	613	CLA	C4B-NB	2.86	1.41	1.37
24	9	605	CHL	C1D-C2D	2.86	1.51	1.45
25	B	612	CLA	C1D-ND	2.86	1.41	1.37
25	C	506	CLA	C1D-ND	2.86	1.41	1.37
25	b	612	CLA	C1D-ND	2.86	1.41	1.37
28	S	1623	NEX	C7-C8	-2.85	1.27	1.32
24	s	601	CHL	C1B-NB	-2.85	1.34	1.37
33	a	408	PHO	CMB-C2B	-2.85	1.45	1.51
24	N	605	CHL	CHB-C1B	2.85	1.45	1.39
25	B	610	CLA	C1D-ND	2.85	1.41	1.37
25	8	602	CLA	C3B-C4B	2.85	1.49	1.42
24	S	608	CHL	C4B-NB	-2.85	1.34	1.37
24	3	607	CHL	MG-NA	-2.85	1.99	2.06
25	1	614	CLA	C3B-C4B	2.85	1.49	1.42
25	5	614	CLA	C4D-ND	-2.85	1.33	1.37
24	1	607	CHL	C4B-NB	-2.85	1.34	1.37
24	n	609	CHL	CHC-C4B	2.85	1.45	1.39
25	7	614	CLA	C3B-C4B	2.85	1.49	1.42
24	S	607	CHL	C4B-NB	-2.85	1.34	1.37
24	q	608	CHL	C4B-NB	-2.85	1.34	1.37
24	3	609	CHL	C4B-NB	-2.85	1.34	1.37
24	4	609	CHL	C4B-NB	-2.85	1.34	1.37
24	8	608	CHL	C1B-NB	-2.85	1.34	1.37
25	N	611	CLA	C4B-NB	2.85	1.41	1.37
28	R	623	NEX	C7-C8	-2.85	1.27	1.32
25	2	612	CLA	C4D-ND	-2.84	1.33	1.37
24	y	605	CHL	C1B-NB	-2.84	1.34	1.37
40	f	101	HEM	FE-ND	2.84	2.03	1.94
24	s	601	CHL	C1D-C2D	2.84	1.50	1.45
39	d	405	PL9	C46-C44	-2.84	1.45	1.51
24	n	608	CHL	C4B-NB	-2.84	1.34	1.37
25	C	501	CLA	C1D-ND	2.84	1.41	1.37
24	S	601	CHL	C1D-C2D	2.84	1.50	1.45
24	6	607	CHL	MG-NA	-2.84	1.99	2.06
24	q	606	CHL	MG-NA	-2.84	1.99	2.06
24	7	607	CHL	C1B-NB	-2.84	1.34	1.37
24	Y	609	CHL	MG-NA	-2.84	1.99	2.06
25	q	614	CLA	C3B-C4B	2.84	1.49	1.42
24	8	601	CHL	C4B-NB	-2.84	1.34	1.37
24	2	601	CHL	C4B-NB	-2.84	1.34	1.37
25	y	603	CLA	C1D-ND	2.84	1.41	1.37
24	g	607	CHL	C1B-NB	-2.83	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	610	CLA	C4B-NB	2.83	1.41	1.37
24	9	609	CHL	C4C-C3C	2.83	1.49	1.45
24	6	606	CHL	MG-NA	-2.83	1.99	2.06
25	s	604	CLA	C4B-NB	2.83	1.41	1.37
24	8	605	CHL	C3B-C4B	2.83	1.49	1.42
25	4	602	CLA	C3B-C4B	2.83	1.49	1.42
24	0	606	CHL	C1D-C2D	2.83	1.50	1.45
25	3	611	CLA	C3B-C4B	2.83	1.49	1.42
24	4	606	CHL	C3D-C2D	2.83	1.46	1.39
24	8	609	CHL	C4B-NB	-2.83	1.34	1.37
24	1	605	CHL	MG-NA	-2.83	1.99	2.06
24	r	608	CHL	C4B-NB	-2.82	1.34	1.37
24	N	609	CHL	CHB-C1B	2.82	1.45	1.39
24	Y	609	CHL	OBD-CAD	2.82	1.27	1.22
24	p	606	CHL	MG-NA	-2.82	1.99	2.06
24	y	601	CHL	MG-NA	-2.82	1.99	2.06
24	y	609	CHL	OBD-CAD	2.82	1.27	1.22
28	9	1623	NEX	C7-C8	-2.82	1.27	1.32
25	B	616	CLA	C4B-NB	2.82	1.41	1.37
25	y	611	CLA	C4B-NB	2.82	1.41	1.37
24	R	608	CHL	C4B-NB	-2.82	1.34	1.37
25	Y	612	CLA	C4B-NB	2.82	1.41	1.37
28	G	1623	NEX	C7-C8	-2.82	1.27	1.32
25	C	510	CLA	C1D-ND	2.82	1.41	1.37
25	Y	603	CLA	C1D-ND	2.82	1.41	1.37
24	1	601	CHL	C1B-NB	-2.82	1.34	1.37
25	b	608	CLA	C4B-NB	2.82	1.41	1.37
24	s	607	CHL	C4B-NB	-2.82	1.34	1.37
25	S	610	CLA	C4B-NB	2.82	1.41	1.37
24	6	608	CHL	C4B-NB	-2.81	1.34	1.37
24	7	607	CHL	C4B-NB	-2.81	1.34	1.37
24	3	605	CHL	C3B-C4B	2.81	1.49	1.42
25	9	612	CLA	C4D-ND	-2.81	1.33	1.37
24	G	609	CHL	CHC-C4B	2.81	1.45	1.39
24	7	601	CHL	C1B-NB	-2.81	1.34	1.37
25	s	611	CLA	C4B-NB	2.81	1.41	1.37
24	q	608	CHL	C1D-C2D	2.81	1.50	1.45
25	c	508	CLA	C1D-ND	2.81	1.41	1.37
24	7	605	CHL	C4B-NB	-2.81	1.34	1.37
24	n	601	CHL	CHB-C1B	2.81	1.45	1.39
24	8	605	CHL	C3D-C2D	2.81	1.46	1.39
24	4	601	CHL	C4B-NB	-2.81	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	608	CHL	C3B-C4B	2.81	1.49	1.42
24	N	608	CHL	C4B-NB	-2.81	1.34	1.37
24	3	605	CHL	C3D-C2D	2.81	1.46	1.39
25	0	612	CLA	C3B-C4B	2.81	1.49	1.42
24	n	609	CHL	CHB-C1B	2.81	1.45	1.39
24	4	601	CHL	C1B-NB	-2.81	1.34	1.37
25	A	407	CLA	C1D-ND	2.81	1.41	1.37
24	y	606	CHL	MG-NA	-2.81	1.99	2.06
24	9	605	CHL	C3D-C2D	2.81	1.46	1.39
24	4	606	CHL	C1D-C2D	2.81	1.50	1.45
25	c	512	CLA	C4B-NB	2.81	1.41	1.37
24	7	608	CHL	C1B-NB	-2.80	1.34	1.37
25	Y	610	CLA	C3B-C4B	2.80	1.49	1.42
24	5	605	CHL	MG-NA	-2.80	1.99	2.06
25	5	614	CLA	C3B-C4B	2.80	1.49	1.42
24	Y	607	CHL	MG-NA	-2.80	1.99	2.06
25	0	613	CLA	C4D-ND	-2.80	1.33	1.37
24	4	608	CHL	C1D-C2D	2.80	1.50	1.45
25	q	610	CLA	C3B-C4B	2.80	1.49	1.42
24	3	601	CHL	C4B-NB	-2.80	1.34	1.37
25	b	603	CLA	C1D-ND	2.80	1.41	1.37
25	S	610	CLA	C3B-C4B	2.80	1.49	1.42
25	8	611	CLA	C3B-C4B	2.80	1.49	1.42
25	s	610	CLA	C3B-C4B	2.80	1.49	1.42
25	C	508	CLA	C1D-ND	2.80	1.41	1.37
25	N	602	CLA	C4B-NB	2.80	1.41	1.37
24	6	601	CHL	MG-NA	-2.80	1.99	2.06
24	9	607	CHL	C1D-C2D	2.79	1.50	1.45
24	g	609	CHL	CHC-C4B	2.79	1.45	1.39
24	4	601	CHL	MG-NA	-2.79	1.99	2.06
24	n	606	CHL	C3B-C4B	2.79	1.49	1.42
24	G	606	CHL	C1B-NB	-2.79	1.34	1.37
24	Y	605	CHL	C1B-NB	-2.79	1.34	1.37
24	n	606	CHL	MG-NA	-2.79	1.99	2.06
24	p	601	CHL	C1D-C2D	2.79	1.50	1.45
24	4	606	CHL	C3B-C4B	2.79	1.49	1.42
33	A	408	PHO	CMD-C2D	-2.79	1.45	1.51
24	0	606	CHL	C3B-C4B	2.79	1.49	1.42
24	G	607	CHL	C1B-NB	-2.79	1.34	1.37
24	3	608	CHL	C3B-C4B	2.79	1.49	1.42
25	a	407	CLA	C1D-ND	2.79	1.41	1.37
24	7	605	CHL	MG-NA	-2.79	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C1D-ND	2.78	1.41	1.37
28	p	1623	NEX	C7-C8	-2.78	1.27	1.32
24	G	605	CHL	C1D-C2D	2.78	1.50	1.45
25	R	616	CLA	C3B-C4B	2.78	1.49	1.42
25	R	602	CLA	MG-NB	-2.78	2.00	2.05
25	y	610	CLA	C3B-C4B	2.78	1.49	1.42
24	2	609	CHL	C1B-NB	-2.78	1.34	1.37
24	y	607	CHL	MG-NA	-2.78	1.99	2.06
25	B	604	CLA	MG-NB	-2.78	2.00	2.05
24	R	606	CHL	MG-NA	-2.78	1.99	2.06
24	r	606	CHL	MG-NA	-2.78	1.99	2.06
25	R	601	CLA	C4B-NB	2.78	1.41	1.37
25	y	612	CLA	C1D-ND	2.78	1.41	1.37
24	1	606	CHL	C4B-NB	-2.78	1.34	1.37
24	4	608	CHL	C3B-C4B	2.78	1.49	1.42
25	B	608	CLA	C4B-NB	2.77	1.41	1.37
24	p	606	CHL	C1B-NB	-2.77	1.34	1.37
24	g	606	CHL	C1B-NB	-2.77	1.34	1.37
24	9	607	CHL	MG-NA	-2.77	1.99	2.06
24	N	606	CHL	C3B-C4B	2.77	1.49	1.42
24	2	607	CHL	C1D-C2D	2.77	1.50	1.45
24	N	606	CHL	MG-NA	-2.77	1.99	2.06
24	5	609	CHL	C4C-C3C	2.77	1.49	1.45
24	4	608	CHL	MG-NA	-2.77	1.99	2.06
25	2	603	CLA	C3B-C4B	2.77	1.49	1.42
25	p	612	CLA	C3B-C4B	2.77	1.49	1.42
25	S	611	CLA	C4B-NB	2.77	1.41	1.37
24	g	605	CHL	C1D-C2D	2.77	1.50	1.45
25	n	611	CLA	C4B-NB	2.77	1.41	1.37
24	5	607	CHL	MG-NA	-2.77	1.99	2.06
24	2	605	CHL	C3D-C2D	2.77	1.46	1.39
24	2	609	CHL	C4C-C3C	2.77	1.49	1.45
24	p	606	CHL	C3D-C2D	2.77	1.46	1.39
33	A	408	PHO	CAC-C3C	-2.77	1.46	1.51
33	a	408	PHO	CAC-C3C	-2.77	1.46	1.51
24	p	608	CHL	C1D-C2D	2.77	1.50	1.45
28	5	1623	NEX	C7-C8	-2.76	1.27	1.32
25	b	610	CLA	C1D-ND	2.76	1.41	1.37
24	n	608	CHL	C1B-NB	-2.76	1.34	1.37
24	Y	601	CHL	MG-NA	-2.76	1.99	2.06
25	r	616	CLA	C3B-C4B	2.76	1.49	1.42
25	0	614	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	601	CHL	C1B-NB	-2.76	1.34	1.37
25	c	508	CLA	C4B-NB	2.76	1.41	1.37
25	S	602	CLA	C3B-C4B	2.76	1.49	1.42
24	4	605	CHL	C3D-C2D	2.76	1.46	1.39
24	p	605	CHL	C3D-C2D	2.76	1.46	1.39
24	1	607	CHL	C1B-NB	-2.76	1.34	1.37
24	Y	605	CHL	MG-NA	-2.76	1.99	2.06
24	y	605	CHL	MG-NA	-2.76	1.99	2.06
24	8	606	CHL	C1B-NB	-2.76	1.34	1.37
33	a	408	PHO	CMD-C2D	-2.76	1.45	1.51
24	5	608	CHL	C1D-C2D	2.76	1.50	1.45
25	D	402	CLA	MG-NB	-2.75	2.00	2.05
25	d	402	CLA	MG-NB	-2.75	2.00	2.05
25	p	613	CLA	C3B-C4B	2.75	1.49	1.42
24	9	601	CHL	CHB-C1B	2.75	1.45	1.39
25	q	604	CLA	C3B-C4B	2.75	1.49	1.42
24	q	606	CHL	C3B-C4B	2.75	1.49	1.42
24	9	608	CHL	C1D-C2D	2.75	1.50	1.45
24	q	605	CHL	C3D-C2D	2.75	1.46	1.39
24	3	601	CHL	MG-NA	-2.75	1.99	2.06
24	Y	606	CHL	MG-NA	-2.75	1.99	2.06
24	5	606	CHL	C3B-C4B	2.75	1.49	1.42
24	0	608	CHL	C4B-NB	-2.75	1.34	1.37
25	8	604	CLA	C3B-C4B	2.75	1.49	1.42
24	5	607	CHL	C3B-C4B	2.75	1.49	1.42
25	b	614	CLA	C1D-ND	2.75	1.41	1.37
25	c	501	CLA	C1D-ND	2.75	1.41	1.37
25	s	602	CLA	C3B-C4B	2.75	1.49	1.42
24	q	601	CHL	MG-NA	-2.75	1.99	2.06
25	6	612	CLA	C3B-C4B	2.74	1.49	1.42
24	S	601	CHL	C1B-NB	-2.74	1.34	1.37
25	p	610	CLA	C3B-C4B	2.74	1.49	1.42
25	b	604	CLA	MG-NB	-2.74	2.00	2.05
24	6	607	CHL	C4B-NB	-2.74	1.34	1.37
25	r	602	CLA	MG-NB	-2.74	2.00	2.05
24	3	607	CHL	C3B-C4B	2.74	1.49	1.42
28	6	1623	NEX	C7-C8	-2.74	1.27	1.32
24	0	606	CHL	C1B-NB	-2.74	1.34	1.37
25	y	612	CLA	C4B-NB	2.74	1.41	1.37
35	a	412	SQD	C6-S	-2.74	1.67	1.77
24	0	609	CHL	MG-NA	-2.74	1.99	2.06
24	4	605	CHL	MG-NA	-2.74	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	602	CLA	C4B-NB	2.74	1.41	1.37
25	r	601	CLA	C4B-NB	2.74	1.41	1.37
24	n	605	CHL	CHB-C1B	2.74	1.45	1.39
25	s	610	CLA	C4B-NB	2.74	1.41	1.37
24	S	606	CHL	C4B-NB	-2.74	1.34	1.37
25	C	508	CLA	C4B-NB	2.74	1.41	1.37
25	5	603	CLA	C3B-C4B	2.74	1.49	1.42
28	3	1623	NEX	C7-C8	-2.73	1.27	1.32
25	B	615	CLA	C1D-ND	2.73	1.41	1.37
25	b	602	CLA	C4B-NB	2.73	1.41	1.37
24	6	606	CHL	C3B-C4B	2.73	1.49	1.42
24	p	607	CHL	MG-NA	-2.73	1.99	2.06
25	8	610	CLA	C3B-C4B	2.73	1.49	1.42
24	r	606	CHL	CHB-C1B	2.73	1.45	1.39
25	B	614	CLA	C1D-ND	2.73	1.41	1.37
25	c	513	CLA	C4B-NB	2.73	1.41	1.37
25	G	604	CLA	C3B-C4B	2.73	1.49	1.42
24	q	607	CHL	C3D-C2D	2.73	1.46	1.39
25	3	604	CLA	C3B-C4B	2.73	1.49	1.42
25	1	610	CLA	C3B-C4B	2.73	1.49	1.42
24	p	607	CHL	C3B-C4B	2.73	1.49	1.42
25	5	612	CLA	C3B-C4B	2.73	1.49	1.42
25	p	603	CLA	C3B-C4B	2.72	1.49	1.42
24	8	607	CHL	CHB-C1B	2.72	1.45	1.39
35	A	412	SQD	C6-S	-2.72	1.67	1.77
25	p	614	CLA	C3B-C4B	2.72	1.49	1.42
24	q	605	CHL	C3B-C4B	2.72	1.49	1.42
25	Y	612	CLA	C1D-ND	2.72	1.41	1.37
24	q	609	CHL	C3B-C4B	2.72	1.49	1.42
24	7	605	CHL	C1B-NB	-2.72	1.34	1.37
24	8	608	CHL	C3B-C4B	2.72	1.49	1.42
24	R	606	CHL	CHB-C1B	2.72	1.45	1.39
24	y	609	CHL	CHB-C4A	-2.72	1.31	1.37
25	D	403	CLA	C4B-NB	2.72	1.41	1.37
24	Y	609	CHL	CHC-C4B	2.72	1.45	1.39
24	n	606	CHL	C4B-NB	-2.72	1.34	1.37
25	A	406	CLA	C1D-ND	2.72	1.41	1.37
25	a	406	CLA	C1D-ND	2.72	1.41	1.37
24	y	609	CHL	CHC-C4B	2.72	1.45	1.39
24	g	608	CHL	C3B-C4B	2.72	1.49	1.42
28	r	623	NEX	C7-C8	-2.72	1.27	1.32
24	R	606	CHL	OBD-CAD	2.71	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	614	CLA	C3B-C4B	2.71	1.49	1.42
25	9	614	CLA	C3B-C4B	2.71	1.49	1.42
24	1	605	CHL	C4B-NB	-2.71	1.34	1.37
24	3	601	CHL	C1D-C2D	2.71	1.50	1.45
24	2	607	CHL	C3D-C2D	2.71	1.46	1.39
25	6	602	CLA	C3B-C4B	2.71	1.49	1.42
25	q	612	CLA	C4D-ND	-2.71	1.34	1.37
24	G	608	CHL	C3B-C4B	2.71	1.49	1.42
25	A	405	CLA	CMC-C2C	-2.71	1.45	1.50
24	q	606	CHL	C4B-NB	-2.71	1.34	1.37
24	0	608	CHL	C1B-NB	-2.71	1.34	1.37
24	r	608	CHL	C1D-ND	-2.71	1.34	1.37
24	2	607	CHL	C4B-NB	-2.71	1.34	1.37
25	b	615	CLA	C1D-ND	2.71	1.41	1.37
25	C	501	CLA	CMD-C2D	-2.71	1.45	1.50
24	6	606	CHL	C1D-C2D	2.71	1.50	1.45
24	9	609	CHL	MG-NA	-2.71	1.99	2.06
24	4	606	CHL	MG-NA	-2.71	1.99	2.06
25	1	604	CLA	C4B-NB	2.71	1.41	1.37
25	8	614	CLA	C3B-C4B	2.71	1.49	1.42
25	3	610	CLA	C3B-C4B	2.71	1.49	1.42
25	D	402	CLA	MG-ND	-2.71	2.00	2.05
25	d	402	CLA	MG-ND	-2.71	2.00	2.05
25	C	512	CLA	C4B-NB	2.70	1.41	1.37
25	7	612	CLA	C3B-C4B	2.70	1.49	1.42
24	N	601	CHL	MG-NA	-2.70	1.99	2.06
25	9	602	CLA	C4B-NB	2.70	1.41	1.37
24	q	601	CHL	C3B-C4B	2.70	1.49	1.42
25	b	616	CLA	C4B-NB	2.70	1.41	1.37
25	6	603	CLA	C3B-C4B	2.70	1.49	1.42
35	b	623	SQD	C6-S	-2.70	1.67	1.77
24	S	601	CHL	MG-NA	-2.70	1.99	2.06
25	g	602	CLA	C3B-C4B	2.70	1.49	1.42
25	5	613	CLA	C3B-C4B	2.70	1.49	1.42
24	0	609	CHL	C1D-C2D	2.70	1.50	1.45
24	Y	609	CHL	CHB-C4A	-2.70	1.31	1.37
25	B	613	CLA	CMD-C2D	-2.70	1.45	1.50
25	C	513	CLA	C4B-NB	2.70	1.41	1.37
24	2	608	CHL	C1D-C2D	2.70	1.50	1.45
24	9	606	CHL	C3D-C2D	2.70	1.46	1.39
24	S	601	CHL	C4B-NB	-2.70	1.34	1.37
25	9	603	CLA	C3B-C4B	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	603	CLA	C3B-C4B	2.69	1.49	1.42
40	f	101	HEM	FE-NC	2.69	2.04	1.95
25	2	614	CLA	C3B-C4B	2.69	1.49	1.42
25	c	501	CLA	CMD-C2D	-2.69	1.45	1.50
24	8	607	CHL	C3B-C4B	2.69	1.49	1.42
24	5	605	CHL	C3D-C2D	2.69	1.46	1.39
24	p	607	CHL	C3D-C2D	2.69	1.46	1.39
24	y	608	CHL	C3B-C4B	2.69	1.49	1.42
25	r	604	CLA	C3B-C4B	2.69	1.49	1.42
24	s	601	CHL	C4B-NB	-2.69	1.34	1.37
24	p	601	CHL	MG-NA	-2.69	1.99	2.06
24	g	606	CHL	MG-NA	-2.69	1.99	2.06
24	s	607	CHL	C3D-C2D	2.69	1.46	1.39
25	N	612	CLA	C3B-C4B	2.69	1.49	1.42
24	9	606	CHL	C1B-NB	-2.69	1.34	1.37
24	6	607	CHL	C3D-C2D	2.69	1.46	1.39
25	a	410	CLA	C4B-NB	2.69	1.41	1.37
24	4	607	CHL	C3B-C4B	2.69	1.49	1.42
25	6	613	CLA	C3B-C4B	2.68	1.49	1.42
24	4	609	CHL	C3B-C4B	2.68	1.49	1.42
35	B	623	SQD	C6-S	-2.68	1.67	1.77
24	2	606	CHL	C3D-C2D	2.68	1.46	1.39
24	1	609	CHL	MG-NA	-2.68	1.99	2.06
25	a	405	CLA	CMC-C2C	-2.68	1.45	1.50
24	9	609	CHL	C3D-C2D	2.68	1.46	1.39
25	0	602	CLA	C3B-C4B	2.68	1.49	1.42
24	1	605	CHL	C1B-NB	-2.68	1.34	1.37
24	S	607	CHL	C3D-C2D	2.68	1.46	1.39
25	b	603	CLA	MG-NB	-2.68	2.00	2.05
24	s	606	CHL	C4B-NB	-2.68	1.34	1.37
25	8	613	CLA	C3B-C4B	2.68	1.49	1.42
24	q	607	CHL	C3B-C4B	2.68	1.49	1.42
24	q	601	CHL	C1B-NB	-2.68	1.34	1.37
24	Y	608	CHL	C3B-C4B	2.68	1.49	1.42
25	1	612	CLA	C3B-C4B	2.68	1.49	1.42
25	g	604	CLA	C3B-C4B	2.68	1.49	1.42
24	G	605	CHL	C3D-C2D	2.68	1.46	1.39
25	A	407	CLA	C4B-NB	2.67	1.41	1.37
25	B	602	CLA	C4B-NB	2.67	1.41	1.37
24	3	606	CHL	C1B-NB	-2.67	1.34	1.37
25	Y	614	CLA	C4B-NB	2.67	1.41	1.37
24	s	608	CHL	MG-NA	-2.67	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	613	CLA	C1B-C2B	2.67	1.49	1.43
24	R	608	CHL	C1D-ND	-2.67	1.34	1.37
24	0	607	CHL	C1B-NB	-2.67	1.34	1.37
24	6	605	CHL	C3D-C2D	2.67	1.46	1.39
25	G	602	CLA	C3B-C4B	2.67	1.49	1.42
25	Y	604	CLA	C1D-ND	2.67	1.41	1.37
24	r	606	CHL	OBD-CAD	2.67	1.27	1.22
25	R	609	CLA	C3B-C4B	2.67	1.49	1.42
24	y	605	CHL	CHB-C1B	2.67	1.45	1.39
25	7	610	CLA	C3B-C4B	2.67	1.49	1.42
25	q	603	CLA	C3B-C4B	2.67	1.49	1.42
25	2	604	CLA	C3B-C4B	2.67	1.49	1.42
25	y	614	CLA	C4B-NB	2.67	1.41	1.37
25	r	604	CLA	CMB-C2B	-2.67	1.45	1.50
24	g	605	CHL	C3D-C2D	2.67	1.46	1.39
24	S	606	CHL	C1D-C2D	2.67	1.50	1.45
25	b	607	CLA	C3B-C4B	2.67	1.49	1.42
24	3	605	CHL	C1B-NB	-2.67	1.34	1.37
25	B	607	CLA	C3B-C4B	2.66	1.49	1.42
25	b	611	CLA	CMD-C2D	-2.66	1.45	1.50
24	N	606	CHL	C4B-NB	-2.66	1.34	1.37
25	R	604	CLA	C3B-C4B	2.66	1.49	1.42
25	r	609	CLA	C3B-C4B	2.66	1.49	1.42
24	Y	607	CHL	CHB-C4A	-2.66	1.31	1.37
25	y	604	CLA	C1D-ND	2.66	1.41	1.37
25	d	403	CLA	C4B-NB	2.66	1.41	1.37
24	y	601	CHL	CHB-C4A	-2.66	1.31	1.37
25	5	610	CLA	C3B-C4B	2.66	1.49	1.42
24	0	601	CHL	C3D-C2D	2.66	1.46	1.39
25	b	613	CLA	CMD-C2D	-2.66	1.45	1.50
25	0	603	CLA	C3B-C4B	2.66	1.49	1.42
25	n	612	CLA	C3B-C4B	2.66	1.49	1.42
24	4	607	CHL	C3D-C2D	2.66	1.46	1.39
24	Y	601	CHL	CHB-C1B	2.66	1.45	1.39
25	B	603	CLA	MG-NB	-2.66	2.00	2.05
25	0	610	CLA	C3B-C4B	2.66	1.49	1.42
24	y	607	CHL	CHB-C4A	-2.66	1.31	1.37
25	4	612	CLA	C4D-ND	-2.66	1.34	1.37
25	Y	613	CLA	MG-ND	-2.66	2.00	2.05
24	s	601	CHL	MG-NA	-2.65	2.00	2.06
24	3	607	CHL	CHB-C1B	2.65	1.45	1.39
24	q	601	CHL	C1D-C2D	2.65	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	605	CHL	C1B-C2B	2.65	1.49	1.43
39	D	405	PL9	C16-C14	-2.65	1.45	1.51
24	4	608	CHL	C1B-NB	-2.65	1.34	1.37
25	0	613	CLA	C1B-C2B	2.65	1.49	1.43
24	5	606	CHL	C1D-C2D	2.65	1.50	1.45
25	2	613	CLA	C3B-C4B	2.65	1.49	1.42
24	4	605	CHL	C3B-C4B	2.65	1.49	1.42
25	9	613	CLA	C3B-C4B	2.65	1.49	1.42
24	1	608	CHL	C1B-NB	-2.65	1.34	1.37
24	3	608	CHL	C1D-C2D	2.65	1.50	1.45
25	R	604	CLA	CMB-C2B	-2.65	1.45	1.50
24	g	606	CHL	C4B-NB	-2.65	1.34	1.37
25	B	604	CLA	C1D-ND	2.65	1.41	1.37
25	C	512	CLA	CMD-C2D	-2.65	1.45	1.50
24	Y	605	CHL	CHB-C1B	2.65	1.45	1.39
24	3	601	CHL	C1B-C2B	2.65	1.49	1.43
24	8	601	CHL	MG-NA	-2.65	2.00	2.06
25	G	603	CLA	C1D-ND	2.65	1.41	1.37
25	q	613	CLA	C3B-C4B	2.64	1.49	1.42
24	4	608	CHL	C3D-C2D	2.64	1.46	1.39
25	9	604	CLA	C3B-C4B	2.64	1.48	1.42
25	c	510	CLA	C3B-C4B	2.64	1.48	1.42
24	s	606	CHL	C1D-C2D	2.64	1.50	1.45
25	q	612	CLA	C3B-C4B	2.64	1.48	1.42
25	a	407	CLA	C4B-NB	2.64	1.41	1.37
24	G	606	CHL	MG-NA	-2.64	2.00	2.06
25	1	602	CLA	C3B-C4B	2.64	1.48	1.42
25	R	612	CLA	C3B-C4B	2.64	1.48	1.42
24	Y	601	CHL	CHB-C4A	-2.64	1.31	1.37
24	9	605	CHL	MG-NA	-2.64	2.00	2.06
25	c	512	CLA	CMD-C2D	-2.64	1.45	1.50
25	a	405	CLA	MG-NB	-2.64	2.00	2.05
39	D	405	PL9	C36-C34	-2.64	1.45	1.51
24	p	608	CHL	C3B-C4B	2.64	1.48	1.42
24	s	608	CHL	C1D-C2D	2.64	1.50	1.45
25	C	510	CLA	C3B-C4B	2.64	1.48	1.42
25	7	604	CLA	CMB-C2B	-2.64	1.45	1.50
24	5	605	CHL	C3B-C4B	2.64	1.48	1.42
25	3	613	CLA	C3B-C4B	2.64	1.48	1.42
24	q	605	CHL	MG-NA	-2.64	2.00	2.06
24	8	601	CHL	C1D-C2D	2.63	1.50	1.45
24	q	605	CHL	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	606	CHL	C4B-NB	-2.63	1.34	1.37
25	n	614	CLA	C3B-C4B	2.63	1.48	1.42
24	0	608	CHL	MG-NA	-2.63	2.00	2.06
24	q	607	CHL	C4B-NB	-2.63	1.34	1.37
25	8	613	CLA	C1B-C2B	2.63	1.49	1.43
25	y	611	CLA	CMD-C2D	-2.63	1.45	1.50
25	5	604	CLA	C3B-C4B	2.63	1.48	1.42
24	2	606	CHL	C1D-C2D	2.63	1.50	1.45
24	9	607	CHL	C3D-C2D	2.63	1.46	1.39
25	B	611	CLA	CMD-C2D	-2.63	1.45	1.50
25	6	610	CLA	C3B-C4B	2.63	1.48	1.42
25	B	609	CLA	C4B-NB	2.63	1.41	1.37
25	b	609	CLA	C4B-NB	2.63	1.41	1.37
24	6	608	CHL	C3B-C4B	2.63	1.48	1.42
24	5	607	CHL	C3D-C2D	2.63	1.46	1.39
24	2	601	CHL	CHB-C1B	2.63	1.45	1.39
24	N	608	CHL	C1B-NB	-2.63	1.34	1.37
25	b	604	CLA	C1D-ND	2.62	1.41	1.37
25	B	604	CLA	CMB-C2B	-2.62	1.45	1.50
24	9	607	CHL	C4B-NB	-2.62	1.34	1.37
24	5	606	CHL	C3D-C2D	2.62	1.46	1.39
24	1	606	CHL	C3B-C4B	2.62	1.48	1.42
24	2	609	CHL	C3D-C2D	2.62	1.46	1.39
25	g	603	CLA	C1D-ND	2.62	1.41	1.37
39	d	405	PL9	C36-C34	-2.62	1.45	1.51
24	3	609	CHL	C1B-NB	-2.62	1.34	1.37
24	6	608	CHL	C1B-NB	-2.62	1.34	1.37
24	7	605	CHL	C1D-C2D	2.62	1.50	1.45
25	C	510	CLA	CMD-C2D	-2.62	1.45	1.50
25	p	604	CLA	C3B-C4B	2.62	1.48	1.42
25	C	509	CLA	MG-NB	-2.62	2.00	2.05
24	S	608	CHL	C1D-C2D	2.62	1.50	1.45
25	g	610	CLA	C3B-C4B	2.62	1.48	1.42
24	p	605	CHL	C3B-C4B	2.61	1.48	1.42
25	8	612	CLA	C3B-C4B	2.61	1.48	1.42
24	8	609	CHL	C1B-NB	-2.61	1.34	1.37
25	B	615	CLA	C4B-NB	2.61	1.41	1.37
24	0	601	CHL	C3B-C4B	2.61	1.48	1.42
39	d	405	PL9	C16-C14	-2.61	1.45	1.51
24	4	601	CHL	C3D-C2D	2.61	1.46	1.39
24	S	608	CHL	MG-NA	-2.61	2.00	2.06
24	n	601	CHL	MG-NA	-2.61	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	614	CLA	C3B-C4B	2.61	1.48	1.42
25	c	502	CLA	CHC-C4B	-2.61	1.33	1.39
24	7	606	CHL	C3B-C4B	2.61	1.48	1.42
25	r	612	CLA	C3B-C4B	2.61	1.48	1.42
24	p	607	CHL	C1D-C2D	2.61	1.50	1.45
25	c	501	CLA	C4B-NB	2.61	1.41	1.37
24	0	608	CHL	C1D-C2D	2.61	1.50	1.45
25	y	613	CLA	MG-ND	-2.61	2.00	2.05
25	9	612	CLA	C1B-C2B	2.61	1.49	1.43
25	C	502	CLA	CHC-C4B	-2.61	1.33	1.39
25	S	605	CLA	C3B-C4B	2.61	1.48	1.42
25	A	410	CLA	C4B-NB	2.61	1.41	1.37
25	4	612	CLA	C3B-C4B	2.61	1.48	1.42
25	G	610	CLA	C3B-C4B	2.61	1.48	1.42
24	0	605	CHL	C3D-C2D	2.61	1.46	1.39
24	5	601	CHL	C3B-C4B	2.61	1.48	1.42
24	6	601	CHL	C3D-C2D	2.61	1.46	1.39
24	S	606	CHL	MG-NA	-2.61	2.00	2.06
25	p	603	CLA	C1B-C2B	2.61	1.49	1.43
25	9	613	CLA	C1B-C2B	2.61	1.49	1.43
24	8	605	CHL	C1B-NB	-2.61	1.34	1.37
25	G	610	CLA	C4B-NB	2.61	1.41	1.37
25	g	610	CLA	C4B-NB	2.61	1.41	1.37
25	N	614	CLA	C3B-C4B	2.61	1.48	1.42
25	b	604	CLA	CMB-C2B	-2.61	1.45	1.50
39	d	405	PL9	C7-C8	-2.61	1.46	1.50
25	c	513	CLA	C3B-C4B	2.61	1.48	1.42
24	4	606	CHL	C4B-NB	-2.60	1.34	1.37
25	B	604	CLA	CMD-C2D	-2.60	1.45	1.50
24	9	601	CHL	MG-NA	-2.60	2.00	2.06
25	c	510	CLA	CMD-C2D	-2.60	1.45	1.50
24	2	601	CHL	MG-NA	-2.60	2.00	2.06
25	C	511	CLA	C1B-NB	-2.60	1.34	1.37
25	C	513	CLA	C3B-C4B	2.60	1.48	1.42
25	A	405	CLA	MG-NB	-2.60	2.00	2.05
25	y	602	CLA	MG-NB	-2.60	2.00	2.05
24	p	601	CHL	C3D-C2D	2.60	1.46	1.39
24	2	609	CHL	C4B-NB	-2.60	1.34	1.37
25	R	610	CLA	CMC-C2C	-2.60	1.45	1.50
24	8	609	CHL	C3D-C2D	2.60	1.46	1.39
25	9	611	CLA	C3B-C4B	2.60	1.48	1.42
24	6	606	CHL	C1B-NB	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	605	CHL	C1D-C2D	2.60	1.50	1.45
25	N	611	CLA	C3B-C4B	2.60	1.48	1.42
25	2	613	CLA	C1B-C2B	2.60	1.49	1.43
25	0	614	CLA	C1B-C2B	2.60	1.49	1.43
25	b	611	CLA	C3B-C4B	2.60	1.48	1.42
25	7	602	CLA	C3B-C4B	2.59	1.48	1.42
28	n	1623	NEX	C7-C8	-2.59	1.27	1.32
25	C	506	CLA	C3B-C4B	2.59	1.48	1.42
24	8	608	CHL	C1D-C2D	2.59	1.50	1.45
24	s	607	CHL	C1D-C2D	2.59	1.50	1.45
25	8	611	CLA	C1B-C2B	2.59	1.49	1.43
25	s	609	CLA	C3B-C4B	2.59	1.48	1.42
24	S	607	CHL	C1D-C2D	2.59	1.50	1.45
25	g	602	CLA	C4B-NB	2.59	1.41	1.37
24	7	601	CHL	MG-NA	-2.59	2.00	2.06
24	8	608	CHL	C4B-NB	-2.59	1.34	1.37
25	p	614	CLA	C1B-C2B	2.59	1.49	1.43
24	9	606	CHL	MG-NA	-2.59	2.00	2.06
24	3	606	CHL	C3D-C2D	2.59	1.46	1.39
25	S	609	CLA	C3B-C4B	2.59	1.48	1.42
24	y	601	CHL	CHB-C1B	2.59	1.45	1.39
25	c	506	CLA	CMB-C2B	-2.59	1.45	1.50
25	r	610	CLA	CMC-C2C	-2.59	1.45	1.50
25	9	603	CLA	C1B-C2B	2.59	1.49	1.43
25	c	509	CLA	MG-NB	-2.59	2.00	2.05
24	4	605	CHL	C4C-C3C	2.59	1.49	1.45
25	5	603	CLA	C1B-C2B	2.59	1.49	1.43
24	0	608	CHL	C3B-C4B	2.59	1.48	1.42
24	6	605	CHL	C4B-NB	-2.59	1.34	1.37
25	3	612	CLA	C3B-C4B	2.59	1.48	1.42
24	2	605	CHL	MG-NA	-2.58	2.00	2.06
25	6	613	CLA	C1B-C2B	2.58	1.49	1.43
24	5	609	CHL	C3D-C2D	2.58	1.46	1.39
25	s	605	CLA	C3B-C4B	2.58	1.48	1.42
25	Y	611	CLA	CMD-C2D	-2.58	1.45	1.50
25	9	612	CLA	C3B-C4B	2.58	1.48	1.42
24	6	609	CHL	C1D-C2D	2.58	1.50	1.45
25	C	505	CLA	C3B-C4B	2.58	1.48	1.42
24	9	601	CHL	C1D-C2D	2.58	1.50	1.45
24	0	607	CHL	C3B-C4B	2.58	1.48	1.42
25	5	604	CLA	C1B-C2B	2.58	1.49	1.43
25	Y	602	CLA	MG-NB	-2.58	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	612	CLA	C3B-C4B	2.58	1.48	1.42
24	Y	607	CHL	CHB-C1B	2.58	1.45	1.39
25	3	613	CLA	C1B-C2B	2.58	1.49	1.43
24	5	608	CHL	C3B-C4B	2.58	1.48	1.42
24	7	608	CHL	C4B-NB	-2.58	1.34	1.37
25	n	611	CLA	C3B-C4B	2.57	1.48	1.42
24	2	605	CHL	C4C-C3C	2.57	1.49	1.45
25	a	410	CLA	MG-NB	-2.57	2.00	2.05
25	c	505	CLA	C3B-C4B	2.57	1.48	1.42
24	5	609	CHL	C4B-NB	-2.57	1.34	1.37
24	g	607	CHL	C1D-C2D	2.57	1.50	1.45
25	B	605	CLA	CMD-C2D	-2.57	1.45	1.50
24	9	605	CHL	C3B-C4B	2.57	1.48	1.42
25	n	602	CLA	C3B-C4B	2.57	1.48	1.42
24	8	606	CHL	C3D-C2D	2.57	1.46	1.39
25	p	604	CLA	C1B-C2B	2.57	1.49	1.43
25	4	611	CLA	C3B-C4B	2.57	1.48	1.42
25	c	512	CLA	C3B-C4B	2.57	1.48	1.42
24	0	609	CHL	C3D-C2D	2.57	1.46	1.39
24	N	607	CHL	C3B-C4B	2.57	1.48	1.42
25	1	604	CLA	CMB-C2B	-2.57	1.45	1.50
25	c	510	CLA	MG-NB	-2.57	2.00	2.05
25	b	611	CLA	CMC-C2C	-2.57	1.45	1.50
25	r	610	CLA	MG-NB	-2.57	2.00	2.05
25	5	613	CLA	C1B-C2B	2.57	1.49	1.43
25	B	611	CLA	C3B-C4B	2.57	1.48	1.42
25	C	502	CLA	C1B-C2B	2.57	1.49	1.43
25	0	613	CLA	C3B-C4B	2.57	1.48	1.42
24	y	607	CHL	CHB-C1B	2.57	1.45	1.39
25	b	604	CLA	CMD-C2D	-2.57	1.45	1.50
24	s	608	CHL	C3D-C2D	2.57	1.46	1.39
25	s	614	CLA	C3B-C4B	2.57	1.48	1.42
25	S	604	CLA	C3B-C4B	2.57	1.48	1.42
24	7	609	CHL	MG-NA	-2.57	2.00	2.06
25	7	611	CLA	C3B-C4B	2.57	1.48	1.42
25	b	605	CLA	CMD-C2D	-2.57	1.45	1.50
25	B	606	CLA	C4B-NB	2.57	1.40	1.37
25	b	606	CLA	C4B-NB	2.57	1.40	1.37
24	6	601	CHL	C3B-C4B	2.57	1.48	1.42
25	a	410	CLA	C3B-C4B	2.56	1.48	1.42
25	s	612	CLA	C3B-C4B	2.56	1.48	1.42
25	9	611	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C4B-NB	2.56	1.40	1.37
25	c	508	CLA	C3B-C4B	2.56	1.48	1.42
24	5	601	CHL	MG-NA	-2.56	2.00	2.06
24	S	607	CHL	C3B-C4B	2.56	1.48	1.42
24	p	609	CHL	C3D-C2D	2.56	1.46	1.39
24	G	605	CHL	MG-NA	-2.56	2.00	2.06
25	7	611	CLA	C1B-C2B	2.56	1.49	1.43
25	1	611	CLA	C3B-C4B	2.56	1.48	1.42
25	N	602	CLA	C3B-C4B	2.56	1.48	1.42
25	3	611	CLA	C1B-C2B	2.56	1.49	1.43
24	6	608	CHL	MG-NA	-2.56	2.00	2.06
24	n	601	CHL	C1D-C2D	2.56	1.50	1.45
24	9	608	CHL	C3B-C4B	2.56	1.48	1.42
24	6	609	CHL	C3D-C2D	2.56	1.46	1.39
24	1	605	CHL	C1D-C2D	2.56	1.50	1.45
24	6	601	CHL	C1D-C2D	2.56	1.50	1.45
24	2	605	CHL	C1B-C2B	2.56	1.49	1.43
25	c	511	CLA	C1B-NB	-2.56	1.34	1.37
25	2	612	CLA	C1B-C2B	2.56	1.49	1.43
24	s	606	CHL	MG-NA	-2.56	2.00	2.06
25	B	609	CLA	C1D-ND	2.56	1.40	1.37
25	b	609	CLA	C1D-ND	2.56	1.40	1.37
24	1	601	CHL	MG-NA	-2.56	2.00	2.06
24	6	607	CHL	C1D-C2D	2.56	1.50	1.45
33	A	409	PHO	C1D-C2D	2.56	1.42	1.39
25	1	611	CLA	C1B-C2B	2.56	1.49	1.43
24	G	607	CHL	MG-NA	-2.56	2.00	2.06
25	g	614	CLA	C3B-C4B	2.55	1.48	1.42
25	s	604	CLA	C3B-C4B	2.55	1.48	1.42
24	4	607	CHL	C4B-NB	-2.55	1.34	1.37
25	C	505	CLA	MG-ND	-2.55	2.00	2.05
25	Y	610	CLA	C4B-NB	2.55	1.40	1.37
25	c	502	CLA	C1B-C2B	2.55	1.49	1.43
24	5	609	CHL	MG-NA	-2.55	2.00	2.06
24	2	609	CHL	MG-NA	-2.55	2.00	2.06
24	N	607	CHL	CHB-C1B	2.55	1.45	1.39
24	Y	608	CHL	C4B-NB	-2.55	1.34	1.37
25	c	510	CLA	C4B-NB	2.55	1.40	1.37
25	A	410	CLA	C3B-C4B	2.55	1.48	1.42
24	3	609	CHL	MG-NA	-2.55	2.00	2.06
25	c	505	CLA	C4B-NB	2.55	1.40	1.37
25	r	603	CLA	C4B-NB	2.55	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	607	CHL	CHB-C4A	-2.55	1.31	1.37
25	q	611	CLA	C3B-C4B	2.55	1.48	1.42
25	y	603	CLA	MG-ND	-2.55	2.00	2.05
25	s	611	CLA	C3B-C4B	2.55	1.48	1.42
24	R	607	CHL	CHB-C4A	-2.55	1.31	1.37
25	B	611	CLA	CMC-C2C	-2.55	1.45	1.50
24	6	605	CHL	MG-NA	-2.55	2.00	2.06
24	3	608	CHL	C4B-NB	-2.55	1.34	1.37
25	C	508	CLA	C3B-C4B	2.55	1.48	1.42
25	C	510	CLA	MG-NB	-2.55	2.00	2.05
25	B	605	CLA	CMB-C2B	-2.55	1.45	1.50
25	c	507	CLA	C1B-NB	-2.55	1.34	1.37
25	C	507	CLA	MG-NB	-2.54	2.00	2.05
24	2	607	CHL	C1B-NB	-2.54	1.34	1.37
25	C	501	CLA	C4B-NB	2.54	1.40	1.37
24	0	607	CHL	C3D-C2D	2.54	1.46	1.39
25	C	503	CLA	C4B-NB	2.54	1.40	1.37
24	Y	607	CHL	C3B-C4B	2.54	1.48	1.42
24	g	605	CHL	C1B-C2B	2.54	1.49	1.43
24	p	606	CHL	C4C-C3C	2.54	1.49	1.45
25	2	611	CLA	C3B-C4B	2.54	1.48	1.42
25	c	506	CLA	C3B-C4B	2.54	1.48	1.42
25	c	502	CLA	CMC-C2C	-2.54	1.45	1.50
39	D	405	PL9	C7-C8	-2.54	1.47	1.50
25	5	612	CLA	C1B-C2B	2.54	1.49	1.43
25	6	614	CLA	C1B-C2B	2.54	1.49	1.43
25	g	613	CLA	C1B-C2B	2.54	1.49	1.43
25	4	613	CLA	C3B-C4B	2.54	1.48	1.42
25	r	611	CLA	C3B-C4B	2.54	1.48	1.42
25	C	502	CLA	MG-NB	-2.54	2.00	2.05
24	p	601	CHL	C3B-C4B	2.54	1.48	1.42
24	3	608	CHL	MG-NA	-2.54	2.00	2.06
24	9	605	CHL	C1B-C2B	2.54	1.49	1.43
25	c	513	CLA	C1B-C2B	2.54	1.49	1.43
25	B	602	CLA	C3B-C4B	2.54	1.48	1.42
24	y	607	CHL	C3B-C4B	2.54	1.48	1.42
25	b	602	CLA	C3B-C4B	2.54	1.48	1.42
33	a	409	PHO	C1D-C2D	2.54	1.42	1.39
25	5	610	CLA	C1B-C2B	2.54	1.49	1.43
24	5	609	CHL	C1B-NB	-2.54	1.34	1.37
24	9	605	CHL	C4C-C3C	2.54	1.49	1.45
24	G	605	CHL	C4C-C3C	2.54	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	q	604	CLA	C1B-C2B	2.54	1.49	1.43
24	G	605	CHL	C1B-C2B	2.53	1.49	1.43
24	n	607	CHL	CHB-C1B	2.53	1.45	1.39
24	p	609	CHL	C4B-NB	-2.53	1.34	1.37
24	7	605	CHL	C3D-C2D	2.53	1.46	1.39
25	7	614	CLA	C1B-C2B	2.53	1.49	1.43
25	C	502	CLA	CMC-C2C	-2.53	1.45	1.50
25	Y	603	CLA	MG-ND	-2.53	2.00	2.05
25	G	614	CLA	C3B-C4B	2.53	1.48	1.42
25	c	505	CLA	C1D-ND	2.53	1.40	1.37
25	N	610	CLA	C3B-C4B	2.53	1.48	1.42
24	5	601	CHL	C3D-C2D	2.53	1.46	1.39
24	s	606	CHL	C3D-C2D	2.53	1.46	1.39
25	C	507	CLA	C1B-NB	-2.53	1.34	1.37
24	0	605	CHL	C1D-C2D	2.53	1.50	1.45
24	3	609	CHL	C3D-C2D	2.53	1.46	1.39
25	B	610	CLA	CMB-C2B	-2.53	1.45	1.50
25	3	614	CLA	C1B-C2B	2.53	1.49	1.43
24	Y	605	CHL	C3D-C2D	2.53	1.46	1.39
24	y	605	CHL	C3D-C2D	2.53	1.46	1.39
24	8	601	CHL	C1B-NB	-2.53	1.34	1.37
24	g	608	CHL	C4B-NB	-2.53	1.34	1.37
24	G	609	CHL	C1D-C2D	2.53	1.50	1.45
25	b	610	CLA	CMB-C2B	-2.53	1.45	1.50
24	1	605	CHL	C3D-C2D	2.53	1.46	1.39
24	s	607	CHL	C3B-C4B	2.53	1.48	1.42
25	3	603	CLA	C3B-C4B	2.53	1.48	1.42
25	y	612	CLA	C3B-C4B	2.53	1.48	1.42
25	C	506	CLA	CMB-C2B	-2.53	1.45	1.50
25	c	511	CLA	C4B-NB	2.53	1.40	1.37
24	4	601	CHL	C1D-C2D	2.53	1.50	1.45
39	d	405	PL9	C26-C24	-2.53	1.46	1.51
24	2	601	CHL	C1D-C2D	2.53	1.50	1.45
24	g	607	CHL	MG-NA	-2.53	2.00	2.06
25	A	405	CLA	C4B-NB	2.53	1.40	1.37
25	C	510	CLA	C4B-NB	2.53	1.40	1.37
25	Y	611	CLA	C1D-ND	2.53	1.40	1.37
25	2	612	CLA	C3B-C4B	2.53	1.48	1.42
25	G	603	CLA	MG-ND	-2.53	2.00	2.05
25	C	513	CLA	C1B-C2B	2.53	1.49	1.43
39	D	405	PL9	C26-C24	-2.53	1.46	1.51
25	R	610	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	603	CLA	C1B-C2B	2.53	1.49	1.43
24	N	601	CHL	C1D-C2D	2.52	1.50	1.45
25	b	615	CLA	C4B-NB	2.52	1.40	1.37
25	8	614	CLA	C1B-C2B	2.52	1.49	1.43
25	R	603	CLA	C4B-NB	2.52	1.40	1.37
25	5	614	CLA	C1B-C2B	2.52	1.49	1.43
24	1	608	CHL	MG-NA	-2.52	2.00	2.06
24	2	608	CHL	C3B-C4B	2.52	1.48	1.42
24	p	605	CHL	C1B-C2B	2.52	1.49	1.43
24	8	607	CHL	C4B-NB	-2.52	1.34	1.37
25	a	405	CLA	C4B-NB	2.52	1.40	1.37
25	b	611	CLA	C1B-NB	-2.52	1.34	1.37
25	c	510	CLA	C1B-NB	-2.52	1.34	1.37
25	R	611	CLA	C3B-C4B	2.52	1.48	1.42
28	r	623	NEX	C1-C6	-2.52	1.50	1.54
33	a	409	PHO	CMB-C2B	-2.52	1.46	1.51
25	S	611	CLA	C3B-C4B	2.52	1.48	1.42
25	c	503	CLA	C3B-C4B	2.52	1.48	1.42
25	B	609	CLA	MG-NB	-2.52	2.00	2.05
25	b	609	CLA	MG-NB	-2.52	2.00	2.05
24	0	601	CHL	C4B-NB	-2.52	1.34	1.37
25	n	603	CLA	C4B-NB	2.52	1.40	1.37
24	S	606	CHL	C3D-C2D	2.52	1.46	1.39
25	B	617	CLA	MG-NB	-2.52	2.00	2.05
24	2	605	CHL	C3B-C4B	2.52	1.48	1.42
24	G	608	CHL	C4B-NB	-2.52	1.34	1.37
24	2	606	CHL	C1B-NB	-2.52	1.34	1.37
25	1	602	CLA	C1B-C2B	2.52	1.49	1.43
24	g	609	CHL	C1D-C2D	2.52	1.50	1.45
25	C	505	CLA	C1D-ND	2.52	1.40	1.37
25	A	410	CLA	MG-NB	-2.52	2.00	2.05
24	5	607	CHL	C1B-NB	-2.52	1.34	1.37
24	g	605	CHL	C3B-C4B	2.52	1.48	1.42
24	6	608	CHL	C1D-C2D	2.52	1.50	1.45
25	n	610	CLA	C3B-C4B	2.52	1.48	1.42
25	B	609	CLA	C1B-NB	-2.52	1.34	1.37
25	b	609	CLA	C1B-NB	-2.52	1.34	1.37
25	b	605	CLA	CMB-C2B	-2.52	1.45	1.50
24	Y	605	CHL	C1D-C2D	2.52	1.50	1.45
24	y	605	CHL	C1D-C2D	2.52	1.50	1.45
25	G	612	CLA	C3B-C4B	2.51	1.48	1.42
25	g	611	CLA	C3B-C4B	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	609	CHL	MG-NA	-2.51	2.00	2.06
24	5	606	CHL	C1B-NB	-2.51	1.34	1.37
24	9	606	CHL	C4B-NB	-2.51	1.34	1.37
25	6	611	CLA	C1B-C2B	2.51	1.49	1.43
24	g	605	CHL	MG-NA	-2.51	2.00	2.06
25	Y	612	CLA	C3B-C4B	2.51	1.48	1.42
24	p	609	CHL	C1B-NB	-2.51	1.34	1.37
25	c	502	CLA	MG-NB	-2.51	2.00	2.05
24	y	609	CHL	CHB-C1B	2.51	1.45	1.39
33	A	409	PHO	CMB-C2B	-2.51	1.46	1.51
25	g	603	CLA	MG-ND	-2.51	2.00	2.05
25	B	611	CLA	C4B-NB	2.51	1.40	1.37
25	G	602	CLA	C4B-NB	2.51	1.40	1.37
25	b	611	CLA	C4B-NB	2.51	1.40	1.37
24	S	608	CHL	C3D-C2D	2.51	1.46	1.39
25	n	604	CLA	C3B-C4B	2.51	1.48	1.42
25	B	610	CLA	CMD-C2D	-2.51	1.45	1.50
25	q	611	CLA	C1B-C2B	2.51	1.49	1.43
24	4	608	CHL	C4B-NB	-2.51	1.34	1.37
24	9	607	CHL	C1B-NB	-2.51	1.34	1.37
25	c	505	CLA	MG-ND	-2.51	2.00	2.05
28	s	1623	NEX	C1-C6	-2.51	1.50	1.54
24	5	606	CHL	MG-NA	-2.51	2.00	2.06
25	6	604	CLA	C3B-C4B	2.51	1.48	1.42
24	8	608	CHL	MG-NA	-2.50	2.00	2.06
25	y	603	CLA	C4B-NB	2.50	1.40	1.37
24	p	601	CHL	C1B-C2B	2.50	1.49	1.43
24	8	601	CHL	C1B-C2B	2.50	1.49	1.43
25	B	612	CLA	C3B-C4B	2.50	1.48	1.42
25	b	612	CLA	C3B-C4B	2.50	1.48	1.42
24	2	608	CHL	C4B-NB	-2.50	1.34	1.37
25	s	602	CLA	MG-NB	-2.50	2.00	2.05
25	4	604	CLA	C1B-C2B	2.50	1.49	1.43
25	2	611	CLA	C1B-C2B	2.50	1.49	1.43
25	g	603	CLA	C1B-C2B	2.50	1.49	1.43
25	B	615	CLA	CMD-C2D	-2.50	1.45	1.50
24	0	607	CHL	MG-NA	-2.50	2.00	2.06
25	N	603	CLA	C4B-NB	2.50	1.40	1.37
24	q	607	CHL	C1B-NB	-2.50	1.34	1.37
25	Y	614	CLA	MG-NB	-2.50	2.00	2.05
25	y	614	CLA	MG-NB	-2.50	2.00	2.05
24	5	606	CHL	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	605	CHL	CHB-C4A	-2.50	1.31	1.37
25	g	612	CLA	C3B-C4B	2.50	1.48	1.42
25	1	614	CLA	C1B-C2B	2.49	1.49	1.43
25	c	503	CLA	C4B-NB	2.49	1.40	1.37
25	G	613	CLA	C1B-C2B	2.49	1.49	1.43
24	0	608	CHL	C3D-C2D	2.49	1.45	1.39
25	n	613	CLA	C3B-C4B	2.49	1.48	1.42
24	9	605	CHL	C4B-NB	-2.49	1.34	1.37
24	9	601	CHL	CHB-C4A	-2.49	1.31	1.37
24	9	607	CHL	C1B-C2B	2.49	1.49	1.43
24	y	605	CHL	C4B-NB	-2.49	1.34	1.37
25	S	610	CLA	CMD-C2D	-2.49	1.45	1.50
24	G	606	CHL	C3B-C4B	2.49	1.48	1.42
24	5	605	CHL	C1B-C2B	2.49	1.49	1.43
25	c	507	CLA	MG-NB	-2.49	2.00	2.05
24	s	606	CHL	C1B-NB	-2.49	1.34	1.37
25	B	611	CLA	MG-NB	-2.49	2.00	2.05
25	4	611	CLA	C1B-C2B	2.49	1.49	1.43
24	5	601	CHL	C1B-NB	-2.49	1.34	1.37
24	N	608	CHL	MG-NA	-2.49	2.00	2.06
25	b	610	CLA	C4B-NB	2.49	1.40	1.37
25	S	602	CLA	MG-NB	-2.49	2.00	2.05
40	F	101	HEM	FE-NC	2.49	2.03	1.95
24	7	606	CHL	C1D-C2D	2.49	1.50	1.45
25	B	611	CLA	CMB-C2B	-2.49	1.45	1.50
24	G	605	CHL	C3B-C4B	2.49	1.48	1.42
25	7	602	CLA	C1B-C2B	2.49	1.49	1.43
24	n	607	CHL	C3B-C4B	2.48	1.48	1.42
25	b	611	CLA	CMB-C2B	-2.48	1.45	1.50
24	g	605	CHL	C4C-C3C	2.48	1.49	1.45
24	4	606	CHL	C1B-NB	-2.48	1.34	1.37
25	g	603	CLA	C3B-C4B	2.48	1.48	1.42
24	5	609	CHL	C1B-C2B	2.48	1.49	1.43
25	Y	604	CLA	MG-NB	-2.48	2.00	2.05
25	g	603	CLA	CMD-C2D	-2.48	1.45	1.50
25	C	503	CLA	C3B-C4B	2.48	1.48	1.42
24	Y	608	CHL	MG-NA	-2.48	2.00	2.06
25	c	508	CLA	CMD-C2D	-2.48	1.45	1.50
24	9	606	CHL	C1D-C2D	2.48	1.50	1.45
25	G	603	CLA	C1B-C2B	2.48	1.49	1.43
25	9	614	CLA	C1B-C2B	2.48	1.49	1.43
25	y	611	CLA	C1D-ND	2.48	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	C1B-NB	-2.48	1.34	1.37
25	q	614	CLA	C1B-C2B	2.48	1.49	1.43
25	s	603	CLA	C3B-C4B	2.48	1.48	1.42
24	5	608	CHL	C1B-NB	-2.48	1.34	1.37
24	g	606	CHL	C3B-C4B	2.48	1.48	1.42
25	s	610	CLA	CMD-C2D	-2.48	1.45	1.50
25	b	604	CLA	CMC-C2C	-2.48	1.45	1.50
25	4	613	CLA	C1B-C2B	2.48	1.49	1.43
25	q	613	CLA	C1B-C2B	2.48	1.49	1.43
24	y	605	CHL	CHB-C4A	-2.47	1.31	1.37
25	b	615	CLA	CMD-C2D	-2.47	1.45	1.50
24	6	609	CHL	MG-NA	-2.47	2.00	2.06
25	4	614	CLA	C1B-C2B	2.47	1.49	1.43
24	3	601	CHL	C1B-NB	-2.47	1.34	1.37
24	S	606	CHL	C1B-NB	-2.47	1.34	1.37
24	q	607	CHL	C4C-C3C	2.47	1.49	1.45
25	b	617	CLA	MG-NB	-2.47	2.00	2.05
25	c	513	CLA	CMD-C2D	-2.47	1.45	1.50
25	S	611	CLA	MG-NB	-2.47	2.00	2.05
24	q	605	CHL	C4C-C3C	2.47	1.49	1.45
24	1	606	CHL	C1D-C2D	2.47	1.50	1.45
24	Y	606	CHL	CHB-C4A	-2.47	1.31	1.37
24	7	601	CHL	C3B-C4B	2.47	1.48	1.42
25	8	603	CLA	C1B-C2B	2.47	1.49	1.43
25	s	609	CLA	C1B-C2B	2.47	1.49	1.43
25	Y	612	CLA	CMD-C2D	-2.47	1.45	1.50
24	0	605	CHL	MG-NA	-2.47	2.00	2.06
24	2	607	CHL	C1B-C2B	2.47	1.49	1.43
24	G	608	CHL	C1D-C2D	2.47	1.50	1.45
25	A	405	CLA	CMD-C2D	-2.47	1.45	1.50
25	a	405	CLA	CMD-C2D	-2.47	1.45	1.50
24	y	608	CHL	MG-NA	-2.47	2.00	2.06
24	0	605	CHL	C3B-C4B	2.47	1.48	1.42
25	s	611	CLA	MG-NB	-2.47	2.00	2.05
25	Y	603	CLA	C4B-NB	2.47	1.40	1.37
25	2	614	CLA	C1B-C2B	2.47	1.49	1.43
25	q	612	CLA	C1B-C2B	2.46	1.49	1.43
33	A	408	PHO	C3B-C2B	-2.46	1.36	1.40
33	a	408	PHO	C3B-C2B	-2.46	1.36	1.40
34	C	515	BCR	C30-C25	-2.46	1.50	1.53
25	C	512	CLA	C3B-C4B	2.46	1.48	1.42
25	y	604	CLA	MG-NB	-2.46	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	612	CLA	MG-ND	-2.46	2.00	2.05
24	6	605	CHL	C1B-C2B	2.46	1.49	1.43
25	3	603	CLA	C1B-C2B	2.46	1.49	1.43
25	b	608	CLA	C3B-C4B	2.46	1.48	1.42
25	B	606	CLA	C3B-C4B	2.46	1.48	1.42
25	G	611	CLA	C3B-C4B	2.46	1.48	1.42
25	S	609	CLA	C1B-C2B	2.46	1.49	1.43
24	2	606	CHL	C4B-NB	-2.46	1.34	1.37
26	y	1620	LUT	C10-C9	-2.46	1.32	1.35
24	2	605	CHL	C1B-NB	-2.46	1.34	1.37
24	p	606	CHL	C4B-NB	-2.46	1.34	1.37
24	N	609	CHL	CHB-C4A	-2.46	1.31	1.37
24	7	609	CHL	C3B-C4B	2.46	1.48	1.42
24	q	606	CHL	C1B-NB	-2.46	1.34	1.37
24	g	606	CHL	C1D-C2D	2.46	1.50	1.45
25	S	603	CLA	C3B-C4B	2.46	1.48	1.42
25	3	610	CLA	C1B-C2B	2.46	1.49	1.43
25	4	610	CLA	C1B-C2B	2.46	1.49	1.43
25	R	611	CLA	C1B-C2B	2.46	1.49	1.43
25	b	611	CLA	MG-NB	-2.46	2.00	2.05
25	0	604	CLA	C3B-C4B	2.46	1.48	1.42
25	Y	604	CLA	CMD-C2D	-2.46	1.45	1.50
25	b	610	CLA	CMD-C2D	-2.46	1.45	1.50
24	y	606	CHL	CHB-C4A	-2.46	1.31	1.37
25	G	603	CLA	CMD-C2D	-2.46	1.45	1.50
25	0	611	CLA	C1B-C2B	2.46	1.49	1.43
24	g	608	CHL	C1D-C2D	2.46	1.50	1.45
25	q	610	CLA	C1B-C2B	2.46	1.49	1.43
24	5	601	CHL	C1B-C2B	2.45	1.49	1.43
25	B	606	CLA	CMD-C2D	-2.45	1.45	1.50
25	B	607	CLA	CMD-C2D	-2.45	1.45	1.50
25	C	508	CLA	CMD-C2D	-2.45	1.45	1.50
24	G	607	CHL	C1D-C2D	2.45	1.50	1.45
24	G	608	CHL	C3D-C2D	2.45	1.45	1.39
25	y	610	CLA	C4B-NB	2.45	1.40	1.37
25	B	604	CLA	CMC-C2C	-2.45	1.45	1.50
25	C	513	CLA	CMD-C2D	-2.45	1.45	1.50
25	B	608	CLA	C3B-C4B	2.45	1.48	1.42
24	q	601	CHL	C3D-C2D	2.45	1.45	1.39
25	r	601	CLA	C1B-C2B	2.45	1.49	1.43
24	7	608	CHL	MG-NA	-2.45	2.00	2.06
24	p	607	CHL	C1B-NB	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	CMD-C2D	-2.45	1.45	1.50
25	N	613	CLA	C1B-C2B	2.45	1.49	1.43
25	8	603	CLA	C3B-C4B	2.45	1.48	1.42
26	Y	1620	LUT	C10-C9	-2.45	1.32	1.35
25	9	604	CLA	C1B-C2B	2.45	1.49	1.43
25	r	611	CLA	C1B-C2B	2.45	1.49	1.43
25	y	604	CLA	CMD-C2D	-2.45	1.45	1.50
24	8	607	CHL	C1D-C2D	2.45	1.50	1.45
25	N	604	CLA	C3B-C4B	2.45	1.48	1.42
25	N	613	CLA	C3B-C4B	2.45	1.48	1.42
25	b	609	CLA	CMD-C2D	-2.45	1.45	1.50
25	b	612	CLA	MG-NB	-2.45	2.00	2.05
25	a	405	CLA	C3B-C4B	2.45	1.48	1.42
24	1	601	CHL	C3B-C4B	2.44	1.48	1.42
25	B	615	CLA	CMB-C2B	-2.44	1.45	1.50
25	b	615	CLA	CMB-C2B	-2.44	1.45	1.50
24	q	605	CHL	C1B-NB	-2.44	1.34	1.37
25	B	611	CLA	C1B-NB	-2.44	1.34	1.37
24	8	601	CHL	C3D-C2D	2.44	1.45	1.39
24	s	606	CHL	C1B-C2B	2.44	1.49	1.43
25	p	610	CLA	C1B-C2B	2.44	1.49	1.43
24	2	605	CHL	C4B-NB	-2.44	1.34	1.37
24	3	607	CHL	C4B-NB	-2.44	1.34	1.37
25	7	613	CLA	C3B-C4B	2.44	1.48	1.42
24	R	606	CHL	CHB-C4A	-2.44	1.31	1.37
25	p	612	CLA	C1B-C2B	2.44	1.49	1.43
24	n	609	CHL	CHB-C4A	-2.44	1.31	1.37
24	S	601	CHL	C3D-C2D	2.44	1.45	1.39
25	D	402	CLA	CMC-C2C	-2.44	1.45	1.50
25	y	611	CLA	CMB-C2B	-2.44	1.45	1.50
24	2	607	CHL	C3B-C4B	2.44	1.48	1.42
25	N	603	CLA	CMB-C2B	-2.44	1.45	1.50
24	9	607	CHL	C3B-C4B	2.44	1.48	1.42
25	R	613	CLA	C1B-C2B	2.44	1.49	1.43
25	C	507	CLA	MG-ND	-2.44	2.00	2.05
24	Y	609	CHL	CHB-C1B	2.44	1.44	1.39
25	C	511	CLA	C4B-NB	2.44	1.40	1.37
25	B	613	CLA	CMC-C2C	-2.44	1.45	1.50
25	b	613	CLA	CMC-C2C	-2.44	1.45	1.50
24	p	609	CHL	C1B-C2B	2.44	1.49	1.43
25	C	512	CLA	MG-ND	-2.44	2.01	2.05
25	y	612	CLA	MG-ND	-2.44	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	603	CLA	C3B-C4B	2.44	1.48	1.42
24	4	605	CHL	C1B-NB	-2.44	1.34	1.37
25	g	614	CLA	MG-NB	-2.44	2.01	2.05
24	4	607	CHL	C1B-NB	-2.44	1.34	1.37
24	n	608	CHL	MG-NA	-2.44	2.00	2.06
25	B	612	CLA	CMD-C2D	-2.44	1.45	1.50
25	b	612	CLA	CMD-C2D	-2.44	1.45	1.50
25	B	612	CLA	MG-NB	-2.44	2.01	2.05
24	2	601	CHL	CHB-C4A	-2.44	1.31	1.37
24	G	605	CHL	C1B-NB	-2.44	1.34	1.37
25	Y	611	CLA	CMB-C2B	-2.44	1.45	1.50
25	Y	613	CLA	CMB-C2B	-2.44	1.45	1.50
25	y	612	CLA	CMD-C2D	-2.44	1.45	1.50
25	s	603	CLA	C1B-C2B	2.44	1.49	1.43
25	r	613	CLA	C1B-C2B	2.43	1.49	1.43
25	B	606	CLA	CMB-C2B	-2.43	1.45	1.50
24	3	601	CHL	C3D-C2D	2.43	1.45	1.39
25	7	603	CLA	C3B-C4B	2.43	1.48	1.42
25	b	607	CLA	CMD-C2D	-2.43	1.45	1.50
24	p	608	CHL	C1B-NB	-2.43	1.34	1.37
25	y	611	CLA	C3B-C4B	2.43	1.48	1.42
25	c	509	CLA	CMD-C2D	-2.43	1.45	1.50
25	b	606	CLA	C3B-C4B	2.43	1.48	1.42
25	N	614	CLA	C1B-C2B	2.43	1.49	1.43
25	8	610	CLA	C1B-C2B	2.43	1.49	1.43
25	c	504	CLA	CMD-C2D	-2.43	1.45	1.50
25	3	612	CLA	C1B-C2B	2.43	1.49	1.43
24	r	606	CHL	CHB-C4A	-2.43	1.31	1.37
25	Y	603	CLA	CMB-C2B	-2.43	1.45	1.50
24	2	608	CHL	C3D-C2D	2.43	1.45	1.39
33	A	409	PHO	CAC-C3C	-2.43	1.47	1.51
25	S	613	CLA	MG-ND	-2.43	2.01	2.05
24	9	601	CHL	C3D-C2D	2.43	1.45	1.39
24	Y	605	CHL	C4B-NB	-2.43	1.34	1.37
25	B	610	CLA	C4B-NB	2.43	1.40	1.37
25	a	407	CLA	CMD-C2D	-2.43	1.45	1.50
25	g	603	CLA	CMB-C2B	-2.42	1.45	1.50
25	B	614	CLA	C1B-NB	-2.42	1.34	1.37
25	C	501	CLA	CMB-C2B	-2.42	1.45	1.50
24	6	605	CHL	C3B-C4B	2.42	1.48	1.42
25	1	613	CLA	C3B-C4B	2.42	1.48	1.42
25	A	405	CLA	C3B-C4B	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	605	CHL	C1B-C2B	2.42	1.49	1.43
25	7	613	CLA	C1B-C2B	2.42	1.49	1.43
25	Y	602	CLA	C3B-C4B	2.42	1.48	1.42
24	N	608	CHL	C3B-C4B	2.42	1.48	1.42
25	b	604	CLA	MG-ND	-2.42	2.01	2.05
25	S	603	CLA	C1B-C2B	2.42	1.49	1.43
25	G	614	CLA	MG-NB	-2.42	2.01	2.05
24	g	608	CHL	C3D-C2D	2.42	1.45	1.39
24	y	608	CHL	C4B-NB	-2.42	1.34	1.37
25	p	611	CLA	C1B-C2B	2.42	1.49	1.43
25	b	606	CLA	CMD-C2D	-2.42	1.45	1.50
24	5	607	CHL	C1D-C2D	2.42	1.50	1.45
25	4	603	CLA	C1B-C2B	2.42	1.49	1.43
24	G	607	CHL	C3D-C2D	2.42	1.45	1.39
24	3	607	CHL	C1D-C2D	2.42	1.50	1.45
25	4	612	CLA	C1B-C2B	2.42	1.48	1.43
25	y	613	CLA	CMB-C2B	-2.42	1.45	1.50
25	R	601	CLA	C1B-C2B	2.42	1.48	1.43
24	p	609	CHL	MG-NA	-2.42	2.00	2.06
25	y	602	CLA	C4B-NB	2.42	1.40	1.37
24	0	606	CHL	C4B-NB	-2.42	1.34	1.37
25	c	504	CLA	C3B-C4B	2.42	1.48	1.42
25	y	603	CLA	CMB-C2B	-2.42	1.45	1.50
24	9	608	CHL	C3D-C2D	2.42	1.45	1.39
25	C	501	CLA	MG-NB	-2.42	2.01	2.05
24	6	608	CHL	C3D-C2D	2.42	1.45	1.39
25	c	501	CLA	MG-NB	-2.41	2.01	2.05
28	R	623	NEX	O24-C25	-2.41	1.42	1.46
25	d	402	CLA	CMB-C2B	-2.41	1.45	1.50
24	9	609	CHL	C1B-C2B	2.41	1.48	1.43
25	B	617	CLA	CMB-C2B	-2.41	1.45	1.50
25	s	604	CLA	CMB-C2B	-2.41	1.45	1.50
25	C	504	CLA	CMD-C2D	-2.41	1.45	1.50
25	9	602	CLA	C3B-C4B	2.41	1.48	1.42
25	C	504	CLA	C3B-C4B	2.41	1.48	1.42
25	Y	610	CLA	CMD-C2D	-2.41	1.45	1.50
25	9	610	CLA	CMC-C2C	-2.41	1.45	1.50
25	2	602	CLA	C3B-C4B	2.41	1.48	1.42
24	g	601	CHL	MG-NA	-2.41	2.00	2.06
25	d	402	CLA	CMC-C2C	-2.41	1.45	1.50
25	Y	611	CLA	C3B-C4B	2.41	1.48	1.42
24	0	607	CHL	C1D-C2D	2.41	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	607	CHL	CHB-C1B	2.41	1.44	1.39
25	0	603	CLA	C1B-C2B	2.41	1.48	1.43
24	q	607	CHL	C1B-C2B	2.41	1.48	1.43
25	B	614	CLA	C4B-NB	2.41	1.40	1.37
25	8	612	CLA	C1B-C2B	2.41	1.48	1.43
25	q	611	CLA	CMD-C2D	-2.41	1.45	1.50
25	c	510	CLA	MG-ND	-2.41	2.01	2.05
25	B	612	CLA	CMB-C2B	-2.41	1.45	1.50
25	b	605	CLA	MG-NB	-2.41	2.01	2.05
24	9	605	CHL	C1B-NB	-2.41	1.34	1.37
24	2	606	CHL	MG-NA	-2.40	2.00	2.06
25	D	402	CLA	CMB-C2B	-2.40	1.45	1.50
25	b	613	CLA	MG-NB	-2.40	2.01	2.05
25	a	405	CLA	CMB-C2B	-2.40	1.45	1.50
25	N	603	CLA	MG-ND	-2.40	2.01	2.05
25	G	603	CLA	CMB-C2B	-2.40	1.45	1.50
25	n	603	CLA	CMB-C2B	-2.40	1.45	1.50
25	q	603	CLA	C1B-C2B	2.40	1.48	1.43
24	0	609	CHL	C3B-C4B	2.40	1.48	1.42
25	C	507	CLA	CMD-C2D	-2.40	1.45	1.50
25	R	603	CLA	CMB-C2B	-2.40	1.45	1.50
25	c	511	CLA	CMD-C2D	-2.40	1.45	1.50
25	r	603	CLA	CMB-C2B	-2.40	1.45	1.50
25	c	501	CLA	MG-ND	-2.40	2.01	2.05
25	n	613	CLA	C1B-C2B	2.40	1.48	1.43
25	C	510	CLA	MG-ND	-2.40	2.01	2.05
25	c	501	CLA	C1B-NB	-2.40	1.34	1.37
25	B	604	CLA	MG-ND	-2.40	2.01	2.05
24	3	606	CHL	C3B-C4B	2.40	1.48	1.42
25	c	508	CLA	CMB-C2B	-2.40	1.45	1.50
25	c	505	CLA	MG-NB	-2.40	2.01	2.05
25	C	501	CLA	CMC-C2C	-2.40	1.45	1.50
25	2	610	CLA	CMC-C2C	-2.40	1.45	1.50
33	a	409	PHO	CAC-C3C	-2.40	1.47	1.51
24	N	609	CHL	C1C-NC	-2.40	1.34	1.37
25	a	407	CLA	MG-NB	-2.40	2.01	2.05
25	s	613	CLA	MG-ND	-2.40	2.01	2.05
25	A	407	CLA	CMD-C2D	-2.40	1.45	1.50
25	1	613	CLA	C1B-C2B	2.40	1.48	1.43
25	R	609	CLA	CMD-C2D	-2.40	1.45	1.50
25	r	609	CLA	CMD-C2D	-2.40	1.45	1.50
24	S	608	CHL	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CMD-C2D	-2.40	1.45	1.50
25	B	615	CLA	MG-NB	-2.40	2.01	2.05
25	a	406	CLA	MG-NB	-2.40	2.01	2.05
25	B	613	CLA	MG-NB	-2.39	2.01	2.05
25	b	617	CLA	CMC-C2C	-2.39	1.45	1.50
24	9	608	CHL	C4B-NB	-2.39	1.34	1.37
25	A	410	CLA	C1B-NB	-2.39	1.34	1.37
25	a	410	CLA	C1B-NB	-2.39	1.34	1.37
24	4	607	CHL	C4C-C3C	2.39	1.49	1.45
25	b	612	CLA	CMB-C2B	-2.39	1.45	1.50
25	b	612	CLA	C4B-NB	2.39	1.40	1.37
25	b	614	CLA	C1B-NB	-2.39	1.34	1.37
25	n	614	CLA	C1B-C2B	2.39	1.48	1.43
25	N	603	CLA	CMD-C2D	-2.39	1.45	1.50
34	c	515	BCR	C30-C25	-2.39	1.50	1.53
24	G	601	CHL	MG-NA	-2.39	2.00	2.06
25	6	603	CLA	C1B-C2B	2.39	1.48	1.43
25	B	605	CLA	MG-NB	-2.39	2.01	2.05
24	n	605	CHL	CHB-C4A	-2.39	1.32	1.37
25	B	604	CLA	C4B-NB	2.39	1.40	1.37
25	b	603	CLA	CMD-C2D	-2.39	1.45	1.50
25	A	405	CLA	CMB-C2B	-2.39	1.45	1.50
24	6	607	CHL	C1B-NB	-2.39	1.34	1.37
24	4	607	CHL	C1B-C2B	2.39	1.48	1.43
25	c	507	CLA	MG-ND	-2.39	2.01	2.05
24	2	609	CHL	C3B-C4B	2.39	1.48	1.42
24	3	608	CHL	C3D-C2D	2.39	1.45	1.39
24	S	606	CHL	C1B-C2B	2.39	1.48	1.43
25	A	405	CLA	C1B-NB	-2.39	1.34	1.37
25	C	509	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	608	CLA	CMD-C2D	-2.39	1.45	1.50
25	c	501	CLA	CMB-C2B	-2.39	1.45	1.50
25	B	609	CLA	CMD-C2D	-2.39	1.45	1.50
24	G	606	CHL	C1D-C2D	2.39	1.50	1.45
24	6	605	CHL	C1B-NB	-2.38	1.34	1.37
25	R	603	CLA	CMD-C2D	-2.38	1.45	1.50
24	p	606	CHL	C1B-C2B	2.38	1.48	1.43
25	1	602	CLA	CMC-C2C	-2.38	1.45	1.50
25	Y	602	CLA	C4B-NB	2.38	1.40	1.37
25	R	602	CLA	C1B-C2B	2.38	1.48	1.43
25	Y	613	CLA	CMC-C2C	-2.38	1.45	1.50
25	c	504	CLA	CMC-C2C	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	613	CLA	CMC-C2C	-2.38	1.45	1.50
24	p	608	CHL	C3D-C2D	2.38	1.45	1.39
25	Y	611	CLA	MG-NB	-2.38	2.01	2.05
25	b	608	CLA	C1B-NB	-2.38	1.34	1.37
25	G	610	CLA	CMC-C2C	-2.38	1.45	1.50
24	5	606	CHL	C4C-C3C	2.38	1.49	1.45
25	y	611	CLA	MG-NB	-2.38	2.01	2.05
25	Y	612	CLA	CMC-C2C	-2.38	1.45	1.50
24	1	609	CHL	C3B-C4B	2.38	1.48	1.42
25	2	602	CLA	C1B-C2B	2.38	1.48	1.43
25	B	617	CLA	CMC-C2C	-2.38	1.45	1.50
25	a	406	CLA	CMD-C2D	-2.38	1.45	1.50
24	9	609	CHL	C3B-C4B	2.38	1.48	1.42
28	r	623	NEX	O24-C25	-2.38	1.42	1.46
25	S	614	CLA	CMD-C2D	-2.38	1.45	1.50
24	9	606	CHL	C1B-C2B	2.38	1.48	1.43
25	c	512	CLA	MG-ND	-2.38	2.01	2.05
24	8	608	CHL	C3D-C2D	2.38	1.45	1.39
24	6	606	CHL	C4B-NB	-2.38	1.34	1.37
24	2	608	CHL	C1B-C2B	2.38	1.48	1.43
25	r	603	CLA	CMD-C2D	-2.38	1.45	1.50
25	n	603	CLA	MG-NB	-2.38	2.01	2.05
24	5	608	CHL	C3D-C2D	2.38	1.45	1.39
25	Y	613	CLA	CMD-C2D	-2.38	1.45	1.50
25	B	608	CLA	CMD-C2D	-2.38	1.45	1.50
25	b	606	CLA	CMB-C2B	-2.38	1.45	1.50
24	N	605	CHL	CHB-C4A	-2.38	1.32	1.37
25	g	610	CLA	CMC-C2C	-2.38	1.45	1.50
24	s	608	CHL	C1B-C2B	2.38	1.48	1.43
24	S	601	CHL	C3B-C4B	2.37	1.48	1.42
24	n	608	CHL	C3B-C4B	2.37	1.48	1.42
25	7	602	CLA	CMC-C2C	-2.37	1.45	1.50
25	N	602	CLA	MG-NB	-2.37	2.01	2.05
25	1	603	CLA	C3B-C4B	2.37	1.48	1.42
25	c	509	CLA	C1B-C2B	2.37	1.48	1.43
25	g	613	CLA	CMD-C2D	-2.37	1.45	1.50
25	Y	611	CLA	MG-ND	-2.37	2.01	2.05
25	b	617	CLA	CMB-C2B	-2.37	1.45	1.50
25	g	602	CLA	CMC-C2C	-2.37	1.45	1.50
24	0	605	CHL	C4B-NB	-2.37	1.34	1.37
24	g	601	CHL	C3B-C4B	2.37	1.48	1.42
24	8	605	CHL	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	MG-NB	-2.37	2.01	2.05
25	N	603	CLA	MG-NB	-2.37	2.01	2.05
25	6	604	CLA	CMB-C2B	-2.37	1.45	1.50
25	R	612	CLA	C1B-C2B	2.37	1.48	1.43
25	r	612	CLA	C1B-C2B	2.37	1.48	1.43
25	s	614	CLA	CMD-C2D	-2.37	1.45	1.50
25	Y	613	CLA	C3B-C4B	2.37	1.48	1.42
24	n	609	CHL	C1D-C2D	2.37	1.50	1.45
25	A	407	CLA	MG-NB	-2.37	2.01	2.05
25	b	611	CLA	MG-ND	-2.37	2.01	2.05
25	0	603	CLA	CMD-C2D	-2.37	1.45	1.50
27	r	622	XAT	O4-C5	-2.37	1.42	1.46
25	n	603	CLA	MG-ND	-2.37	2.01	2.05
25	S	604	CLA	CMB-C2B	-2.37	1.45	1.50
24	R	607	CHL	CHB-C1B	2.37	1.44	1.39
24	q	606	CHL	C2C-C1C	2.37	1.49	1.44
25	5	611	CLA	C1B-C2B	2.37	1.48	1.43
24	r	606	CHL	C1D-C2D	2.36	1.50	1.45
25	R	610	CLA	C3B-C4B	2.36	1.48	1.42
24	2	606	CHL	C3B-C4B	2.36	1.48	1.42
25	y	613	CLA	C3B-C4B	2.36	1.48	1.42
25	b	614	CLA	CMC-C2C	-2.36	1.45	1.50
25	B	612	CLA	C4B-NB	2.36	1.40	1.37
25	1	603	CLA	CMB-C2B	-2.36	1.45	1.50
25	1	614	CLA	CMD-C2D	-2.36	1.45	1.50
25	B	614	CLA	CMC-C2C	-2.36	1.45	1.50
25	7	611	CLA	CMD-C2D	-2.36	1.45	1.50
24	3	605	CHL	C4C-C3C	2.36	1.49	1.45
24	6	606	CHL	C3D-C2D	2.36	1.45	1.39
25	S	613	CLA	C3B-C4B	2.36	1.48	1.42
24	2	606	CHL	C1B-C2B	2.36	1.48	1.43
24	9	608	CHL	C1B-C2B	2.36	1.48	1.43
25	S	614	CLA	C1B-C2B	2.36	1.48	1.43
25	c	509	CLA	CMC-C2C	-2.36	1.45	1.50
24	G	601	CHL	C3B-C4B	2.36	1.48	1.42
24	8	606	CHL	C4C-C3C	2.36	1.49	1.45
25	y	610	CLA	CMD-C2D	-2.36	1.45	1.50
25	b	615	CLA	MG-NB	-2.36	2.01	2.05
25	n	611	CLA	C1B-C2B	2.36	1.48	1.43
25	A	406	CLA	MG-NB	-2.36	2.01	2.05
24	4	605	CHL	C4B-NB	-2.36	1.34	1.37
24	N	605	CHL	C1D-C2D	2.36	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	602	CLA	MG-NB	-2.36	2.01	2.05
25	C	504	CLA	CMC-C2C	-2.36	1.45	1.50
24	4	606	CHL	C2C-C1C	2.36	1.49	1.44
25	A	406	CLA	CMD-C2D	-2.36	1.45	1.50
25	C	504	CLA	CMB-C2B	-2.36	1.45	1.50
25	b	616	CLA	CMD-C2D	-2.36	1.45	1.50
25	y	611	CLA	MG-ND	-2.36	2.01	2.05
24	8	607	CHL	C3D-C2D	2.36	1.45	1.39
24	N	608	CHL	C1B-C2B	2.36	1.48	1.43
25	1	611	CLA	CMD-C2D	-2.36	1.45	1.50
24	7	608	CHL	C1B-C2B	2.36	1.48	1.43
24	n	607	CHL	C1D-ND	-2.36	1.34	1.37
25	B	615	CLA	CMC-C2C	-2.36	1.45	1.50
24	9	608	CHL	MG-NA	-2.36	2.00	2.06
25	b	615	CLA	C3B-C4B	2.36	1.48	1.42
25	G	613	CLA	CMD-C2D	-2.36	1.45	1.50
25	s	611	CLA	CMD-C2D	-2.36	1.45	1.50
25	B	614	CLA	MG-ND	-2.35	2.01	2.05
24	n	607	CHL	CHB-C4A	-2.35	1.32	1.37
24	6	607	CHL	C3B-C4B	2.35	1.48	1.42
24	R	606	CHL	C1D-C2D	2.35	1.50	1.45
25	y	614	CLA	C3B-C4B	2.35	1.48	1.42
24	8	605	CHL	C4C-C3C	2.35	1.49	1.45
25	y	610	CLA	CMC-C2C	-2.35	1.45	1.50
24	3	607	CHL	C3D-C2D	2.35	1.45	1.39
25	r	604	CLA	CMD-C2D	-2.35	1.45	1.50
24	q	606	CHL	C4C-C3C	2.35	1.49	1.45
25	G	602	CLA	CMC-C2C	-2.35	1.45	1.50
25	y	604	CLA	C1B-NB	-2.35	1.34	1.37
25	C	509	CLA	C1B-C2B	2.35	1.48	1.43
25	Y	610	CLA	CMC-C2C	-2.35	1.45	1.50
25	Y	614	CLA	CMD-C2D	-2.35	1.45	1.50
25	b	615	CLA	CMC-C2C	-2.35	1.45	1.50
25	C	503	CLA	MG-NB	-2.35	2.01	2.05
24	8	606	CHL	C3B-C4B	2.35	1.48	1.42
25	b	614	CLA	C3B-C4B	2.35	1.48	1.42
25	B	613	CLA	C1B-NB	-2.35	1.34	1.37
25	b	613	CLA	C1B-NB	-2.35	1.34	1.37
25	B	616	CLA	CMB-C2B	-2.35	1.45	1.50
25	c	504	CLA	CMB-C2B	-2.35	1.45	1.50
24	q	608	CHL	C1B-C2B	2.35	1.48	1.43
25	r	602	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	MG-ND	-2.35	2.01	2.05
25	b	604	CLA	C4B-NB	2.35	1.40	1.37
25	b	614	CLA	C4B-NB	2.35	1.40	1.37
25	G	602	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	502	CLA	CMD-C2D	-2.35	1.45	1.50
24	3	605	CHL	C1B-C2B	2.35	1.48	1.43
25	2	613	CLA	CMD-C2D	-2.35	1.45	1.50
25	C	508	CLA	CMB-C2B	-2.35	1.45	1.50
25	n	603	CLA	CMD-C2D	-2.35	1.45	1.50
25	G	613	CLA	C3B-C4B	2.35	1.48	1.42
25	r	601	CLA	CMD-C2D	-2.35	1.45	1.50
24	s	601	CHL	C3D-C2D	2.35	1.45	1.39
24	p	608	CHL	C1B-C2B	2.35	1.48	1.43
25	g	614	CLA	CMD-C2D	-2.35	1.45	1.50
25	C	501	CLA	MG-ND	-2.35	2.01	2.05
24	g	605	CHL	C1B-NB	-2.35	1.34	1.37
25	B	614	CLA	C3B-C4B	2.34	1.48	1.42
25	S	605	CLA	C1B-C2B	2.34	1.48	1.43
24	1	607	CHL	C3D-C2D	2.34	1.45	1.39
25	B	615	CLA	C3B-C4B	2.34	1.48	1.42
25	r	610	CLA	C1B-C2B	2.34	1.48	1.43
27	Y	1622	XAT	O24-C25	-2.34	1.42	1.46
25	n	602	CLA	CMD-C2D	-2.34	1.45	1.50
25	y	602	CLA	C3B-C4B	2.34	1.48	1.42
25	4	611	CLA	CMD-C2D	-2.34	1.45	1.50
24	G	605	CHL	C4B-NB	-2.34	1.34	1.37
25	R	603	CLA	C1B-C2B	2.34	1.48	1.43
25	r	603	CLA	C1B-C2B	2.34	1.48	1.43
24	9	606	CHL	C3B-C4B	2.34	1.48	1.42
25	r	616	CLA	C1B-C2B	2.34	1.48	1.43
27	n	1622	XAT	O4-C5	-2.34	1.42	1.46
25	B	606	CLA	MG-NB	-2.34	2.01	2.05
25	B	617	CLA	CMD-C2D	-2.34	1.45	1.50
24	0	606	CHL	C3D-C2D	2.34	1.45	1.39
25	S	602	CLA	CMD-C2D	-2.34	1.45	1.50
25	g	613	CLA	C3B-C4B	2.34	1.48	1.42
24	8	601	CHL	C3B-C4B	2.34	1.48	1.42
25	y	612	CLA	CMC-C2C	-2.34	1.45	1.50
24	5	606	CHL	C4B-NB	-2.34	1.34	1.37
25	N	603	CLA	C1B-C2B	2.34	1.48	1.43
25	n	603	CLA	C1B-C2B	2.34	1.48	1.43
25	0	610	CLA	CMD-C2D	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	CMB-C2B	-2.33	1.45	1.50
25	Y	603	CLA	CMC-C2C	-2.33	1.45	1.50
25	B	614	CLA	CMB-C2B	-2.33	1.45	1.50
27	N	1622	XAT	O4-C5	-2.33	1.42	1.46
24	n	608	CHL	C1B-C2B	2.33	1.48	1.43
25	R	610	CLA	C1B-C2B	2.33	1.48	1.43
25	a	410	CLA	CMC-C2C	-2.33	1.45	1.50
25	p	602	CLA	C1B-C2B	2.33	1.48	1.43
24	N	607	CHL	CHB-C4A	-2.33	1.32	1.37
25	b	608	CLA	CMB-C2B	-2.33	1.45	1.50
24	3	607	CHL	CHB-C4A	-2.33	1.32	1.37
25	C	511	CLA	CMB-C2B	-2.33	1.45	1.50
24	2	608	CHL	MG-NA	-2.33	2.00	2.06
24	y	601	CHL	C1D-ND	-2.33	1.34	1.37
25	c	502	CLA	C1B-NB	-2.33	1.34	1.37
25	9	611	CLA	CMD-C2D	-2.33	1.45	1.50
25	4	614	CLA	CMD-C2D	-2.33	1.45	1.50
25	R	604	CLA	CMD-C2D	-2.33	1.45	1.50
24	4	608	CHL	C1B-C2B	2.33	1.48	1.43
25	7	614	CLA	CMD-C2D	-2.33	1.45	1.50
25	b	606	CLA	MG-NB	-2.33	2.01	2.05
25	Y	603	CLA	CMD-C2D	-2.33	1.45	1.50
25	7	603	CLA	MG-ND	-2.33	2.01	2.05
25	r	610	CLA	C3B-C4B	2.33	1.48	1.42
25	c	503	CLA	CMD-C2D	-2.33	1.45	1.50
25	N	610	CLA	CMB-C2B	-2.33	1.45	1.50
25	R	609	CLA	CMB-C2B	-2.33	1.45	1.50
24	0	607	CHL	C4B-NB	-2.33	1.34	1.37
24	s	601	CHL	C3B-C4B	2.33	1.48	1.42
25	b	606	CLA	CMC-C2C	-2.33	1.45	1.50
25	7	603	CLA	CMB-C2B	-2.33	1.45	1.50
24	2	609	CHL	C1B-C2B	2.33	1.48	1.43
25	0	604	CLA	CMB-C2B	-2.33	1.45	1.50
25	b	610	CLA	MG-NB	-2.32	2.01	2.05
24	9	608	CHL	C1B-NB	-2.32	1.34	1.37
25	B	613	CLA	C4B-NB	2.32	1.40	1.37
25	b	613	CLA	C4B-NB	2.32	1.40	1.37
25	B	611	CLA	MG-ND	-2.32	2.01	2.05
25	B	616	CLA	CMD-C2D	-2.32	1.45	1.50
24	N	606	CHL	CHB-C4A	-2.32	1.32	1.37
25	A	410	CLA	MG-ND	-2.32	2.01	2.05
25	c	511	CLA	MG-NB	-2.32	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	601	CHL	CHB-C4A	-2.32	1.32	1.37
25	c	503	CLA	C1B-C2B	2.32	1.48	1.43
25	s	614	CLA	C1B-C2B	2.32	1.48	1.43
25	c	511	CLA	CMC-C2C	-2.32	1.45	1.50
25	1	603	CLA	C1B-C2B	2.32	1.48	1.43
25	G	612	CLA	CMD-C2D	-2.32	1.45	1.50
25	c	509	CLA	CMB-C2B	-2.32	1.45	1.50
25	B	603	CLA	CMD-C2D	-2.32	1.45	1.50
25	R	601	CLA	CMD-C2D	-2.32	1.45	1.50
24	5	605	CHL	C1B-NB	-2.32	1.34	1.37
25	9	613	CLA	CMD-C2D	-2.32	1.45	1.50
25	b	605	CLA	CMC-C2C	-2.32	1.45	1.50
25	R	616	CLA	C1B-C2B	2.32	1.48	1.43
25	Y	613	CLA	C1B-C2B	2.32	1.48	1.43
24	q	609	CHL	C4C-C3C	2.32	1.49	1.45
25	B	606	CLA	CMC-C2C	-2.32	1.45	1.50
25	g	602	CLA	C1B-NB	-2.32	1.34	1.37
24	7	607	CHL	C3D-C2D	2.32	1.45	1.39
25	S	611	CLA	CMD-C2D	-2.32	1.45	1.50
25	g	604	CLA	CMB-C2B	-2.32	1.45	1.50
25	G	604	CLA	CMB-C2B	-2.32	1.45	1.50
24	G	601	CHL	CHB-C4A	-2.32	1.32	1.37
25	C	508	CLA	MG-NB	-2.32	2.01	2.05
25	r	603	CLA	MG-NB	-2.32	2.01	2.05
25	C	509	CLA	CMB-C2B	-2.32	1.45	1.50
25	A	410	CLA	CMC-C2C	-2.32	1.45	1.50
25	n	611	CLA	CMD-C2D	-2.32	1.45	1.50
25	y	602	CLA	C1B-C2B	2.32	1.48	1.43
25	q	614	CLA	CMD-C2D	-2.32	1.45	1.50
25	b	614	CLA	CMB-C2B	-2.32	1.45	1.50
25	N	611	CLA	C1B-C2B	2.32	1.48	1.43
25	B	608	CLA	C1B-NB	-2.32	1.34	1.37
25	y	610	CLA	CMB-C2B	-2.32	1.45	1.50
25	S	613	CLA	C1B-C2B	2.32	1.48	1.43
25	c	507	CLA	C1B-C2B	2.32	1.48	1.43
24	7	608	CHL	C3B-C4B	2.32	1.48	1.42
25	C	502	CLA	CMD-C2D	-2.32	1.45	1.50
25	G	602	CLA	C1B-NB	-2.31	1.34	1.37
25	b	609	CLA	CMC-C2C	-2.31	1.45	1.50
24	S	607	CHL	C1B-C2B	2.31	1.48	1.43
25	n	613	CLA	CMD-C2D	-2.31	1.45	1.50
27	R	622	XAT	O4-C5	-2.31	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	603	CLA	CMC-C2C	-2.31	1.45	1.50
25	y	613	CLA	CMD-C2D	-2.31	1.45	1.50
25	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
25	r	610	CLA	CMD-C2D	-2.31	1.45	1.50
25	7	613	CLA	CMD-C2D	-2.31	1.45	1.50
34	b	620	BCR	C1-C6	-2.31	1.50	1.53
25	Y	610	CLA	CMB-C2B	-2.31	1.45	1.50
24	q	605	CHL	C4B-NB	-2.31	1.34	1.37
25	Y	604	CLA	C1B-NB	-2.31	1.34	1.37
25	C	503	CLA	CMD-C2D	-2.31	1.45	1.50
25	S	602	CLA	CMB-C2B	-2.31	1.45	1.50
25	s	613	CLA	CMB-C2B	-2.31	1.45	1.50
25	y	614	CLA	CMD-C2D	-2.31	1.45	1.50
34	B	620	BCR	C1-C6	-2.31	1.50	1.53
24	s	608	CHL	C3B-C4B	2.31	1.48	1.42
25	C	511	CLA	CMC-C2C	-2.31	1.45	1.50
25	b	609	CLA	CMB-C2B	-2.31	1.45	1.50
25	r	609	CLA	CMB-C2B	-2.31	1.45	1.50
24	3	606	CHL	C4C-C3C	2.31	1.49	1.45
25	r	602	CLA	C1B-NB	-2.31	1.34	1.37
24	0	605	CHL	C1B-NB	-2.31	1.34	1.37
25	2	602	CLA	CMD-C2D	-2.31	1.45	1.50
25	c	508	CLA	MG-NB	-2.31	2.01	2.05
25	G	610	CLA	C1B-C2B	2.31	1.48	1.43
25	g	610	CLA	C1B-C2B	2.31	1.48	1.43
25	R	612	CLA	CMB-C2B	-2.31	1.45	1.50
25	R	601	CLA	C3B-C4B	2.31	1.48	1.42
25	6	603	CLA	CMD-C2D	-2.31	1.45	1.50
25	b	614	CLA	MG-NB	-2.31	2.01	2.05
25	s	613	CLA	C3B-C4B	2.31	1.48	1.42
25	R	616	CLA	CMD-C2D	-2.30	1.45	1.50
25	B	607	CLA	CMC-C2C	-2.30	1.45	1.50
25	N	611	CLA	CMD-C2D	-2.30	1.45	1.50
25	7	603	CLA	C1B-C2B	2.30	1.48	1.43
25	g	611	CLA	MG-NB	-2.30	2.01	2.05
25	b	616	CLA	CMB-C2B	-2.30	1.45	1.50
25	9	602	CLA	C1B-C2B	2.30	1.48	1.43
33	A	408	PHO	C3B-CAB	-2.30	1.43	1.47
33	a	408	PHO	C3B-CAB	-2.30	1.43	1.47
25	y	604	CLA	C3B-C4B	2.30	1.48	1.42
25	r	601	CLA	C3B-C4B	2.30	1.48	1.42
25	g	602	CLA	CMD-C2D	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	608	CHL	MG-NA	-2.30	2.00	2.06
24	N	607	CHL	C1D-ND	-2.30	1.35	1.37
25	R	603	CLA	MG-NB	-2.30	2.01	2.05
25	N	602	CLA	CMD-C2D	-2.30	1.45	1.50
25	c	503	CLA	MG-NB	-2.30	2.01	2.05
24	g	607	CHL	C3D-C2D	2.30	1.45	1.39
25	n	610	CLA	CMB-C2B	-2.30	1.45	1.50
27	g	1622	XAT	O4-C5	-2.30	1.42	1.46
25	N	604	CLA	CMD-C2D	-2.30	1.45	1.50
25	y	613	CLA	C1B-C2B	2.30	1.48	1.43
25	6	610	CLA	CMD-C2D	-2.30	1.45	1.50
24	S	608	CHL	C3B-C4B	2.30	1.48	1.42
25	r	602	CLA	C3B-C4B	2.30	1.48	1.42
25	s	613	CLA	C1B-C2B	2.30	1.48	1.43
25	6	613	CLA	CMD-C2D	-2.30	1.45	1.50
24	0	601	CHL	C1D-C2D	2.30	1.49	1.45
25	B	613	CLA	CMB-C2B	-2.30	1.45	1.50
25	S	613	CLA	CMD-C2D	-2.30	1.45	1.50
25	b	613	CLA	CMB-C2B	-2.30	1.45	1.50
25	s	613	CLA	CMD-C2D	-2.30	1.45	1.50
25	r	611	CLA	CMB-C2B	-2.30	1.45	1.50
25	n	610	CLA	MG-NB	-2.30	2.01	2.05
27	Y	1622	XAT	O4-C5	-2.30	1.42	1.46
25	b	603	CLA	C4B-NB	2.30	1.40	1.37
25	b	617	CLA	CMD-C2D	-2.30	1.45	1.50
25	C	503	CLA	C1B-C2B	2.30	1.48	1.43
25	C	509	CLA	CMC-C2C	-2.30	1.45	1.50
26	R	620	LUT	C1-C6	-2.30	1.50	1.53
25	G	614	CLA	CMD-C2D	-2.30	1.45	1.50
25	Y	602	CLA	C1B-C2B	2.30	1.48	1.43
25	0	602	CLA	C1B-C2B	2.30	1.48	1.43
25	B	609	CLA	CMC-C2C	-2.29	1.45	1.50
25	r	616	CLA	CMD-C2D	-2.29	1.45	1.50
24	N	606	CHL	C1D-C2D	2.29	1.49	1.45
24	S	608	CHL	C4C-C3C	2.29	1.49	1.45
24	8	606	CHL	C1B-C2B	2.29	1.48	1.43
24	s	607	CHL	C1B-C2B	2.29	1.48	1.43
25	B	606	CLA	C1B-C2B	2.29	1.48	1.43
25	n	612	CLA	CMD-C2D	-2.29	1.45	1.50
25	a	405	CLA	C1B-NB	-2.29	1.35	1.37
25	b	606	CLA	C1B-C2B	2.29	1.48	1.43
25	s	605	CLA	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	606	CHL	C1B-C2B	2.29	1.48	1.43
24	1	606	CHL	C3D-C2D	2.29	1.45	1.39
24	1	609	CHL	C3D-C2D	2.29	1.45	1.39
25	C	506	CLA	CMC-C2C	-2.29	1.45	1.50
24	5	609	CHL	C3B-C4B	2.29	1.48	1.42
24	p	607	CHL	C4B-NB	-2.29	1.35	1.37
25	7	612	CLA	CMD-C2D	-2.29	1.45	1.50
24	g	606	CHL	C1B-C2B	2.29	1.48	1.43
25	G	614	CLA	C1B-C2B	2.29	1.48	1.43
25	A	407	CLA	C1B-C2B	2.29	1.48	1.43
25	B	614	CLA	MG-NB	-2.29	2.01	2.05
24	6	607	CHL	C1B-C2B	2.29	1.48	1.43
25	b	607	CLA	CMC-C2C	-2.29	1.45	1.50
25	y	603	CLA	C3B-C4B	2.29	1.48	1.42
24	0	601	CHL	C1B-C2B	2.29	1.48	1.43
25	B	616	CLA	MG-ND	-2.29	2.01	2.05
25	S	604	CLA	MG-NB	-2.29	2.01	2.05
25	N	613	CLA	CMD-C2D	-2.29	1.45	1.50
25	c	511	CLA	CMB-C2B	-2.29	1.45	1.50
25	C	511	CLA	MG-NB	-2.29	2.01	2.05
25	d	402	CLA	C3B-C4B	2.29	1.48	1.42
25	a	407	CLA	C1B-C2B	2.29	1.48	1.43
25	6	604	CLA	MG-NB	-2.29	2.01	2.05
24	3	606	CHL	C1B-C2B	2.29	1.48	1.43
24	Y	601	CHL	C1D-ND	-2.29	1.35	1.37
25	c	501	CLA	C1B-C2B	2.29	1.48	1.43
25	5	603	CLA	CMD-C2D	-2.29	1.46	1.50
25	A	406	CLA	CMB-C2B	-2.29	1.46	1.50
25	R	602	CLA	CMB-C2B	-2.29	1.46	1.50
25	0	610	CLA	C1B-C2B	2.29	1.48	1.43
25	Y	614	CLA	C3B-C4B	2.29	1.48	1.42
24	G	609	CHL	CHB-C4A	-2.29	1.32	1.37
24	n	605	CHL	C1D-C2D	2.29	1.49	1.45
25	B	616	CLA	CMC-C2C	-2.29	1.46	1.50
25	B	612	CLA	MG-ND	-2.29	2.01	2.05
25	b	612	CLA	MG-ND	-2.29	2.01	2.05
25	g	614	CLA	C1B-C2B	2.28	1.48	1.43
24	7	606	CHL	C3D-C2D	2.28	1.45	1.39
25	d	403	CLA	C3B-C4B	2.28	1.48	1.42
24	p	608	CHL	MG-NA	-2.28	2.00	2.06
25	B	603	CLA	C4B-NB	2.28	1.40	1.37
25	b	607	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	607	CHL	C1B-C2B	2.28	1.48	1.43
24	2	608	CHL	C1B-NB	-2.28	1.35	1.37
24	p	601	CHL	C1B-NB	-2.28	1.35	1.37
25	6	602	CLA	C1B-C2B	2.28	1.48	1.43
25	D	403	CLA	C3B-C4B	2.28	1.48	1.42
25	4	610	CLA	CMC-C2C	-2.28	1.46	1.50
25	d	403	CLA	CMB-C2B	-2.28	1.46	1.50
25	s	605	CLA	CMD-C2D	-2.28	1.46	1.50
28	8	1623	NEX	C7-C8	-2.28	1.28	1.32
25	8	602	CLA	CMD-C2D	-2.28	1.46	1.50
24	r	608	CHL	CHB-C4A	-2.28	1.32	1.37
25	G	612	CLA	C1B-C2B	2.28	1.48	1.43
24	3	609	CHL	C3B-C4B	2.28	1.48	1.42
24	g	605	CHL	C4B-NB	-2.28	1.35	1.37
27	y	1622	XAT	O4-C5	-2.28	1.42	1.46
24	y	601	CHL	C3B-C4B	2.28	1.48	1.42
25	B	608	CLA	CMC-C2C	-2.28	1.46	1.50
25	d	403	CLA	MG-NB	-2.28	2.01	2.05
25	S	605	CLA	CMD-C2D	-2.28	1.46	1.50
25	1	603	CLA	MG-ND	-2.28	2.01	2.05
25	C	501	CLA	C1B-NB	-2.28	1.35	1.37
25	y	603	CLA	MG-NB	-2.28	2.01	2.05
25	y	603	CLA	CMD-C2D	-2.28	1.46	1.50
24	N	609	CHL	C1D-C2D	2.28	1.49	1.45
24	3	609	CHL	C1C-NC	-2.28	1.34	1.37
24	0	607	CHL	C1B-C2B	2.28	1.48	1.43
25	C	502	CLA	C1B-NB	-2.28	1.35	1.37
24	7	609	CHL	C3D-C2D	2.28	1.45	1.39
24	5	608	CHL	C1B-C2B	2.28	1.48	1.43
25	b	602	CLA	CMC-C2C	-2.28	1.46	1.50
24	7	607	CHL	C1D-C2D	2.28	1.49	1.45
25	s	610	CLA	MG-NB	-2.28	2.01	2.05
25	C	501	CLA	C1B-C2B	2.28	1.48	1.43
25	S	610	CLA	CMB-C2B	-2.28	1.46	1.50
24	8	607	CHL	CHB-C4A	-2.27	1.32	1.37
25	1	613	CLA	CMD-C2D	-2.27	1.46	1.50
25	g	612	CLA	CMD-C2D	-2.27	1.46	1.50
25	B	610	CLA	MG-NB	-2.27	2.01	2.05
25	B	602	CLA	CMD-C2D	-2.27	1.46	1.50
27	y	1622	XAT	O24-C25	-2.27	1.43	1.46
25	D	403	CLA	MG-NB	-2.27	2.01	2.05
25	S	613	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	MG-ND	-2.27	2.01	2.05
25	b	613	CLA	MG-ND	-2.27	2.01	2.05
25	5	614	CLA	CMD-C2D	-2.27	1.46	1.50
25	D	402	CLA	C1D-ND	2.27	1.40	1.37
25	C	507	CLA	C1B-C2B	2.27	1.48	1.43
25	2	611	CLA	CMD-C2D	-2.27	1.46	1.50
25	r	612	CLA	CMB-C2B	-2.27	1.46	1.50
24	n	606	CHL	CHB-C4A	-2.27	1.32	1.37
34	C	515	BCR	C1-C6	-2.27	1.50	1.53
25	Y	604	CLA	C3B-C4B	2.27	1.48	1.42
25	N	610	CLA	MG-NB	-2.27	2.01	2.05
25	9	612	CLA	CMD-C2D	-2.27	1.46	1.50
25	s	610	CLA	CMB-C2B	-2.27	1.46	1.50
25	d	402	CLA	C1D-ND	2.27	1.40	1.37
25	g	612	CLA	C1B-C2B	2.27	1.48	1.43
25	Y	602	CLA	CMD-C2D	-2.27	1.46	1.50
25	a	410	CLA	MG-ND	-2.27	2.01	2.05
27	G	1622	XAT	O4-C5	-2.27	1.43	1.46
25	2	604	CLA	C1B-C2B	2.27	1.48	1.43
25	b	616	CLA	MG-ND	-2.27	2.01	2.05
25	A	406	CLA	MG-ND	-2.27	2.01	2.05
25	s	602	CLA	CMB-C2B	-2.27	1.46	1.50
25	D	403	CLA	CMD-C2D	-2.27	1.46	1.50
25	g	611	CLA	CMD-C2D	-2.27	1.46	1.50
25	s	603	CLA	CMB-C2B	-2.27	1.46	1.50
25	C	509	CLA	MG-ND	-2.27	2.01	2.05
25	R	610	CLA	CMD-C2D	-2.27	1.46	1.50
25	6	602	CLA	MG-NB	-2.27	2.01	2.05
25	s	604	CLA	MG-NB	-2.27	2.01	2.05
25	R	602	CLA	C1B-NB	-2.27	1.35	1.37
25	6	610	CLA	C1B-C2B	2.27	1.48	1.43
25	n	612	CLA	CMB-C2B	-2.27	1.46	1.50
24	s	608	CHL	C4C-C3C	2.26	1.48	1.45
25	0	604	CLA	C1B-C2B	2.26	1.48	1.43
25	7	610	CLA	C1B-C2B	2.26	1.48	1.43
25	3	603	CLA	MG-ND	-2.26	2.01	2.05
25	c	506	CLA	CMC-C2C	-2.26	1.46	1.50
24	7	607	CHL	C3B-C4B	2.26	1.48	1.42
25	B	616	CLA	CHC-C4B	-2.26	1.34	1.39
25	D	403	CLA	CMB-C2B	-2.26	1.46	1.50
24	G	606	CHL	C3D-C2D	2.26	1.45	1.39
25	p	603	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	C3B-C4B	2.26	1.48	1.42
25	Y	603	CLA	C3B-C4B	2.26	1.48	1.42
25	b	613	CLA	C3B-C4B	2.26	1.48	1.42
24	4	606	CHL	C4C-C3C	2.26	1.48	1.45
25	S	610	CLA	MG-NB	-2.26	2.01	2.05
24	g	609	CHL	CHB-C4A	-2.26	1.32	1.37
24	2	601	CHL	C3D-C2D	2.26	1.45	1.39
25	c	506	CLA	CMD-C2D	-2.26	1.46	1.50
24	6	607	CHL	C4C-C3C	2.26	1.48	1.45
25	B	617	CLA	C3B-C4B	2.26	1.48	1.42
24	y	601	CHL	C1D-C2D	2.26	1.49	1.45
25	a	406	CLA	CMB-C2B	-2.26	1.46	1.50
25	1	612	CLA	CMD-C2D	-2.26	1.46	1.50
24	2	601	CHL	C3B-C4B	2.26	1.48	1.42
25	C	509	CLA	C1B-NB	-2.26	1.35	1.37
25	D	402	CLA	C3B-C4B	2.26	1.48	1.42
24	g	606	CHL	C3D-C2D	2.26	1.45	1.39
25	G	611	CLA	MG-NB	-2.26	2.01	2.05
24	2	606	CHL	C4C-C3C	2.26	1.48	1.45
25	y	602	CLA	CMD-C2D	-2.26	1.46	1.50
25	B	613	CLA	C1B-C2B	2.26	1.48	1.43
25	b	613	CLA	C1B-C2B	2.26	1.48	1.43
25	C	505	CLA	CMB-C2B	-2.26	1.46	1.50
25	G	610	CLA	CMD-C2D	-2.26	1.46	1.50
25	r	602	CLA	CMB-C2B	-2.26	1.46	1.50
25	0	602	CLA	MG-NB	-2.26	2.01	2.05
25	c	509	CLA	MG-ND	-2.26	2.01	2.05
26	r	620	LUT	C1-C6	-2.26	1.50	1.53
25	B	607	CLA	CMB-C2B	-2.25	1.46	1.50
25	5	602	CLA	C1B-C2B	2.25	1.48	1.43
24	n	601	CHL	CHB-C4A	-2.25	1.32	1.37
25	C	512	CLA	CMB-C2B	-2.25	1.46	1.50
25	n	604	CLA	CMD-C2D	-2.25	1.46	1.50
25	g	602	CLA	MG-NB	-2.25	2.01	2.05
25	R	602	CLA	C3B-C4B	2.25	1.48	1.42
25	b	616	CLA	CHC-C4B	-2.25	1.34	1.39
26	Y	1621	LUT	C22-C21	-2.25	1.51	1.54
25	b	616	CLA	CMC-C2C	-2.25	1.46	1.50
25	3	603	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	609	CLA	CMB-C2B	-2.25	1.46	1.50
24	1	605	CHL	C1B-C2B	2.25	1.48	1.43
24	6	601	CHL	C1B-C2B	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	C1B-C2B	2.25	1.48	1.43
25	N	612	CLA	CMD-C2D	-2.25	1.46	1.50
25	c	503	CLA	CMC-C2C	-2.25	1.46	1.50
25	2	603	CLA	CMD-C2D	-2.25	1.46	1.50
25	G	611	CLA	CMD-C2D	-2.25	1.46	1.50
25	b	602	CLA	CMB-C2B	-2.25	1.46	1.50
24	1	607	CHL	C1D-C2D	2.25	1.49	1.45
25	G	604	CLA	CMD-C2D	-2.25	1.46	1.50
25	a	410	CLA	CMB-C2B	-2.25	1.46	1.50
24	8	609	CHL	C3B-C4B	2.25	1.48	1.42
25	d	403	CLA	CMD-C2D	-2.25	1.46	1.50
25	b	602	CLA	C1B-C2B	2.25	1.48	1.43
24	1	601	CHL	CHB-C4A	-2.25	1.32	1.37
25	C	502	CLA	MG-ND	-2.25	2.01	2.05
25	q	611	CLA	CMC-C2C	-2.25	1.46	1.50
25	4	602	CLA	C1B-C2B	2.25	1.48	1.43
25	Y	603	CLA	MG-NB	-2.25	2.01	2.05
25	B	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	a	407	CLA	MG-ND	-2.25	2.01	2.05
24	Y	601	CHL	C3B-C4B	2.25	1.48	1.42
25	b	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	G	602	CLA	C1B-C2B	2.25	1.48	1.43
25	A	407	CLA	MG-ND	-2.25	2.01	2.05
25	C	506	CLA	MG-NB	-2.25	2.01	2.05
25	C	506	CLA	CMD-C2D	-2.24	1.46	1.50
25	G	611	CLA	CMC-C2C	-2.24	1.46	1.50
25	g	611	CLA	CMC-C2C	-2.24	1.46	1.50
24	R	608	CHL	CHB-C4A	-2.24	1.32	1.37
25	C	512	CLA	C1B-C2B	2.24	1.48	1.43
24	9	606	CHL	C4C-C3C	2.24	1.48	1.45
25	B	602	CLA	MG-NB	-2.24	2.01	2.05
25	Y	612	CLA	CMB-C2B	-2.24	1.46	1.50
25	y	612	CLA	CMB-C2B	-2.24	1.46	1.50
25	B	603	CLA	C3B-C4B	2.24	1.48	1.42
25	C	507	CLA	C3B-C4B	2.24	1.48	1.42
25	g	613	CLA	MG-ND	-2.24	2.01	2.05
25	y	614	CLA	CMB-C2B	-2.24	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.24	1.46	1.50
34	c	515	BCR	C1-C6	-2.24	1.50	1.53
24	g	609	CHL	MG-ND	-2.24	2.01	2.05
25	B	614	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	614	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	612	CLA	CMD-C2D	-2.24	1.46	1.50
25	s	602	CLA	CMD-C2D	-2.24	1.46	1.50
25	3	602	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	602	CLA	CMC-C2C	-2.24	1.46	1.50
25	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
25	S	614	CLA	MG-NB	-2.24	2.01	2.05
25	1	604	CLA	C1B-C2B	2.24	1.48	1.43
24	6	601	CHL	C4B-NB	-2.24	1.35	1.37
24	y	605	CHL	C3B-C4B	2.24	1.48	1.42
25	2	612	CLA	CMD-C2D	-2.24	1.46	1.50
25	8	604	CLA	CMB-C2B	-2.24	1.46	1.50
25	R	604	CLA	CMC-C2C	-2.24	1.46	1.50
25	R	610	CLA	CMB-C2B	-2.24	1.46	1.50
25	r	610	CLA	CMB-C2B	-2.24	1.46	1.50
25	N	614	CLA	CMB-C2B	-2.24	1.46	1.50
25	b	603	CLA	C3B-C4B	2.24	1.48	1.42
24	N	609	CHL	C3D-C2D	2.24	1.45	1.39
24	5	605	CHL	C4B-NB	-2.24	1.35	1.37
24	1	607	CHL	C3B-C4B	2.23	1.48	1.42
25	7	604	CLA	MG-NB	-2.23	2.01	2.05
25	r	612	CLA	MG-NB	-2.23	2.01	2.05
25	S	612	CLA	CMD-C2D	-2.23	1.46	1.50
25	2	610	CLA	C1B-C2B	2.23	1.48	1.43
24	g	607	CHL	C3B-C4B	2.23	1.48	1.42
27	r	622	XAT	O24-C25	-2.23	1.43	1.46
25	r	613	CLA	CMB-C2B	-2.23	1.46	1.50
25	A	405	CLA	MG-ND	-2.23	2.01	2.05
25	a	405	CLA	MG-ND	-2.23	2.01	2.05
25	R	611	CLA	CMC-C2C	-2.23	1.46	1.50
25	g	612	CLA	CMB-C2B	-2.23	1.46	1.50
25	n	614	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	503	CLA	C1B-NB	-2.23	1.35	1.37
24	G	609	CHL	MG-ND	-2.23	2.01	2.05
25	R	613	CLA	CMB-C2B	-2.23	1.46	1.50
25	c	502	CLA	MG-ND	-2.23	2.01	2.05
25	C	503	CLA	CMC-C2C	-2.23	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.23	1.46	1.50
25	b	606	CLA	MG-ND	-2.23	2.01	2.05
25	c	509	CLA	C1B-NB	-2.23	1.35	1.37
25	N	611	CLA	MG-NB	-2.23	2.01	2.05
25	N	613	CLA	CMB-C2B	-2.23	1.46	1.50
25	Y	612	CLA	C1B-NB	-2.23	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	CMB-C2B	-2.23	1.46	1.50
24	R	607	CHL	C3D-C2D	2.23	1.45	1.39
25	R	602	CLA	CMD-C2D	-2.23	1.46	1.50
25	n	603	CLA	CHC-C4B	-2.23	1.34	1.39
24	6	606	CHL	C1B-C2B	2.23	1.48	1.43
25	A	410	CLA	CMD-C2D	-2.23	1.46	1.50
25	S	611	CLA	CMB-C2B	-2.23	1.46	1.50
25	a	410	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	616	CLA	C1B-C2B	2.23	1.48	1.43
25	S	603	CLA	CMB-C2B	-2.23	1.46	1.50
25	y	611	CLA	CMC-C2C	-2.23	1.46	1.50
24	5	607	CHL	C1B-C2B	2.22	1.48	1.43
25	B	602	CLA	C1B-C2B	2.22	1.48	1.43
25	N	612	CLA	CMB-C2B	-2.22	1.46	1.50
25	s	614	CLA	MG-NB	-2.22	2.01	2.05
24	7	605	CHL	C1B-C2B	2.22	1.48	1.43
25	R	603	CLA	C3B-C4B	2.22	1.48	1.42
25	G	613	CLA	MG-ND	-2.22	2.01	2.05
25	a	406	CLA	MG-ND	-2.22	2.01	2.05
24	s	606	CHL	C3B-C4B	2.22	1.48	1.42
25	n	604	CLA	MG-NB	-2.22	2.01	2.05
25	3	604	CLA	CMB-C2B	-2.22	1.46	1.50
25	D	403	CLA	CMC-C2C	-2.22	1.46	1.50
24	Y	605	CHL	C3B-C4B	2.22	1.48	1.42
25	1	610	CLA	C1B-C2B	2.22	1.48	1.43
25	1	604	CLA	MG-NB	-2.22	2.01	2.05
25	B	610	CLA	MG-ND	-2.22	2.01	2.05
25	G	612	CLA	CMB-C2B	-2.22	1.46	1.50
25	8	603	CLA	MG-ND	-2.22	2.01	2.05
24	1	608	CHL	C3D-C2D	2.22	1.45	1.39
24	q	606	CHL	C1B-C2B	2.22	1.48	1.43
24	p	605	CHL	C1B-NB	-2.22	1.35	1.37
25	7	603	CLA	CMD-C2D	-2.22	1.46	1.50
25	y	602	CLA	CMC-C2C	-2.22	1.46	1.50
24	N	608	CHL	C1D-C2D	2.22	1.49	1.45
24	7	601	CHL	CHB-C4A	-2.22	1.32	1.37
24	n	609	CHL	C3D-C2D	2.22	1.45	1.39
24	7	607	CHL	C1B-C2B	2.22	1.48	1.43
24	1	609	CHL	C1D-C2D	2.22	1.49	1.45
25	n	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	s	611	CLA	CMB-C2B	-2.22	1.46	1.50
25	Y	602	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	611	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	608	CLA	C1B-C2B	2.22	1.48	1.43
24	n	606	CHL	C1D-C2D	2.22	1.49	1.45
25	2	602	CLA	MG-NB	-2.22	2.01	2.05
25	R	611	CLA	CMB-C2B	-2.22	1.46	1.50
25	C	504	CLA	MG-NB	-2.22	2.01	2.05
25	b	617	CLA	C3B-C4B	2.22	1.48	1.42
24	4	609	CHL	MG-ND	-2.22	2.01	2.05
25	R	612	CLA	MG-NB	-2.22	2.01	2.05
24	Y	601	CHL	C1D-C2D	2.22	1.49	1.45
24	n	609	CHL	C1C-NC	-2.22	1.34	1.37
25	c	506	CLA	MG-NB	-2.22	2.01	2.05
25	Y	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	Y	614	CLA	CMC-C2C	-2.22	1.46	1.50
25	y	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	y	614	CLA	CMC-C2C	-2.22	1.46	1.50
25	c	512	CLA	MG-NB	-2.21	2.01	2.05
24	1	607	CHL	C1B-C2B	2.21	1.48	1.43
24	S	606	CHL	C3B-C4B	2.21	1.48	1.42
24	Y	606	CHL	C1C-NC	-2.21	1.34	1.37
25	b	615	CLA	MG-ND	-2.21	2.01	2.05
25	G	614	CLA	CMC-C2C	-2.21	1.46	1.50
25	b	617	CLA	C1B-NB	-2.21	1.35	1.37
24	9	607	CHL	C4C-C3C	2.21	1.48	1.45
24	G	607	CHL	C3B-C4B	2.21	1.47	1.42
25	1	602	CLA	MG-NB	-2.21	2.01	2.05
24	1	605	CHL	C3B-C4B	2.21	1.47	1.42
24	8	609	CHL	CHB-C4A	-2.21	1.32	1.37
25	g	611	CLA	C1B-C2B	2.21	1.48	1.43
25	n	611	CLA	CMB-C2B	-2.21	1.46	1.50
24	Y	601	CHL	C1C-NC	-2.21	1.34	1.37
25	R	616	CLA	CMC-C2C	-2.21	1.46	1.50
25	g	614	CLA	CMC-C2C	-2.21	1.46	1.50
24	8	609	CHL	C1C-NC	-2.21	1.34	1.37
25	6	604	CLA	CMD-C2D	-2.21	1.46	1.50
25	C	512	CLA	CMC-C2C	-2.21	1.46	1.50
25	6	611	CLA	CMD-C2D	-2.21	1.46	1.50
25	C	512	CLA	MG-NB	-2.21	2.01	2.05
24	p	609	CHL	C3B-C4B	2.21	1.47	1.42
25	N	604	CLA	MG-NB	-2.21	2.01	2.05
25	Y	614	CLA	CMB-C2B	-2.21	1.46	1.50
25	B	603	CLA	C1B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	602	CLA	MG-ND	-2.21	2.01	2.05
25	g	610	CLA	CMD-C2D	-2.21	1.46	1.50
24	q	609	CHL	C2C-C1C	2.21	1.49	1.44
24	6	609	CHL	CHB-C4A	-2.21	1.32	1.37
25	A	410	CLA	CMB-C2B	-2.20	1.46	1.50
25	q	612	CLA	CMD-C2D	-2.20	1.46	1.50
24	9	601	CHL	C3B-C4B	2.20	1.47	1.42
25	R	616	CLA	CMB-C2B	-2.20	1.46	1.50
24	2	608	CHL	C2C-C1C	2.20	1.49	1.44
27	N	1622	XAT	C22-C21	-2.20	1.51	1.54
25	0	611	CLA	CMD-C2D	-2.20	1.46	1.50
25	6	612	CLA	C1B-C2B	2.20	1.48	1.43
24	7	605	CHL	C3B-C4B	2.20	1.47	1.42
25	c	505	CLA	C1B-NB	-2.20	1.35	1.37
25	C	505	CLA	CMC-C2C	-2.20	1.46	1.50
25	0	612	CLA	C1B-C2B	2.20	1.48	1.43
25	R	611	CLA	CMD-C2D	-2.20	1.46	1.50
25	B	609	CLA	MG-ND	-2.20	2.01	2.05
25	G	602	CLA	MG-NB	-2.20	2.01	2.05
25	b	609	CLA	MG-ND	-2.20	2.01	2.05
25	b	610	CLA	MG-ND	-2.20	2.01	2.05
40	f	101	HEM	C2A-C3A	-2.20	1.33	1.38
25	S	613	CLA	CMC-C2C	-2.20	1.46	1.50
25	b	616	CLA	MG-NB	-2.20	2.01	2.05
25	G	614	CLA	CMB-C2B	-2.20	1.46	1.50
25	1	611	CLA	MG-ND	-2.20	2.01	2.05
25	3	613	CLA	CMD-C2D	-2.20	1.46	1.50
25	R	612	CLA	CMD-C2D	-2.20	1.46	1.50
25	Y	611	CLA	CMC-C2C	-2.20	1.46	1.50
25	A	406	CLA	C3B-C4B	2.20	1.47	1.42
25	B	606	CLA	MG-ND	-2.20	2.01	2.05
25	r	603	CLA	MG-ND	-2.20	2.01	2.05
25	4	604	CLA	CMC-C2C	-2.20	1.46	1.50
25	n	603	CLA	CMC-C2C	-2.20	1.46	1.50
25	r	611	CLA	CMD-C2D	-2.20	1.46	1.50
25	g	604	CLA	MG-NB	-2.20	2.01	2.05
25	7	612	CLA	C1B-C2B	2.20	1.48	1.43
25	r	616	CLA	CMC-C2C	-2.20	1.46	1.50
25	8	610	CLA	CMD-C2D	-2.20	1.46	1.50
25	c	513	CLA	CMB-C2B	-2.20	1.46	1.50
24	g	601	CHL	C1D-C2D	2.20	1.49	1.45
25	g	602	CLA	C1B-C2B	2.20	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	609	CHL	CHB-C4A	-2.20	1.32	1.37
25	C	513	CLA	CMB-C2B	-2.20	1.46	1.50
25	d	403	CLA	CMC-C2C	-2.20	1.46	1.50
25	3	602	CLA	C1B-C2B	2.20	1.48	1.43
24	r	607	CHL	C3D-C2D	2.20	1.45	1.39
25	A	407	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	505	CLA	C1B-NB	-2.19	1.35	1.37
25	q	613	CLA	CMD-C2D	-2.19	1.46	1.50
25	9	610	CLA	C1B-C2B	2.19	1.48	1.43
25	G	604	CLA	MG-NB	-2.19	2.01	2.05
24	y	606	CHL	C1C-NC	-2.19	1.34	1.37
25	g	611	CLA	CMB-C2B	-2.19	1.46	1.50
25	4	612	CLA	CMD-C2D	-2.19	1.46	1.50
25	N	611	CLA	CMB-C2B	-2.19	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.19	1.46	1.50
25	c	512	CLA	CMB-C2B	-2.19	1.46	1.50
25	C	507	CLA	C4B-NB	2.19	1.40	1.37
25	G	611	CLA	CMB-C2B	-2.19	1.46	1.50
24	2	607	CHL	C4C-C3C	2.19	1.48	1.45
24	S	601	CHL	C1B-C2B	2.19	1.48	1.43
24	8	609	CHL	C1B-C2B	2.19	1.48	1.43
24	s	601	CHL	C1B-C2B	2.19	1.48	1.43
25	S	604	CLA	C1B-C2B	2.19	1.48	1.43
25	7	611	CLA	MG-ND	-2.19	2.01	2.05
25	n	613	CLA	CMB-C2B	-2.19	1.46	1.50
25	S	612	CLA	C1B-C2B	2.19	1.48	1.43
25	y	602	CLA	CMB-C2B	-2.19	1.46	1.50
25	B	616	CLA	MG-NB	-2.19	2.01	2.05
25	1	602	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.19	1.46	1.50
25	g	604	CLA	CMD-C2D	-2.19	1.46	1.50
24	0	609	CHL	C1B-C2B	2.19	1.48	1.43
25	8	602	CLA	C1B-C2B	2.19	1.48	1.43
25	n	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	n	603	CLA	CAC-C3C	-2.19	1.45	1.51
25	7	604	CLA	C3B-C4B	2.19	1.47	1.42
25	N	603	CLA	CMC-C2C	-2.19	1.46	1.50
25	8	603	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.19	1.46	1.50
25	c	504	CLA	MG-NB	-2.19	2.01	2.05
25	N	602	CLA	CMB-C2B	-2.19	1.46	1.50
25	c	512	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C3B-C4B	2.19	1.47	1.42
25	6	604	CLA	C1B-C2B	2.19	1.48	1.43
25	q	602	CLA	C1B-C2B	2.19	1.48	1.43
25	N	603	CLA	CHC-C4B	-2.19	1.34	1.39
24	6	609	CHL	C3B-C4B	2.19	1.47	1.42
25	2	602	CLA	CMC-C2C	-2.19	1.46	1.50
25	n	610	CLA	CMD-C2D	-2.19	1.46	1.50
25	r	604	CLA	CMC-C2C	-2.19	1.46	1.50
25	4	602	CLA	CMC-C2C	-2.19	1.46	1.50
25	s	612	CLA	CMB-C2B	-2.19	1.46	1.50
24	2	601	CHL	C4C-C3C	2.18	1.48	1.45
24	q	608	CHL	C4C-C3C	2.18	1.48	1.45
24	0	606	CHL	C1B-C2B	2.18	1.48	1.43
25	8	613	CLA	CMD-C2D	-2.18	1.46	1.50
25	b	603	CLA	C1B-NB	-2.18	1.35	1.37
25	R	603	CLA	MG-ND	-2.18	2.01	2.05
25	c	503	CLA	CMB-C2B	-2.18	1.46	1.50
24	4	606	CHL	C1B-C2B	2.18	1.48	1.43
25	C	511	CLA	C1B-C2B	2.18	1.48	1.43
24	n	607	CHL	C1D-C2D	2.18	1.49	1.45
25	2	611	CLA	MG-ND	-2.18	2.01	2.05
24	n	606	CHL	C3D-C2D	2.18	1.45	1.39
25	3	610	CLA	CMD-C2D	-2.18	1.46	1.50
25	R	602	CLA	CMC-C2C	-2.18	1.46	1.50
25	b	602	CLA	MG-NB	-2.18	2.01	2.05
24	R	607	CHL	C1D-ND	-2.18	1.35	1.37
25	y	612	CLA	C1B-NB	-2.18	1.35	1.37
25	4	611	CLA	CMC-C2C	-2.18	1.46	1.50
24	r	606	CHL	C3B-C4B	2.18	1.47	1.42
25	r	603	CLA	C3B-C4B	2.18	1.47	1.42
25	n	604	CLA	CMC-C2C	-2.18	1.46	1.50
24	2	605	CHL	C4D-CHA	2.18	1.46	1.38
25	B	617	CLA	C1B-NB	-2.18	1.35	1.37
24	N	606	CHL	C3D-C2D	2.18	1.45	1.39
25	s	612	CLA	C1B-C2B	2.18	1.48	1.43
24	p	608	CHL	C4C-C3C	2.18	1.48	1.45
25	r	602	CLA	CMD-C2D	-2.18	1.46	1.50
25	s	604	CLA	C1B-C2B	2.18	1.48	1.43
24	4	608	CHL	C4C-C3C	2.18	1.48	1.45
25	p	604	CLA	CMB-C2B	-2.18	1.46	1.50
25	B	609	CLA	C1B-C2B	2.18	1.48	1.43
25	b	609	CLA	C1B-C2B	2.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	MG-ND	-2.18	2.01	2.05
25	S	612	CLA	MG-ND	-2.18	2.01	2.05
24	9	609	CHL	CMC-C2C	2.18	1.49	1.45
25	S	602	CLA	CMC-C2C	-2.18	1.46	1.50
25	9	611	CLA	MG-ND	-2.18	2.01	2.05
25	g	614	CLA	CMB-C2B	-2.18	1.46	1.50
24	N	605	CHL	C3D-C2D	2.18	1.45	1.39
25	R	613	CLA	C3B-C4B	2.18	1.47	1.42
25	r	613	CLA	C3B-C4B	2.18	1.47	1.42
25	a	406	CLA	C3B-C4B	2.17	1.47	1.42
25	N	603	CLA	CAC-C3C	-2.17	1.45	1.51
24	G	601	CHL	C1D-C2D	2.17	1.49	1.45
24	3	601	CHL	C3B-C4B	2.17	1.47	1.42
25	9	603	CLA	CMD-C2D	-2.17	1.46	1.50
24	r	607	CHL	C1D-ND	-2.17	1.35	1.37
25	Y	602	CLA	CMB-C2B	-2.17	1.46	1.50
25	7	602	CLA	CMD-C2D	-2.17	1.46	1.50
25	r	616	CLA	CMB-C2B	-2.17	1.46	1.50
25	R	609	CLA	C1B-C2B	2.17	1.48	1.43
24	y	601	CHL	C1C-NC	-2.17	1.34	1.37
25	c	513	CLA	CMC-C2C	-2.17	1.46	1.50
33	A	408	PHO	CBD-CGD	-2.17	1.49	1.52
25	B	606	CLA	C1B-NB	-2.17	1.35	1.37
25	B	608	CLA	C1B-C2B	2.17	1.48	1.43
28	1	1623	NEX	O24-C25	-2.17	1.43	1.46
25	B	610	CLA	CMC-C2C	-2.17	1.46	1.50
25	N	602	CLA	CMC-C2C	-2.17	1.46	1.50
24	q	609	CHL	C1B-C2B	2.17	1.48	1.43
25	p	610	CLA	CMD-C2D	-2.17	1.46	1.50
25	9	602	CLA	MG-NB	-2.17	2.01	2.05
25	g	610	CLA	CMB-C2B	-2.17	1.46	1.50
25	r	612	CLA	CMD-C2D	-2.17	1.46	1.50
25	G	603	CLA	MG-NB	-2.17	2.01	2.05
25	g	603	CLA	MG-NB	-2.17	2.01	2.05
24	6	609	CHL	C1B-C2B	2.17	1.48	1.43
24	N	607	CHL	C1D-C2D	2.17	1.49	1.45
25	G	611	CLA	C1B-C2B	2.17	1.48	1.43
25	a	407	CLA	CMB-C2B	-2.17	1.46	1.50
25	q	604	CLA	CMC-C2C	-2.17	1.46	1.50
25	B	603	CLA	C1B-C2B	2.17	1.48	1.43
25	N	613	CLA	CMC-C2C	-2.17	1.46	1.50
25	y	612	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	603	CLA	CMB-C2B	-2.17	1.46	1.50
26	N	1621	LUT	C22-C21	-2.16	1.52	1.54
25	5	602	CLA	CMC-C2C	-2.16	1.46	1.50
24	6	605	CHL	C4C-C3C	2.16	1.48	1.45
24	8	605	CHL	C4B-NB	-2.16	1.35	1.37
25	s	611	CLA	MG-ND	-2.16	2.01	2.05
25	p	603	CLA	CMB-C2B	-2.16	1.46	1.50
25	b	617	CLA	MG-ND	-2.16	2.01	2.05
25	n	602	CLA	CMB-C2B	-2.16	1.46	1.50
25	1	612	CLA	MG-ND	-2.16	2.01	2.05
25	0	604	CLA	CMD-C2D	-2.16	1.46	1.50
27	R	622	XAT	O24-C25	-2.16	1.43	1.46
25	c	504	CLA	MG-ND	-2.16	2.01	2.05
25	N	604	CLA	CMC-C2C	-2.16	1.46	1.50
25	s	612	CLA	MG-ND	-2.16	2.01	2.05
25	1	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	4	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.16	1.46	1.50
24	7	608	CHL	C3D-C2D	2.16	1.45	1.39
25	n	611	CLA	MG-NB	-2.16	2.01	2.05
25	s	610	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	610	CLA	C3B-C4B	2.16	1.47	1.42
25	N	611	CLA	CMC-C2C	-2.16	1.46	1.50
25	n	603	CLA	C1B-NB	-2.16	1.35	1.37
25	y	603	CLA	C1B-NB	-2.16	1.35	1.37
25	1	612	CLA	C1B-C2B	2.16	1.48	1.43
25	r	609	CLA	C1B-C2B	2.16	1.48	1.43
25	n	610	CLA	C1B-C2B	2.16	1.48	1.43
25	S	610	CLA	CMC-C2C	-2.16	1.46	1.50
24	9	605	CHL	C4D-CHA	2.16	1.46	1.38
24	5	608	CHL	C4B-NB	-2.16	1.35	1.37
25	c	507	CLA	CMB-C2B	-2.16	1.46	1.50
25	b	610	CLA	C3B-C4B	2.16	1.47	1.42
25	1	610	CLA	CMD-C2D	-2.16	1.46	1.50
25	7	604	CLA	CMC-C2C	-2.16	1.46	1.50
25	C	503	CLA	CMB-C2B	-2.16	1.46	1.50
25	G	610	CLA	CMB-C2B	-2.16	1.46	1.50
27	n	1622	XAT	C22-C21	-2.16	1.51	1.54
25	S	603	CLA	CMD-C2D	-2.16	1.46	1.50
24	G	607	CHL	C1B-C2B	2.16	1.48	1.43
25	C	504	CLA	C1B-C2B	2.16	1.48	1.43
25	9	603	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	612	CLA	C1B-C2B	2.15	1.48	1.43
25	c	512	CLA	C1B-C2B	2.15	1.48	1.43
24	p	601	CHL	C4B-NB	-2.15	1.35	1.37
25	r	604	CLA	C1B-NB	-2.15	1.35	1.37
25	Y	610	CLA	C1B-C2B	2.15	1.48	1.43
25	7	610	CLA	CMD-C2D	-2.15	1.46	1.50
24	0	609	CHL	C4C-C3C	2.15	1.48	1.45
25	S	612	CLA	CMB-C2B	-2.15	1.46	1.50
25	6	603	CLA	MG-ND	-2.15	2.01	2.05
25	C	513	CLA	CMC-C2C	-2.15	1.46	1.50
25	N	610	CLA	C1B-C2B	2.15	1.48	1.43
24	6	609	CHL	C4C-C3C	2.15	1.48	1.45
25	C	503	CLA	MG-ND	-2.15	2.01	2.05
25	2	604	CLA	CMB-C2B	-2.15	1.46	1.50
25	7	612	CLA	CMB-C2B	-2.15	1.46	1.50
25	n	604	CLA	C1B-C2B	2.15	1.48	1.43
25	G	613	CLA	CHC-C4B	-2.15	1.34	1.39
25	S	611	CLA	CMC-C2C	-2.15	1.46	1.50
24	0	608	CHL	CHB-C4A	-2.15	1.32	1.37
25	C	507	CLA	CMB-C2B	-2.15	1.46	1.50
25	c	504	CLA	C1B-C2B	2.15	1.48	1.43
25	4	604	CLA	CMB-C2B	-2.15	1.46	1.50
25	8	602	CLA	CMB-C2B	-2.15	1.46	1.50
25	r	602	CLA	CMC-C2C	-2.15	1.46	1.50
25	n	602	CLA	MG-ND	-2.15	2.01	2.05
25	p	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	C	510	CLA	CMC-C2C	-2.15	1.46	1.50
25	y	604	CLA	MG-ND	-2.15	2.01	2.05
25	R	610	CLA	C1B-NB	-2.15	1.35	1.37
25	Y	603	CLA	C1B-NB	-2.15	1.35	1.37
25	N	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	S	604	CLA	CMD-C2D	-2.15	1.46	1.50
25	B	604	CLA	C3B-C4B	2.15	1.47	1.42
24	3	609	CHL	C1B-C2B	2.15	1.48	1.43
25	n	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	s	613	CLA	CMC-C2C	-2.15	1.46	1.50
25	Y	612	CLA	MG-NB	-2.15	2.01	2.05
24	3	605	CHL	C4B-NB	-2.14	1.35	1.37
24	2	608	CHL	C4C-C3C	2.14	1.48	1.45
24	G	609	CHL	C3D-C2D	2.14	1.45	1.39
24	7	609	CHL	C1D-C2D	2.14	1.49	1.45
24	9	608	CHL	C2C-C1C	2.14	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	612	CLA	MG-ND	-2.14	2.01	2.05
25	g	612	CLA	MG-ND	-2.14	2.01	2.05
24	5	601	CHL	CHB-C4A	-2.14	1.32	1.37
25	c	511	CLA	C1B-C2B	2.14	1.48	1.43
24	p	608	CHL	C4B-NB	-2.14	1.35	1.37
40	F	101	HEM	C2A-C3A	-2.14	1.33	1.38
24	6	608	CHL	C1B-C2B	2.14	1.48	1.43
25	3	611	CLA	CMD-C2D	-2.14	1.46	1.50
25	R	613	CLA	CMC-C2C	-2.14	1.46	1.50
24	4	601	CHL	C1B-C2B	2.14	1.48	1.43
24	9	601	CHL	C1B-C2B	2.14	1.48	1.43
25	S	605	CLA	CMB-C2B	-2.14	1.46	1.50
25	N	602	CLA	MG-ND	-2.14	2.01	2.05
25	s	611	CLA	CMC-C2C	-2.14	1.46	1.50
25	s	610	CLA	MG-ND	-2.14	2.01	2.05
25	5	604	CLA	CMB-C2B	-2.14	1.46	1.50
24	4	605	CHL	C2C-C1C	2.14	1.49	1.44
25	B	603	CLA	MG-ND	-2.14	2.01	2.05
24	y	608	CHL	C1C-NC	-2.14	1.34	1.37
25	9	604	CLA	CMB-C2B	-2.14	1.46	1.50
25	r	603	CLA	CMC-C2C	-2.14	1.46	1.50
25	Y	604	CLA	MG-ND	-2.14	2.01	2.05
25	7	602	CLA	MG-NB	-2.14	2.01	2.05
25	3	612	CLA	CMB-C2B	-2.14	1.46	1.50
24	g	607	CHL	C1B-C2B	2.14	1.48	1.43
26	y	1621	LUT	C22-C21	-2.14	1.52	1.54
25	b	604	CLA	C3B-C4B	2.14	1.47	1.42
25	b	607	CLA	MG-NB	-2.14	2.01	2.05
25	p	613	CLA	CMB-C2B	-2.14	1.46	1.50
25	r	612	CLA	MG-ND	-2.14	2.01	2.05
25	3	602	CLA	CMB-C2B	-2.14	1.46	1.50
25	5	610	CLA	CMC-C2C	-2.14	1.46	1.50
25	N	610	CLA	CMD-C2D	-2.14	1.46	1.50
25	A	406	CLA	CMC-C2C	-2.14	1.46	1.50
25	a	406	CLA	CMC-C2C	-2.14	1.46	1.50
24	N	601	CHL	CHB-C4A	-2.14	1.32	1.37
25	A	406	CLA	CHC-C4B	-2.14	1.34	1.39
25	C	501	CLA	CHC-C4B	-2.14	1.34	1.39
24	N	605	CHL	C3B-C4B	2.14	1.47	1.42
24	R	606	CHL	C3B-C4B	2.14	1.47	1.42
24	9	601	CHL	C4C-C3C	2.13	1.48	1.45
25	R	612	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	609	CHL	CHB-C4A	-2.13	1.32	1.37
24	p	607	CHL	CHB-C4A	-2.13	1.32	1.37
25	A	407	CLA	CMC-C2C	-2.13	1.46	1.50
24	n	608	CHL	C1D-C2D	2.13	1.49	1.45
25	S	611	CLA	MG-ND	-2.13	2.01	2.05
25	a	407	CLA	CMC-C2C	-2.13	1.46	1.50
24	7	609	CHL	C1B-C2B	2.13	1.48	1.43
25	2	612	CLA	CMB-C2B	-2.13	1.46	1.50
25	r	601	CLA	CMC-C2C	-2.13	1.46	1.50
25	N	604	CLA	C1B-C2B	2.13	1.48	1.43
24	R	606	CHL	C3D-C2D	2.13	1.44	1.39
25	8	612	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	606	CLA	C1B-NB	-2.13	1.35	1.37
25	2	611	CLA	MG-NB	-2.13	2.01	2.05
25	0	603	CLA	MG-ND	-2.13	2.01	2.05
25	R	603	CLA	CMC-C2C	-2.13	1.46	1.50
25	s	604	CLA	CMD-C2D	-2.13	1.46	1.50
25	0	604	CLA	CMC-C2C	-2.13	1.46	1.50
26	n	1621	LUT	C22-C21	-2.13	1.52	1.54
25	c	513	CLA	MG-ND	-2.13	2.01	2.05
25	8	604	CLA	C1B-C2B	2.13	1.48	1.43
25	0	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	b	603	CLA	MG-ND	-2.13	2.01	2.05
25	1	610	CLA	CMB-C2B	-2.13	1.46	1.50
25	g	613	CLA	CMC-C2C	-2.13	1.46	1.50
25	7	613	CLA	MG-ND	-2.13	2.01	2.05
25	y	610	CLA	C1B-C2B	2.13	1.48	1.43
25	6	612	CLA	CMB-C2B	-2.13	1.46	1.50
25	B	603	CLA	CMB-C2B	-2.13	1.46	1.50
25	B	610	CLA	C1B-NB	-2.13	1.35	1.37
34	C	517	BCR	C30-C25	-2.13	1.50	1.53
24	1	609	CHL	C1B-C2B	2.13	1.48	1.43
25	n	602	CLA	C1B-C2B	2.13	1.48	1.43
25	S	610	CLA	MG-ND	-2.13	2.01	2.05
25	c	510	CLA	CMB-C2B	-2.13	1.46	1.50
25	9	614	CLA	CMD-C2D	-2.13	1.46	1.50
25	n	611	CLA	MG-ND	-2.13	2.01	2.05
25	1	602	CLA	CMB-C2B	-2.13	1.46	1.50
25	5	613	CLA	CMD-C2D	-2.13	1.46	1.50
24	1	609	CHL	CHB-C4A	-2.13	1.32	1.37
33	A	409	PHO	C3B-C2B	-2.13	1.37	1.40
25	9	602	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	602	CLA	CMD-C2D	-2.12	1.46	1.50
25	N	602	CLA	C1B-C2B	2.12	1.48	1.43
28	g	1623	NEX	O24-C25	-2.12	1.43	1.46
25	s	602	CLA	CMC-C2C	-2.12	1.46	1.50
25	4	604	CLA	CMD-C2D	-2.12	1.46	1.50
25	B	605	CLA	C1B-NB	-2.12	1.35	1.37
25	C	511	CLA	C3B-C4B	2.12	1.47	1.42
25	4	613	CLA	CMD-C2D	-2.12	1.46	1.50
25	q	603	CLA	CMB-C2B	-2.12	1.46	1.50
25	g	613	CLA	CHC-C4B	-2.12	1.34	1.39
25	r	611	CLA	MG-NB	-2.12	2.01	2.05
25	b	605	CLA	C3B-C4B	2.12	1.47	1.42
25	S	611	CLA	C1B-C2B	2.12	1.48	1.43
33	a	408	PHO	CBD-CGD	-2.12	1.49	1.52
25	D	403	CLA	MG-ND	-2.12	2.01	2.05
25	a	406	CLA	CHC-C4B	-2.12	1.34	1.39
24	4	609	CHL	C4C-C3C	2.12	1.48	1.45
25	b	611	CLA	C1B-C2B	2.12	1.48	1.43
25	N	603	CLA	C1B-NB	-2.12	1.35	1.37
25	C	504	CLA	MG-ND	-2.12	2.01	2.05
24	2	601	CHL	C1B-C2B	2.12	1.48	1.43
25	8	611	CLA	CMD-C2D	-2.12	1.46	1.50
24	p	607	CHL	C4C-C3C	2.12	1.48	1.45
25	d	403	CLA	MG-ND	-2.12	2.01	2.05
25	B	605	CLA	C3B-C4B	2.12	1.47	1.42
25	1	611	CLA	CMB-C2B	-2.12	1.46	1.50
25	B	611	CLA	C1B-C2B	2.12	1.48	1.43
25	6	603	CLA	CMB-C2B	-2.12	1.46	1.50
25	n	612	CLA	C1B-C2B	2.11	1.48	1.43
25	R	604	CLA	C1B-NB	-2.11	1.35	1.37
24	7	606	CHL	C1B-C2B	2.11	1.48	1.43
25	Y	602	CLA	C1B-NB	-2.11	1.35	1.37
25	N	614	CLA	CMC-C2C	-2.11	1.46	1.50
25	s	603	CLA	CMD-C2D	-2.11	1.46	1.50
25	b	603	CLA	C1B-C2B	2.11	1.48	1.43
25	y	614	CLA	C1B-C2B	2.11	1.48	1.43
25	7	611	CLA	CMB-C2B	-2.11	1.46	1.50
25	c	501	CLA	CHC-C4B	-2.11	1.34	1.39
25	3	604	CLA	C1B-C2B	2.11	1.48	1.43
25	R	601	CLA	CMC-C2C	-2.11	1.46	1.50
25	p	611	CLA	CMD-C2D	-2.11	1.46	1.50
24	y	607	CHL	C1D-C2D	2.11	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	407	CLA	C3B-C4B	2.11	1.47	1.42
24	Y	608	CHL	C1C-NC	-2.11	1.34	1.37
24	p	605	CHL	C4C-C3C	2.11	1.48	1.45
25	n	611	CLA	CMC-C2C	-2.11	1.46	1.50
24	7	608	CHL	C1D-C2D	2.11	1.49	1.45
25	n	614	CLA	MG-NB	-2.11	2.01	2.05
27	0	1622	XAT	O24-C25	-2.11	1.43	1.46
25	c	507	CLA	CMC-C2C	-2.11	1.46	1.50
25	G	613	CLA	CMC-C2C	-2.11	1.46	1.50
24	q	607	CHL	C4D-CHA	2.11	1.45	1.38
25	q	604	CLA	CMB-C2B	-2.11	1.46	1.50
25	7	611	CLA	MG-NB	-2.11	2.01	2.05
24	r	606	CHL	C3D-C2D	2.11	1.44	1.39
25	1	604	CLA	C3B-C4B	2.11	1.47	1.42
33	a	409	PHO	C3B-C2B	-2.11	1.37	1.40
25	n	610	CLA	CMC-C2C	-2.11	1.46	1.50
25	5	603	CLA	CMB-C2B	-2.11	1.46	1.50
25	B	617	CLA	MG-ND	-2.11	2.01	2.05
25	2	603	CLA	MG-ND	-2.11	2.01	2.05
24	S	606	CHL	C4C-C3C	2.11	1.48	1.45
25	D	403	CLA	C1B-NB	-2.11	1.35	1.37
25	d	403	CLA	C1B-NB	-2.11	1.35	1.37
25	1	604	CLA	CMD-C2D	-2.10	1.46	1.50
25	0	612	CLA	CMD-C2D	-2.10	1.46	1.50
24	n	605	CHL	C3B-C4B	2.10	1.47	1.42
25	B	609	CLA	C3B-C4B	2.10	1.47	1.42
25	b	609	CLA	C3B-C4B	2.10	1.47	1.42
24	0	606	CHL	C4C-C3C	2.10	1.48	1.45
28	Y	1623	NEX	O24-C25	-2.10	1.43	1.46
24	Y	607	CHL	C1D-C2D	2.10	1.49	1.45
25	7	610	CLA	CMB-C2B	-2.10	1.46	1.50
25	C	507	CLA	CMC-C2C	-2.10	1.46	1.50
25	C	510	CLA	CMB-C2B	-2.10	1.46	1.50
27	n	1622	XAT	O24-C25	-2.10	1.43	1.46
25	r	611	CLA	MG-ND	-2.10	2.01	2.05
24	y	606	CHL	C3D-C2D	2.10	1.44	1.39
25	6	610	CLA	CMC-C2C	-2.10	1.46	1.50
25	n	612	CLA	MG-ND	-2.10	2.01	2.05
24	1	601	CHL	C1B-C2B	2.10	1.48	1.43
25	1	612	CLA	CMB-C2B	-2.10	1.46	1.50
25	C	509	CLA	C3B-C4B	2.10	1.47	1.42
25	c	509	CLA	C3B-C4B	2.10	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	604	CLA	MG-ND	-2.10	2.01	2.05
25	9	611	CLA	MG-NB	-2.10	2.01	2.05
25	R	613	CLA	CMD-C2D	-2.10	1.46	1.50
24	9	608	CHL	C4C-C3C	2.10	1.48	1.45
25	C	513	CLA	MG-ND	-2.10	2.01	2.05
25	4	611	CLA	CMB-C2B	-2.10	1.46	1.50
25	c	506	CLA	C1B-C2B	2.10	1.48	1.43
25	1	613	CLA	CMB-C2B	-2.10	1.46	1.50
25	c	511	CLA	C3B-C4B	2.10	1.47	1.42
25	G	604	CLA	CMC-C2C	-2.09	1.46	1.50
24	n	605	CHL	C3D-C2D	2.09	1.44	1.39
25	7	612	CLA	MG-NB	-2.09	2.01	2.05
25	c	508	CLA	MG-ND	-2.09	2.01	2.05
25	N	612	CLA	CMC-C2C	-2.09	1.46	1.50
25	s	611	CLA	C1B-C2B	2.09	1.48	1.43
25	7	612	CLA	MG-ND	-2.09	2.01	2.05
25	b	608	CLA	MG-ND	-2.09	2.01	2.05
25	r	601	CLA	MG-ND	-2.09	2.01	2.05
25	6	612	CLA	CMD-C2D	-2.09	1.46	1.50
25	A	407	CLA	C3B-C4B	2.09	1.47	1.42
34	c	517	BCR	C30-C25	-2.09	1.50	1.53
25	b	603	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	607	CLA	MG-NB	-2.09	2.01	2.05
25	N	611	CLA	MG-ND	-2.09	2.01	2.05
25	a	406	CLA	C4B-NB	2.09	1.40	1.37
25	b	605	CLA	C1B-NB	-2.09	1.35	1.37
25	c	503	CLA	C1B-NB	-2.09	1.35	1.37
25	R	611	CLA	MG-ND	-2.09	2.01	2.05
24	Y	606	CHL	C3D-C2D	2.09	1.44	1.39
25	2	614	CLA	CMD-C2D	-2.09	1.46	1.50
25	S	609	CLA	CMB-C2B	-2.09	1.46	1.50
25	r	613	CLA	CMC-C2C	-2.09	1.46	1.50
25	R	601	CLA	MG-NB	-2.09	2.01	2.05
25	c	507	CLA	C4B-NB	2.09	1.40	1.37
25	B	605	CLA	MG-ND	-2.09	2.01	2.05
28	n	1623	NEX	O24-C25	-2.09	1.43	1.46
24	s	606	CHL	C4C-C3C	2.09	1.48	1.45
24	5	601	CHL	C4B-NB	-2.09	1.35	1.37
25	A	406	CLA	C4B-NB	2.09	1.40	1.37
25	D	402	CLA	C1B-C2B	2.09	1.48	1.43
25	s	605	CLA	CMB-C2B	-2.09	1.46	1.50
25	s	609	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	MG-ND	-2.09	2.01	2.05
24	1	608	CHL	C1D-C2D	2.09	1.49	1.45
25	y	604	CLA	CHC-C4B	-2.09	1.34	1.39
25	p	612	CLA	CMD-C2D	-2.09	1.46	1.50
24	1	608	CHL	C1B-C2B	2.09	1.48	1.43
25	1	613	CLA	MG-ND	-2.09	2.01	2.05
25	9	614	CLA	CMB-C2B	-2.09	1.46	1.50
24	y	609	CHL	C1D-ND	-2.09	1.35	1.37
24	5	605	CHL	C4C-C3C	2.09	1.48	1.45
25	p	610	CLA	CMC-C2C	-2.09	1.46	1.50
25	b	610	CLA	C1B-NB	-2.09	1.35	1.37
25	1	611	CLA	MG-NB	-2.09	2.01	2.05
24	q	601	CHL	C1B-C2B	2.09	1.48	1.43
25	8	604	CLA	CMD-C2D	-2.09	1.46	1.50
25	1	604	CLA	CMC-C2C	-2.08	1.46	1.50
25	0	612	CLA	CMB-C2B	-2.08	1.46	1.50
24	p	601	CHL	CHB-C4A	-2.08	1.32	1.37
24	R	608	CHL	MG-ND	-2.08	2.01	2.05
26	1	1620	LUT	C22-C21	-2.08	1.52	1.54
26	7	1620	LUT	C22-C21	-2.08	1.52	1.54
24	7	601	CHL	C1B-C2B	2.08	1.48	1.43
25	d	403	CLA	C1B-C2B	2.08	1.48	1.43
25	3	610	CLA	CMC-C2C	-2.08	1.46	1.50
25	C	511	CLA	MG-ND	-2.08	2.01	2.05
25	n	614	CLA	CMC-C2C	-2.08	1.46	1.50
24	2	609	CHL	CHB-C4A	-2.08	1.32	1.37
24	1	606	CHL	C1B-C2B	2.08	1.48	1.43
25	b	615	CLA	C1B-C2B	2.08	1.48	1.43
25	5	611	CLA	CHC-C1C	2.08	1.42	1.38
24	p	605	CHL	C4B-NB	-2.08	1.35	1.37
25	1	604	CLA	MG-ND	-2.08	2.01	2.05
25	s	612	CLA	CMC-C2C	-2.08	1.46	1.50
24	1	608	CHL	CHB-C4A	-2.08	1.32	1.37
25	g	604	CLA	CMC-C2C	-2.08	1.46	1.50
28	N	1623	NEX	O24-C25	-2.08	1.43	1.46
24	6	605	CHL	C4D-CHA	2.08	1.45	1.38
25	n	612	CLA	CMC-C2C	-2.08	1.46	1.50
24	y	608	CHL	CHB-C4A	-2.08	1.32	1.37
25	y	602	CLA	C1B-NB	-2.08	1.35	1.37
25	y	611	CLA	C1B-NB	-2.08	1.35	1.37
24	G	607	CHL	CHB-C4A	-2.08	1.32	1.37
25	1	614	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	MG-ND	-2.08	2.01	2.05
25	7	612	CLA	CMC-C2C	-2.08	1.46	1.50
25	r	613	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	506	CLA	MG-ND	-2.08	2.01	2.05
25	7	602	CLA	CMB-C2B	-2.08	1.46	1.50
25	3	604	CLA	MG-NB	-2.08	2.01	2.05
25	G	604	CLA	C1B-C2B	2.07	1.48	1.43
25	1	603	CLA	CMC-C2C	-2.07	1.46	1.50
24	5	605	CHL	C2C-C1C	2.07	1.49	1.44
25	C	506	CLA	C1B-C2B	2.07	1.48	1.43
25	b	616	CLA	C3B-C4B	2.07	1.47	1.42
25	4	614	CLA	CMB-C2B	-2.07	1.46	1.50
25	g	613	CLA	CMB-C2B	-2.07	1.46	1.50
25	7	604	CLA	CMD-C2D	-2.07	1.46	1.50
25	D	402	CLA	C1B-NB	-2.07	1.35	1.37
25	d	402	CLA	C1B-NB	-2.07	1.35	1.37
25	2	602	CLA	CMB-C2B	-2.07	1.46	1.50
25	R	611	CLA	MG-NB	-2.07	2.01	2.05
24	3	608	CHL	CHB-C4A	-2.07	1.32	1.37
24	Y	608	CHL	CHB-C4A	-2.07	1.32	1.37
25	B	602	CLA	MG-ND	-2.07	2.01	2.05
25	6	610	CLA	CMB-C2B	-2.07	1.46	1.50
25	1	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	C	513	CLA	MG-NB	-2.07	2.01	2.05
25	p	602	CLA	CMC-C2C	-2.07	1.46	1.50
25	D	403	CLA	C1B-C2B	2.07	1.48	1.43
25	G	603	CLA	CMC-C2C	-2.07	1.46	1.50
25	G	613	CLA	CMB-C2B	-2.07	1.46	1.50
25	g	603	CLA	CMC-C2C	-2.07	1.46	1.50
24	Y	609	CHL	C1D-ND	-2.07	1.35	1.37
24	2	601	CHL	MG-ND	-2.07	2.01	2.05
25	2	613	CLA	MG-ND	-2.07	2.01	2.05
25	s	609	CLA	CMB-C2B	-2.07	1.46	1.50
25	Y	610	CLA	MG-NB	-2.07	2.01	2.05
25	0	604	CLA	MG-NB	-2.07	2.01	2.05
25	c	503	CLA	MG-ND	-2.07	2.01	2.05
25	5	611	CLA	CMD-C2D	-2.07	1.46	1.50
25	N	610	CLA	CMC-C2C	-2.07	1.46	1.50
25	Y	614	CLA	C1B-C2B	2.07	1.48	1.43
24	8	601	CHL	CHB-C4A	-2.07	1.32	1.37
24	5	608	CHL	C4C-C3C	2.07	1.48	1.45
25	N	612	CLA	MG-ND	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	609	CHL	C3D-C2D	2.07	1.44	1.39
24	8	608	CHL	C1B-C2B	2.07	1.48	1.43
24	1	608	CHL	C4B-NB	-2.07	1.35	1.37
25	4	602	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	616	CLA	MG-ND	-2.07	2.01	2.05
25	4	614	CLA	CMC-C2C	-2.07	1.46	1.50
24	6	601	CHL	CHB-C4A	-2.07	1.32	1.37
25	p	611	CLA	CMB-C2B	-2.07	1.46	1.50
25	p	602	CLA	CMB-C2B	-2.07	1.46	1.50
25	r	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	n	604	CLA	MG-ND	-2.06	2.01	2.05
25	3	604	CLA	CMD-C2D	-2.06	1.46	1.50
25	r	610	CLA	C1B-NB	-2.06	1.35	1.37
25	s	604	CLA	MG-ND	-2.06	2.01	2.05
25	q	614	CLA	CMB-C2B	-2.06	1.46	1.50
25	s	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	Y	611	CLA	C1B-NB	-2.06	1.35	1.37
25	S	602	CLA	C1B-C2B	2.06	1.48	1.43
26	g	1621	LUT	C22-C21	-2.06	1.52	1.54
24	g	606	CHL	CHB-C4A	-2.06	1.32	1.37
27	N	1622	XAT	O24-C25	-2.06	1.43	1.46
24	y	606	CHL	MG-ND	-2.06	2.01	2.05
24	N	608	CHL	C3D-C2D	2.06	1.44	1.39
25	G	602	CLA	MG-ND	-2.06	2.01	2.05
25	0	602	CLA	CMC-C2C	-2.06	1.46	1.50
25	9	612	CLA	CMB-C2B	-2.06	1.46	1.50
25	8	604	CLA	MG-NB	-2.06	2.01	2.05
25	6	613	CLA	CMB-C2B	-2.06	1.46	1.50
24	r	607	CHL	C3B-C4B	2.06	1.47	1.42
24	4	601	CHL	C4C-C3C	2.06	1.48	1.45
25	5	613	CLA	CMB-C2B	-2.06	1.46	1.50
25	4	603	CLA	CMC-C2C	-2.06	1.46	1.50
25	0	603	CLA	CMB-C2B	-2.06	1.46	1.50
25	7	604	CLA	MG-ND	-2.06	2.01	2.05
24	q	601	CHL	C4C-C3C	2.06	1.48	1.45
25	S	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	q	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	g	607	CHL	CHB-C4A	-2.06	1.32	1.37
25	C	511	CLA	CHC-C4B	-2.06	1.34	1.39
25	c	511	CLA	CHC-C4B	-2.06	1.34	1.39
24	9	601	CHL	MG-ND	-2.06	2.01	2.05
25	R	601	CLA	MG-ND	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	610	CLA	MG-NB	-2.06	2.01	2.05
25	c	511	CLA	MG-ND	-2.06	2.01	2.05
25	g	604	CLA	C1B-C2B	2.06	1.48	1.43
24	S	601	CHL	CHB-C4A	-2.06	1.32	1.37
24	8	608	CHL	CHB-C4A	-2.06	1.32	1.37
25	N	604	CLA	MG-ND	-2.06	2.01	2.05
28	2	1623	NEX	O24-C25	-2.06	1.43	1.46
25	1	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	S	609	CLA	CMD-C2D	-2.06	1.46	1.50
25	7	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	p	614	CLA	CMB-C2B	-2.06	1.46	1.50
25	d	402	CLA	C1B-C2B	2.06	1.48	1.43
25	r	609	CLA	CMC-C2C	-2.06	1.46	1.50
24	0	601	CHL	CHB-C4A	-2.06	1.32	1.37
25	A	406	CLA	C1B-C2B	2.06	1.48	1.43
25	a	406	CLA	C1B-C2B	2.06	1.48	1.43
34	B	619	BCR	C1-C6	-2.06	1.50	1.53
34	b	619	BCR	C1-C6	-2.06	1.50	1.53
25	8	604	CLA	CMC-C2C	-2.06	1.46	1.50
25	q	610	CLA	CMC-C2C	-2.06	1.46	1.50
24	5	607	CHL	CHB-C4A	-2.06	1.32	1.37
25	r	604	CLA	C1B-C2B	2.05	1.48	1.43
25	Y	604	CLA	CHC-C4B	-2.05	1.34	1.39
25	5	610	CLA	CMD-C2D	-2.05	1.46	1.50
25	R	609	CLA	CMC-C2C	-2.05	1.46	1.50
25	3	602	CLA	MG-NB	-2.05	2.01	2.05
25	p	602	CLA	CHC-C1C	2.05	1.42	1.38
25	7	604	CLA	C1B-C2B	2.05	1.48	1.43
25	6	602	CLA	CMC-C2C	-2.05	1.46	1.50
25	7	610	CLA	CMC-C2C	-2.05	1.46	1.50
25	1	612	CLA	MG-NB	-2.05	2.01	2.05
25	5	602	CLA	CHC-C1C	2.05	1.42	1.38
25	3	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	R	612	CLA	CMC-C2C	-2.05	1.46	1.50
25	8	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	7	613	CLA	CMC-C2C	-2.05	1.46	1.50
25	2	611	CLA	CMB-C2B	-2.05	1.46	1.50
25	6	602	CLA	CMD-C2D	-2.05	1.46	1.50
28	s	1623	NEX	O24-C25	-2.05	1.43	1.46
25	8	602	CLA	MG-NB	-2.05	2.01	2.05
24	n	601	CHL	C1B-C2B	2.05	1.48	1.43
25	2	612	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	1623	NEX	O24-C25	-2.05	1.43	1.46
25	p	602	CLA	CMD-C2D	-2.05	1.46	1.50
24	R	607	CHL	C3B-C4B	2.05	1.47	1.42
24	5	607	CHL	C4B-NB	-2.05	1.35	1.37
25	2	614	CLA	CMB-C2B	-2.05	1.46	1.50
25	B	615	CLA	C1B-C2B	2.05	1.48	1.43
24	2	609	CHL	CMC-C2C	2.05	1.49	1.45
25	b	605	CLA	MG-ND	-2.05	2.01	2.05
25	c	502	CLA	CAC-C3C	-2.05	1.45	1.51
24	3	608	CHL	C1B-C2B	2.05	1.48	1.43
25	s	605	CLA	CMC-C2C	-2.05	1.46	1.50
24	4	609	CHL	C1D-ND	-2.05	1.35	1.37
24	3	607	CHL	C2C-C1C	2.05	1.49	1.44
24	6	608	CHL	CHB-C4A	-2.05	1.32	1.37
25	y	603	CLA	CHC-C4B	-2.05	1.34	1.39
27	0	1622	XAT	O4-C5	-2.05	1.43	1.46
24	2	608	CHL	CMC-C2C	2.04	1.49	1.45
25	3	610	CLA	CMB-C2B	-2.04	1.46	1.50
25	0	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	9	611	CLA	CMB-C2B	-2.04	1.46	1.50
25	r	609	CLA	MG-NB	-2.04	2.01	2.05
27	6	1622	XAT	O4-C5	-2.04	1.43	1.46
24	y	607	CHL	C3A-C2A	-2.04	1.48	1.54
24	N	601	CHL	C1B-C2B	2.04	1.48	1.43
24	Y	608	CHL	C1B-C2B	2.04	1.48	1.43
25	5	612	CLA	CMB-C2B	-2.04	1.46	1.50
25	8	610	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	605	CLA	C1B-C2B	2.04	1.48	1.43
25	9	610	CLA	CMD-C2D	-2.04	1.46	1.50
25	4	613	CLA	CMB-C2B	-2.04	1.46	1.50
25	a	407	CLA	C1B-NB	-2.04	1.35	1.37
24	4	609	CHL	C1B-C2B	2.04	1.48	1.43
25	1	614	CLA	CMB-C2B	-2.04	1.46	1.50
25	G	612	CLA	MG-NB	-2.04	2.01	2.05
25	7	614	CLA	CMB-C2B	-2.04	1.46	1.50
25	6	604	CLA	CMC-C2C	-2.04	1.46	1.50
33	a	409	PHO	C3B-CAB	-2.04	1.43	1.47
24	5	606	CHL	C2C-C1C	2.04	1.48	1.44
25	5	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	q	602	CLA	CMC-C2C	-2.04	1.46	1.50
25	6	614	CLA	CHC-C1C	2.04	1.42	1.38
28	q	1623	NEX	O24-C25	-2.04	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	612	CLA	CMC-C2C	-2.04	1.46	1.50
24	r	606	CHL	C4C-C3C	2.04	1.48	1.45
28	7	1623	NEX	O24-C25	-2.04	1.43	1.46
25	g	612	CLA	MG-NB	-2.04	2.01	2.05
27	6	1622	XAT	O24-C25	-2.04	1.43	1.46
25	a	407	CLA	CHC-C4B	-2.04	1.34	1.39
25	R	604	CLA	C1B-C2B	2.04	1.48	1.43
25	5	614	CLA	CMB-C2B	-2.04	1.46	1.50
25	0	602	CLA	CMB-C2B	-2.04	1.46	1.50
25	R	604	CLA	MG-NB	-2.04	2.01	2.05
25	5	611	CLA	CMB-C2B	-2.04	1.46	1.50
24	0	609	CHL	CHB-C4A	-2.04	1.32	1.37
24	0	605	CHL	C4C-C3C	2.04	1.48	1.45
24	g	601	CHL	C1C-NC	-2.04	1.34	1.37
24	7	601	CHL	C3D-C2D	2.04	1.44	1.39
28	4	1623	NEX	O24-C25	-2.04	1.43	1.46
24	9	609	CHL	CHB-C4A	-2.04	1.32	1.37
25	C	508	CLA	MG-ND	-2.04	2.01	2.05
25	G	612	CLA	CMC-C2C	-2.04	1.46	1.50
25	g	612	CLA	CMC-C2C	-2.03	1.46	1.50
24	2	608	CHL	C4D-CHA	2.03	1.45	1.38
25	C	510	CLA	C1B-C2B	2.03	1.48	1.43
24	1	601	CHL	C3D-C2D	2.03	1.44	1.39
25	N	614	CLA	MG-NB	-2.03	2.01	2.05
25	q	603	CLA	CMD-C2D	-2.03	1.46	1.50
25	Y	603	CLA	CHC-C4B	-2.03	1.34	1.39
24	1	606	CHL	CHB-C4A	-2.03	1.32	1.37
25	7	602	CLA	MG-ND	-2.03	2.01	2.05
25	c	506	CLA	C1B-NB	-2.03	1.35	1.37
25	3	612	CLA	CMD-C2D	-2.03	1.46	1.50
25	4	603	CLA	MG-ND	-2.03	2.01	2.05
25	b	608	CLA	MG-NB	-2.03	2.01	2.05
25	0	612	CLA	MG-ND	-2.03	2.01	2.05
24	q	609	CHL	C1D-ND	-2.03	1.35	1.37
24	n	601	CHL	C3B-C4B	2.03	1.47	1.42
25	p	604	CLA	CMD-C2D	-2.03	1.46	1.50
24	Y	607	CHL	C3D-C2D	2.03	1.44	1.39
25	S	614	CLA	CMB-C2B	-2.03	1.46	1.50
25	q	611	CLA	CMB-C2B	-2.03	1.46	1.50
25	6	610	CLA	MG-NB	-2.03	2.01	2.05
25	r	604	CLA	MG-NB	-2.03	2.01	2.05
24	Y	606	CHL	C1D-ND	-2.03	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	602	CLA	CMC-C2C	-2.03	1.46	1.50
25	y	610	CLA	MG-NB	-2.03	2.01	2.05
25	S	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	B	615	CLA	CAC-C3C	-2.03	1.45	1.51
25	b	615	CLA	CAC-C3C	-2.03	1.45	1.51
34	D	404	BCR	C1-C6	-2.03	1.51	1.53
25	8	612	CLA	CMD-C2D	-2.03	1.46	1.50
39	d	405	PL9	C40-C39	-2.03	1.45	1.50
25	c	513	CLA	MG-NB	-2.03	2.01	2.05
25	r	601	CLA	MG-NB	-2.03	2.01	2.05
25	g	602	CLA	CMB-C2B	-2.03	1.46	1.50
34	c	517	BCR	C1-C6	-2.03	1.51	1.53
28	9	1623	NEX	O24-C25	-2.03	1.43	1.46
25	9	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	608	CLA	MG-NB	-2.03	2.01	2.05
25	q	602	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	506	CLA	MG-ND	-2.03	2.01	2.05
25	S	605	CLA	MG-ND	-2.03	2.01	2.05
25	6	612	CLA	CMC-C2C	-2.03	1.46	1.50
24	G	606	CHL	CHB-C4A	-2.03	1.32	1.37
24	n	608	CHL	C3D-C2D	2.03	1.44	1.39
25	c	510	CLA	C1B-C2B	2.03	1.48	1.43
25	C	502	CLA	CAC-C3C	-2.03	1.45	1.51
24	0	605	CHL	CHB-C4A	-2.03	1.32	1.37
25	0	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	2	604	CLA	CMC-C2C	-2.02	1.46	1.50
25	9	602	CLA	CMC-C2C	-2.02	1.46	1.50
25	9	603	CLA	MG-ND	-2.02	2.01	2.05
25	B	614	CLA	C1B-C2B	2.02	1.48	1.43
33	A	409	PHO	C3B-CAB	-2.02	1.43	1.47
25	d	402	CLA	CAA-C2A	-2.02	1.50	1.54
25	G	602	CLA	CMB-C2B	-2.02	1.46	1.50
24	Y	608	CHL	C1D-C2D	2.02	1.49	1.45
34	C	517	BCR	C1-C6	-2.02	1.51	1.53
25	s	614	CLA	CMB-C2B	-2.02	1.46	1.50
24	6	606	CHL	C4C-C3C	2.02	1.48	1.45
24	R	606	CHL	C3A-C2A	-2.02	1.48	1.54
24	0	609	CHL	C2C-C1C	2.02	1.48	1.44
25	7	613	CLA	CMB-C2B	-2.02	1.46	1.50
25	7	604	CLA	CHC-C4B	-2.02	1.34	1.39
25	5	604	CLA	CMD-C2D	-2.02	1.46	1.50
24	q	601	CHL	CHB-C4A	-2.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	1623	NEX	O24-C25	-2.02	1.43	1.46
25	0	611	CLA	CMB-C2B	-2.02	1.46	1.50
25	b	616	CLA	C1B-NB	-2.02	1.35	1.37
24	r	608	CHL	MG-ND	-2.02	2.01	2.05
25	2	610	CLA	CMD-C2D	-2.02	1.46	1.50
24	Y	606	CHL	MG-ND	-2.02	2.01	2.05
24	p	601	CHL	C4C-C3C	2.02	1.48	1.45
24	8	607	CHL	C2C-C1C	2.02	1.48	1.44
24	r	606	CHL	C3A-C2A	-2.02	1.48	1.54
25	3	604	CLA	CMC-C2C	-2.02	1.46	1.50
25	G	604	CLA	MG-ND	-2.02	2.01	2.05
24	y	608	CHL	C1B-C2B	2.02	1.48	1.43
25	1	613	CLA	C1B-NB	-2.02	1.35	1.37
25	A	407	CLA	C1B-NB	-2.02	1.35	1.37
24	Y	607	CHL	C3A-C2A	-2.02	1.48	1.54
25	y	603	CLA	CAC-C3C	-2.02	1.45	1.51
25	A	407	CLA	CHC-C4B	-2.02	1.34	1.39
25	5	612	CLA	CMD-C2D	-2.01	1.46	1.50
27	1	1622	XAT	O4-C5	-2.01	1.43	1.46
25	1	611	CLA	CMC-C2C	-2.01	1.46	1.50
25	3	603	CLA	CMB-C2B	-2.01	1.46	1.50
25	4	612	CLA	CMB-C2B	-2.01	1.46	1.50
24	s	601	CHL	CHB-C4A	-2.01	1.32	1.37
24	q	608	CHL	C3B-C2B	2.01	1.48	1.41
25	b	614	CLA	C1B-C2B	2.01	1.48	1.43
25	s	602	CLA	C1B-C2B	2.01	1.48	1.43
25	R	616	CLA	MG-ND	-2.01	2.01	2.05
24	G	601	CHL	C1B-C2B	2.01	1.48	1.43
24	g	601	CHL	C1B-C2B	2.01	1.48	1.43
25	C	501	CLA	C3B-C4B	2.01	1.47	1.42
25	C	504	CLA	CAC-C3C	-2.01	1.46	1.51
25	2	613	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	610	CLA	C1B-C2B	2.01	1.48	1.43
39	D	405	PL9	C40-C39	-2.01	1.45	1.50
25	3	614	CLA	CMD-C2D	-2.01	1.46	1.50
25	q	602	CLA	CHC-C1C	2.01	1.42	1.38
28	y	1623	NEX	C22-C21	-2.01	1.51	1.54
25	r	603	CLA	CHC-C4B	-2.01	1.34	1.39
25	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	501	CLA	C3B-C4B	2.01	1.47	1.42
25	0	613	CLA	CMD-C2D	-2.01	1.46	1.50
24	R	607	CHL	MG-ND	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	605	CHL	C4D-CHA	2.01	1.45	1.38
25	6	602	CLA	CMB-C2B	-2.01	1.46	1.50
25	S	605	CLA	CMC-C2C	-2.01	1.46	1.50
28	Y	1623	NEX	C22-C21	-2.01	1.51	1.54
25	0	610	CLA	CMC-C2C	-2.01	1.46	1.50
25	8	610	CLA	CMC-C2C	-2.01	1.46	1.50
25	9	603	CLA	CMC-C2C	-2.01	1.46	1.50
25	Y	603	CLA	CAC-C3C	-2.01	1.46	1.51
24	Y	606	CHL	C1D-C2D	2.01	1.49	1.45
25	B	616	CLA	C3B-C4B	2.01	1.47	1.42
25	9	613	CLA	CMC-C2C	-2.01	1.46	1.50
24	2	607	CHL	C4D-CHA	2.01	1.45	1.38
24	y	607	CHL	C3D-C2D	2.01	1.44	1.39
25	B	617	CLA	C4B-NB	2.01	1.40	1.37
25	b	617	CLA	C4B-NB	2.01	1.40	1.37
40	f	101	HEM	FE-NB	2.01	2.01	1.94
24	2	605	CHL	C3B-C2B	2.01	1.48	1.41
37	c	524	DGD	O2G-C2G	-2.01	1.41	1.46
24	8	608	CHL	C4C-C3C	2.01	1.48	1.45
25	b	611	CLA	CHC-C4B	-2.01	1.34	1.39
25	8	614	CLA	CMB-C2B	-2.01	1.46	1.50
25	0	614	CLA	CHC-C1C	2.01	1.42	1.38
24	1	609	CHL	C1C-NC	-2.01	1.34	1.37
25	C	507	CLA	CHC-C4B	-2.01	1.34	1.39
24	r	608	CHL	C1D-C2D	2.00	1.49	1.45
27	1	1622	XAT	O24-C25	-2.00	1.43	1.46
24	y	608	CHL	C1D-C2D	2.00	1.49	1.45
25	9	604	CLA	CMC-C2C	-2.00	1.46	1.50
25	9	614	CLA	MG-NB	-2.00	2.01	2.05
25	b	617	CLA	C1B-C2B	2.00	1.48	1.43
25	B	611	CLA	CHC-C4B	-2.00	1.34	1.39
34	d	404	BCR	C1-C6	-2.00	1.51	1.53
24	N	605	CHL	C1B-C2B	2.00	1.48	1.43
25	7	603	CLA	CMC-C2C	-2.00	1.46	1.50
25	p	613	CLA	CMD-C2D	-2.00	1.46	1.50
24	N	607	CHL	C2C-C1C	2.00	1.48	1.44
24	r	608	CHL	C3D-C2D	2.00	1.44	1.39
25	q	603	CLA	CMC-C2C	-2.00	1.46	1.50
25	B	610	CLA	CHC-C4B	-2.00	1.34	1.39
25	S	609	CLA	CMC-C2C	-2.00	1.46	1.50
25	7	611	CLA	CMC-C2C	-2.00	1.46	1.50
37	C	524	DGD	O2G-C2G	-2.00	1.41	1.46

All (6530) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	412	SQD	O9-S-C6	-19.98	83.20	106.94
35	A	412	SQD	O9-S-C6	-19.85	83.34	106.94
27	Y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	6	1622	XAT	C37-C21-C36	-17.56	81.47	107.37
27	0	1622	XAT	C37-C21-C36	-17.49	81.58	107.37
27	1	1622	XAT	C37-C21-C36	-17.00	82.29	107.37
27	7	1622	XAT	C37-C21-C36	-16.64	82.82	107.37
27	Y	1622	XAT	C37-C21-C22	-15.26	82.46	108.98
27	y	1622	XAT	C37-C21-C22	-15.26	82.46	108.98
27	1	1622	XAT	C37-C21-C22	-15.05	82.82	108.98
27	7	1622	XAT	C37-C21-C22	-15.05	82.84	108.98
27	6	1622	XAT	C37-C21-C22	-14.93	83.04	108.98
27	0	1622	XAT	C37-C21-C22	-14.84	83.20	108.98
35	A	412	SQD	O8-S-O9	-11.92	82.14	111.27
35	a	412	SQD	O8-S-O9	-11.90	82.20	111.27
28	2	1623	NEX	O24-C25-C24	11.26	121.84	113.38
24	Y	605	CHL	C2B-C1B-NB	10.80	117.47	110.23
24	y	605	CHL	C2B-C1B-NB	10.77	117.45	110.23
24	9	601	CHL	C2B-C1B-NB	10.75	117.44	110.23
24	y	607	CHL	C2B-C1B-NB	10.68	117.39	110.23
24	5	601	CHL	C2B-C1B-NB	10.67	117.38	110.23
28	9	1623	NEX	O24-C25-C24	10.64	121.38	113.38
24	Y	607	CHL	C2B-C1B-NB	10.60	117.33	110.23
24	2	601	CHL	C2B-C1B-NB	10.59	117.33	110.23
24	r	607	CHL	C2B-C1B-NB	10.51	117.28	110.23
24	3	607	CHL	C2B-C1B-NB	10.47	117.25	110.23
28	5	1623	NEX	O24-C25-C24	10.44	121.22	113.38
24	1	601	CHL	CMD-C2D-C1D	10.43	143.09	124.71
24	p	601	CHL	C2B-C1B-NB	10.38	117.19	110.23
24	R	607	CHL	C2B-C1B-NB	10.36	117.17	110.23
24	7	601	CHL	CMD-C2D-C1D	10.35	142.95	124.71
28	s	1623	NEX	O24-C25-C24	10.33	121.14	113.38
24	n	601	CHL	C2B-C1B-NB	10.30	117.14	110.23
28	S	1623	NEX	O24-C25-C24	10.29	121.11	113.38
27	n	1622	XAT	O24-C25-C24	10.29	121.11	113.38
27	N	1622	XAT	O24-C25-C24	10.24	121.08	113.38
24	G	601	CHL	CMD-C2D-C1D	10.24	142.76	124.71
24	n	607	CHL	C2B-C1B-NB	10.23	117.09	110.23
24	N	607	CHL	C2B-C1B-NB	10.19	117.06	110.23
24	q	609	CHL	CHD-C1D-ND	-10.17	115.11	124.45
24	8	607	CHL	C2B-C1B-NB	10.06	116.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	601	CHL	C2B-C1B-NB	9.90	116.87	110.23
35	a	412	SQD	O7-S-C6	9.89	118.69	106.94
28	0	1623	NEX	O24-C25-C24	9.87	120.80	113.38
28	p	1623	NEX	O24-C25-C24	9.85	120.78	113.38
24	g	601	CHL	CMD-C2D-C1D	9.82	142.02	124.71
28	R	623	NEX	O24-C25-C24	9.81	120.75	113.38
24	2	609	CHL	C2B-C1B-NB	9.80	116.80	110.23
35	A	412	SQD	O7-S-C6	9.79	118.58	106.94
28	r	623	NEX	O24-C25-C24	9.79	120.74	113.38
24	r	606	CHL	C2B-C1B-NB	9.73	116.75	110.23
24	R	606	CHL	C2B-C1B-NB	9.73	116.75	110.23
24	N	609	CHL	C2B-C1B-NB	9.66	116.71	110.23
24	7	601	CHL	C2B-C1B-NB	9.66	116.71	110.23
24	y	601	CHL	C2B-C1B-NB	9.65	116.70	110.23
24	5	608	CHL	C2B-C1B-NB	9.62	116.68	110.23
24	p	608	CHL	C2B-C1B-NB	9.62	116.68	110.23
24	1	601	CHL	C2B-C1B-NB	9.61	116.68	110.23
24	3	608	CHL	C2B-C1B-NB	9.61	116.67	110.23
24	g	609	CHL	CMD-C2D-C1D	9.60	141.63	124.71
24	G	609	CHL	CMD-C2D-C1D	9.59	141.61	124.71
24	G	601	CHL	C2B-C1B-NB	9.58	116.65	110.23
24	0	607	CHL	C2B-C1B-NB	9.57	116.65	110.23
24	8	601	CHL	C2B-C1B-NB	9.55	116.64	110.23
24	2	608	CHL	C2B-C1B-NB	9.55	116.63	110.23
24	0	605	CHL	C2B-C1B-NB	9.52	116.61	110.23
24	N	605	CHL	C2B-C1B-NB	9.51	116.61	110.23
24	n	609	CHL	C2B-C1B-NB	9.51	116.61	110.23
24	6	601	CHL	C2B-C1B-NB	9.49	116.60	110.23
24	9	609	CHL	C2B-C1B-NB	9.49	116.60	110.23
24	1	608	CHL	C2B-C1B-NB	9.49	116.59	110.23
24	g	601	CHL	C2B-C1B-NB	9.48	116.59	110.23
24	n	605	CHL	C2B-C1B-NB	9.46	116.57	110.23
24	N	601	CHL	CMD-C2D-C1D	9.45	141.36	124.71
28	8	1623	NEX	O24-C25-C24	9.43	120.47	113.38
24	8	608	CHL	C2B-C1B-NB	9.41	116.54	110.23
24	p	607	CHL	C2B-C1B-NB	9.40	116.54	110.23
24	n	601	CHL	CMD-C2D-C1D	9.39	141.27	124.71
24	9	608	CHL	C2B-C1B-NB	9.38	116.52	110.23
24	Y	601	CHL	C2B-C1B-NB	9.37	116.51	110.23
24	g	607	CHL	C2B-C1B-NB	9.36	116.50	110.23
24	n	606	CHL	C2B-C1B-NB	9.32	116.48	110.23
24	G	607	CHL	C2B-C1B-NB	9.31	116.47	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	601	CHL	C2B-C1B-NB	9.29	116.46	110.23
24	n	608	CHL	C2B-C1B-NB	9.27	116.45	110.23
24	3	609	CHL	C2B-C1B-NB	9.25	116.44	110.23
24	q	601	CHL	C2B-C1B-NB	9.25	116.43	110.23
28	3	1623	NEX	O24-C25-C24	9.25	120.33	113.38
24	4	609	CHL	CHD-C1D-ND	-9.22	115.98	124.45
24	6	608	CHL	C2B-C1B-NB	9.22	116.41	110.23
27	5	1622	XAT	O24-C25-C24	9.21	120.30	113.38
24	Y	609	CHL	C2B-C1B-NB	9.20	116.40	110.23
24	y	609	CHL	C2B-C1B-NB	9.17	116.38	110.23
24	N	606	CHL	C2B-C1B-NB	9.16	116.38	110.23
24	6	607	CHL	C2B-C1B-NB	9.15	116.36	110.23
24	6	605	CHL	C2B-C1B-NB	9.15	116.36	110.23
24	y	606	CHL	C2B-C1B-NB	9.14	116.36	110.23
24	0	608	CHL	C2B-C1B-NB	9.14	116.36	110.23
24	7	608	CHL	C2B-C1B-NB	9.11	116.34	110.23
24	s	601	CHL	CMD-C2D-C1D	9.08	140.72	124.71
24	6	609	CHL	C2B-C1B-NB	9.08	116.32	110.23
25	c	502	CLA	C4A-NA-C1A	9.08	110.79	106.71
24	7	609	CHL	C2B-C1B-NB	9.08	116.32	110.23
24	1	609	CHL	C2B-C1B-NB	9.07	116.31	110.23
24	Y	606	CHL	C2B-C1B-NB	9.06	116.30	110.23
24	N	607	CHL	CMD-C2D-C1D	9.06	140.67	124.71
24	0	601	CHL	C2B-C1B-NB	9.05	116.30	110.23
28	q	1623	NEX	O24-C25-C24	9.04	120.17	113.38
24	N	608	CHL	C2B-C1B-NB	9.02	116.28	110.23
24	n	607	CHL	CMD-C2D-C1D	9.02	140.61	124.71
28	n	1623	NEX	O24-C25-C24	9.01	120.15	113.38
24	n	605	CHL	CMD-C2D-C1D	9.01	140.59	124.71
24	2	601	CHL	CMD-C2D-C1D	9.00	140.57	124.71
24	8	609	CHL	C2B-C1B-NB	8.99	116.26	110.23
24	G	605	CHL	C2B-C1B-NB	8.97	116.25	110.23
25	C	502	CLA	C4A-NA-C1A	8.95	110.73	106.71
24	g	605	CHL	C2B-C1B-NB	8.94	116.23	110.23
24	N	605	CHL	CMD-C2D-C1D	8.94	140.47	124.71
35	A	412	SQD	O9-S-O7	-8.93	83.04	113.95
24	5	607	CHL	C2B-C1B-NB	8.92	116.21	110.23
28	N	1623	NEX	O24-C25-C24	8.89	120.06	113.38
35	a	412	SQD	O9-S-O7	-8.89	83.18	113.95
24	y	606	CHL	C2C-C3C-C4C	-8.89	100.15	106.49
28	4	1623	NEX	O24-C25-C24	8.88	120.05	113.38
24	g	606	CHL	C2B-C1B-NB	8.88	116.18	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	601	CHL	CMD-C2D-C1D	8.88	140.36	124.71
24	8	607	CHL	C1D-ND-C4D	-8.87	100.03	106.33
24	5	609	CHL	CMD-C2D-C1D	8.87	140.34	124.71
24	S	601	CHL	C2B-C1B-NB	8.85	116.16	110.23
24	s	608	CHL	C2B-C1B-NB	8.84	116.16	110.23
24	r	606	CHL	CMD-C2D-C1D	8.84	140.29	124.71
33	a	409	PHO	C4D-CHA-CBD	-8.83	104.52	108.52
24	S	601	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	p	609	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	9	608	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	R	606	CHL	CMD-C2D-C1D	8.82	140.25	124.71
33	A	409	PHO	C4D-CHA-CBD	-8.82	104.53	108.52
24	3	607	CHL	C1D-ND-C4D	-8.82	100.07	106.33
24	Y	606	CHL	C2C-C3C-C4C	-8.81	100.21	106.49
24	9	609	CHL	CMD-C2D-C1D	8.81	140.24	124.71
24	S	608	CHL	C2B-C1B-NB	8.81	116.14	110.23
24	p	605	CHL	CMD-C2D-C1D	8.81	140.23	124.71
24	y	608	CHL	C1D-ND-C4D	-8.80	100.08	106.33
24	G	606	CHL	C2B-C1B-NB	8.80	116.13	110.23
24	s	606	CHL	C2B-C1B-NB	8.79	116.13	110.23
24	3	609	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
24	Y	607	CHL	CMD-C2D-C1D	8.76	140.15	124.71
24	5	601	CHL	CMD-C2D-C1D	8.75	140.14	124.71
24	y	607	CHL	CMD-C2D-C1D	8.75	140.13	124.71
24	S	606	CHL	C2B-C1B-NB	8.75	116.09	110.23
24	Y	608	CHL	C1D-ND-C4D	-8.74	100.12	106.33
24	0	606	CHL	CMD-C2D-C1D	8.74	140.12	124.71
24	2	608	CHL	CMD-C2D-C1D	8.74	140.12	124.71
27	3	1622	XAT	O24-C25-C24	8.73	119.94	113.38
24	1	606	CHL	C2B-C1B-NB	8.73	116.08	110.23
24	7	601	CHL	C1D-ND-C4D	-8.72	100.14	106.33
24	2	609	CHL	CMD-C2D-C1D	8.71	140.07	124.71
28	6	1623	NEX	O24-C25-C24	8.71	119.92	113.38
24	9	607	CHL	C2B-C1B-NB	8.71	116.07	110.23
24	7	608	CHL	C2C-C3C-C4C	-8.70	100.28	106.49
24	Y	606	CHL	CMD-C2D-C1D	8.70	140.05	124.71
24	3	606	CHL	CMD-C2D-C1D	8.70	140.04	124.71
24	8	606	CHL	CMD-C2D-C1D	8.69	140.03	124.71
24	6	609	CHL	CMD-C2D-C1D	8.68	140.01	124.71
24	q	605	CHL	CMD-C2D-C1D	8.68	140.00	124.71
24	y	606	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	N	608	CHL	CMD-C2D-C1D	8.67	139.99	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	601	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	n	608	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	y	608	CHL	CMD-C2D-C1D	8.66	139.98	124.71
24	Y	608	CHL	CMD-C2D-C1D	8.66	139.98	124.71
27	8	1622	XAT	O24-C25-C24	8.66	119.89	113.38
24	N	607	CHL	C1D-ND-C4D	-8.66	100.19	106.33
24	3	601	CHL	CMD-C2D-C1D	8.65	139.95	124.71
24	1	601	CHL	C1D-ND-C4D	-8.64	100.19	106.33
24	4	608	CHL	C2B-C1B-NB	8.64	116.02	110.23
24	4	601	CHL	C2B-C1B-NB	8.63	116.02	110.23
24	7	606	CHL	CMD-C2D-C1D	8.62	139.91	124.71
24	1	608	CHL	C2C-C3C-C4C	-8.62	100.34	106.49
24	n	607	CHL	C1D-ND-C4D	-8.62	100.21	106.33
24	s	601	CHL	C2B-C1B-NB	8.62	116.01	110.23
28	g	1623	NEX	O24-C25-C24	8.60	119.84	113.38
24	4	607	CHL	C2B-C1B-NB	8.60	116.00	110.23
24	y	609	CHL	C2C-C3C-C4C	-8.59	100.36	106.49
24	0	609	CHL	C2B-C1B-NB	8.59	115.99	110.23
24	4	607	CHL	CMD-C2D-C1D	8.59	139.85	124.71
24	p	609	CHL	C2B-C1B-NB	8.58	115.99	110.23
24	1	606	CHL	CMD-C2D-C1D	8.58	139.84	124.71
24	5	605	CHL	CMD-C2D-C1D	8.58	139.84	124.71
24	1	605	CHL	C2B-C1B-NB	8.58	115.98	110.23
24	6	608	CHL	CMD-C2D-C1D	8.58	139.83	124.71
24	0	608	CHL	CMD-C2D-C1D	8.58	139.83	124.71
24	Y	609	CHL	C2C-C3C-C4C	-8.57	100.38	106.49
24	8	608	CHL	CMD-C2D-C1D	8.57	139.81	124.71
24	4	605	CHL	CMD-C2D-C1D	8.56	139.79	124.71
24	q	609	CHL	CMD-C2D-C1D	8.56	139.79	124.71
27	2	1622	XAT	O4-C5-C4	8.55	119.80	113.38
24	p	608	CHL	CMD-C2D-C1D	8.55	139.78	124.71
24	7	605	CHL	C2B-C1B-NB	8.54	115.96	110.23
24	5	608	CHL	C1D-ND-C4D	-8.54	100.27	106.33
27	y	1622	XAT	C36-C21-C22	8.54	123.82	108.98
27	Y	1622	XAT	C36-C21-C22	8.53	123.81	108.98
24	0	609	CHL	CMD-C2D-C1D	8.53	139.75	124.71
24	7	608	CHL	CMD-C2D-C1D	8.53	139.74	124.71
24	1	609	CHL	CMD-C2D-C1D	8.52	139.74	124.71
28	G	1623	NEX	O24-C25-C24	8.52	119.78	113.38
24	5	608	CHL	CMD-C2D-C1D	8.51	139.72	124.71
24	N	606	CHL	CMD-C2D-C1D	8.51	139.71	124.71
24	8	601	CHL	CMD-C2D-C1D	8.51	139.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	607	CHL	CMD-C2D-C1D	8.51	139.70	124.71
24	p	608	CHL	C1D-ND-C4D	-8.51	100.29	106.33
24	8	609	CHL	C2C-C3C-C4C	-8.50	100.43	106.49
24	1	607	CHL	C2B-C1B-NB	8.49	115.92	110.23
24	Y	601	CHL	CMD-C2D-C1D	8.49	139.68	124.71
24	8	607	CHL	CMD-C2D-C1D	8.48	139.66	124.71
24	n	606	CHL	CMD-C2D-C1D	8.47	139.65	124.71
24	2	607	CHL	C2B-C1B-NB	8.47	115.91	110.23
24	7	609	CHL	CMD-C2D-C1D	8.47	139.64	124.71
24	p	605	CHL	CHD-C1D-ND	-8.47	116.67	124.45
24	3	607	CHL	CMD-C2D-C1D	8.46	139.63	124.71
24	7	606	CHL	C2B-C1B-NB	8.46	115.90	110.23
24	7	605	CHL	CMD-C2D-C1D	8.45	139.61	124.71
24	3	608	CHL	CMD-C2D-C1D	8.45	139.60	124.71
24	p	601	CHL	CMD-C2D-C1D	8.43	139.58	124.71
24	Y	607	CHL	C1D-ND-C4D	-8.43	100.34	106.33
24	y	608	CHL	C2B-C1B-NB	8.43	115.88	110.23
24	4	608	CHL	CMD-C2D-C1D	8.42	139.56	124.71
28	1	1623	NEX	O24-C25-C24	8.42	119.71	113.38
24	q	601	CHL	CMD-C2D-C1D	8.42	139.56	124.71
24	5	609	CHL	C2B-C1B-NB	8.42	115.88	110.23
24	Y	609	CHL	CMD-C2D-C1D	8.42	139.55	124.71
24	y	607	CHL	C1D-ND-C4D	-8.41	100.36	106.33
24	9	607	CHL	CMD-C2D-C1D	8.41	139.54	124.71
24	6	601	CHL	C1D-ND-C4D	-8.41	100.36	106.33
24	n	601	CHL	C1D-ND-C4D	-8.40	100.37	106.33
24	7	607	CHL	C2B-C1B-NB	8.40	115.86	110.23
24	g	606	CHL	CMD-C2D-C1D	8.39	139.50	124.71
24	s	608	CHL	CMD-C2D-C1D	8.39	139.50	124.71
24	6	606	CHL	C2B-C1B-NB	8.38	115.85	110.23
24	n	609	CHL	CMD-C2D-C1D	8.38	139.48	124.71
24	G	606	CHL	CMD-C2D-C1D	8.38	139.48	124.71
27	9	1622	XAT	O4-C5-C4	8.37	119.67	113.38
24	1	608	CHL	CMD-C2D-C1D	8.37	139.47	124.71
24	G	608	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	8	605	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	q	607	CHL	C2B-C1B-NB	8.36	115.84	110.23
24	q	608	CHL	CHD-C1D-ND	-8.36	116.77	124.45
24	6	606	CHL	CMD-C2D-C1D	8.36	139.44	124.71
24	N	609	CHL	CMD-C2D-C1D	8.35	139.44	124.71
24	Y	608	CHL	C2B-C1B-NB	8.35	115.83	110.23
24	S	608	CHL	CMD-C2D-C1D	8.35	139.42	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	CMD-C2D-C1D	8.34	139.40	124.71
24	n	606	CHL	C1D-ND-C4D	-8.33	100.42	106.33
24	p	606	CHL	CMD-C2D-C1D	8.32	139.37	124.71
24	1	605	CHL	CMD-C2D-C1D	8.32	139.37	124.71
24	0	607	CHL	C1D-ND-C4D	-8.31	100.43	106.33
24	5	605	CHL	CHD-C1D-ND	-8.31	116.82	124.45
24	3	605	CHL	CMD-C2D-C1D	8.30	139.34	124.71
24	y	609	CHL	CMD-C2D-C1D	8.29	139.32	124.71
24	q	605	CHL	C2B-C1B-NB	8.29	115.79	110.23
24	q	607	CHL	CMD-C2D-C1D	8.27	139.29	124.71
24	8	601	CHL	C1D-ND-C4D	-8.27	100.46	106.33
27	p	1622	XAT	O24-C25-C24	8.26	119.59	113.38
24	g	608	CHL	C2B-C1B-NB	8.26	115.77	110.23
24	N	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
24	8	605	CHL	CHD-C1D-ND	-8.24	116.88	124.45
24	5	605	CHL	C1D-ND-C4D	-8.24	100.48	106.33
24	4	609	CHL	CMD-C2D-C1D	8.22	139.20	124.71
24	q	608	CHL	C2C-C3C-C4C	-8.22	100.63	106.49
24	p	601	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	g	601	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	8	609	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	G	605	CHL	CMD-C2D-C1D	8.21	139.18	124.71
24	9	605	CHL	CMD-C2D-C1D	8.20	139.17	124.71
24	3	605	CHL	CHD-C1D-ND	-8.19	116.93	124.45
24	0	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71
24	g	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71
24	2	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71
24	S	606	CHL	C2C-C3C-C4C	-8.18	100.66	106.49
24	R	607	CHL	C2C-C3C-C4C	-8.17	100.67	106.49
24	s	606	CHL	C2C-C3C-C4C	-8.17	100.67	106.49
24	Y	609	CHL	C1D-ND-C4D	-8.16	100.53	106.33
24	r	608	CHL	CMD-C2D-C1D	8.16	139.10	124.71
24	G	608	CHL	C2B-C1B-NB	8.15	115.70	110.23
24	N	608	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	9	609	CHL	C2C-C3C-C4C	-8.15	100.68	106.49
24	R	608	CHL	CMD-C2D-C1D	8.15	139.07	124.71
24	N	606	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	4	606	CHL	C2B-C1B-NB	8.15	115.69	110.23
24	g	606	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	0	606	CHL	C2B-C1B-NB	8.14	115.69	110.23
24	G	606	CHL	C1D-ND-C4D	-8.14	100.55	106.33
24	r	607	CHL	C2C-C3C-C4C	-8.14	100.69	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	605	CHL	C2B-C1B-NB	8.12	115.68	110.23
24	6	605	CHL	CMD-C2D-C1D	8.11	139.01	124.71
24	2	609	CHL	C2C-C3C-C4C	-8.11	100.71	106.49
24	S	606	CHL	CMD-C2D-C1D	8.11	139.00	124.71
24	0	609	CHL	C2C-C3C-C4C	-8.10	100.71	106.49
24	3	601	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	y	609	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	1	608	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	G	601	CHL	C1D-ND-C4D	-8.09	100.58	106.33
24	5	606	CHL	CMD-C2D-C1D	8.09	138.97	124.71
24	s	606	CHL	CMD-C2D-C1D	8.08	138.96	124.71
24	S	608	CHL	C2C-C3C-C4C	-8.07	100.73	106.49
24	3	609	CHL	C1D-ND-C4D	-8.07	100.60	106.33
24	2	607	CHL	CMD-C2D-C1D	8.07	138.94	124.71
24	y	608	CHL	C2C-C3C-C4C	-8.06	100.74	106.49
24	2	606	CHL	CMD-C2D-C1D	8.05	138.91	124.71
24	G	607	CHL	CMD-C2D-C1D	8.04	138.89	124.71
24	s	608	CHL	C2C-C3C-C4C	-8.03	100.76	106.49
24	9	605	CHL	C2B-C1B-NB	8.03	115.62	110.23
24	4	605	CHL	C2B-C1B-NB	8.03	115.61	110.23
24	n	608	CHL	C2C-C3C-C4C	-8.03	100.77	106.49
24	n	608	CHL	C1D-ND-C4D	-8.01	100.64	106.33
24	R	607	CHL	CMD-C2D-C1D	8.01	138.83	124.71
24	r	608	CHL	C2B-C1B-NB	8.01	115.60	110.23
24	r	607	CHL	CMD-C2D-C1D	8.01	138.83	124.71
24	5	607	CHL	C1D-ND-C4D	-8.01	100.65	106.33
24	6	608	CHL	C2C-C3C-C4C	-8.00	100.78	106.49
24	S	606	CHL	C1D-ND-C4D	-8.00	100.66	106.33
24	4	608	CHL	C2C-C3C-C4C	-7.99	100.79	106.49
24	y	601	CHL	C1D-ND-C4D	-7.99	100.66	106.33
24	R	608	CHL	C2B-C1B-NB	7.99	115.59	110.23
24	Y	605	CHL	CMD-C2D-C1D	7.98	138.78	124.71
24	y	605	CHL	CMD-C2D-C1D	7.98	138.78	124.71
24	7	608	CHL	C1D-ND-C4D	-7.98	100.67	106.33
24	4	606	CHL	CMD-C2D-C1D	7.98	138.77	124.71
24	Y	608	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
24	5	605	CHL	C2B-C1B-NB	7.97	115.57	110.23
24	q	606	CHL	CMD-C2D-C1D	7.96	138.74	124.71
24	R	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	r	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	9	608	CHL	C1D-ND-C4D	-7.94	100.69	106.33
24	6	607	CHL	C2C-C3C-C4C	-7.94	100.83	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	606	CHL	C1D-ND-C4D	-7.94	100.70	106.33
24	2	608	CHL	C1D-ND-C4D	-7.93	100.70	106.33
24	s	606	CHL	C1D-ND-C4D	-7.93	100.70	106.33
24	N	608	CHL	C2C-C3C-C4C	-7.93	100.84	106.49
24	q	605	CHL	CHD-C1D-ND	-7.93	117.17	124.45
24	R	606	CHL	C2C-C3C-C4C	-7.93	100.84	106.49
24	p	605	CHL	C2B-C1B-NB	7.92	115.54	110.23
24	r	606	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
24	5	601	CHL	C1D-ND-C4D	-7.91	100.71	106.33
24	Y	601	CHL	C1D-ND-C4D	-7.89	100.73	106.33
24	q	606	CHL	C2B-C1B-NB	7.89	115.52	110.23
24	6	607	CHL	CMD-C2D-C1D	7.89	138.61	124.71
24	q	608	CHL	CMD-C2D-C1D	7.88	138.60	124.71
24	Y	607	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
27	0	1622	XAT	O4-C5-C4	7.87	119.29	113.38
24	S	607	CHL	CMD-C2D-C1D	7.86	138.57	124.71
24	2	606	CHL	C2B-C1B-NB	7.84	115.49	110.23
24	6	601	CHL	CMD-C2D-C1D	7.84	138.53	124.71
24	0	607	CHL	CMD-C2D-C1D	7.84	138.53	124.71
24	q	601	CHL	C1D-ND-C4D	-7.84	100.77	106.33
24	y	607	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
24	p	609	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
24	s	607	CHL	CMD-C2D-C1D	7.83	138.51	124.71
27	1	1622	XAT	C36-C21-C22	7.82	122.57	108.98
24	7	607	CHL	CMD-C2D-C1D	7.81	138.49	124.71
24	4	601	CHL	CMD-C2D-C1D	7.81	138.48	124.71
28	y	1623	NEX	O24-C25-C24	7.81	119.25	113.38
24	1	605	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
24	g	607	CHL	C2C-C3C-C4C	-7.79	100.94	106.49
24	8	606	CHL	C2B-C1B-NB	7.79	115.45	110.23
28	Y	1623	NEX	O24-C25-C24	7.79	119.23	113.38
24	9	606	CHL	CMD-C2D-C1D	7.78	138.43	124.71
24	G	607	CHL	C1D-ND-C4D	-7.77	100.81	106.33
24	8	605	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
24	4	605	CHL	CHD-C1D-ND	-7.77	117.31	124.45
24	G	607	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
24	6	609	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
24	0	601	CHL	C1D-ND-C4D	-7.76	100.82	106.33
24	7	605	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
24	1	607	CHL	CMD-C2D-C1D	7.74	138.35	124.71
24	7	609	CHL	C1D-ND-C4D	-7.74	100.84	106.33
24	3	605	CHL	C2C-C3C-C4C	-7.73	100.98	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	607	CHL	CMD-C2D-C1D	7.73	138.34	124.71
27	6	1622	XAT	O4-C5-C4	7.73	119.19	113.38
27	7	1622	XAT	C36-C21-C22	7.72	122.40	108.98
27	6	1622	XAT	C36-C21-C22	7.72	122.39	108.98
24	p	607	CHL	C1D-ND-C4D	-7.72	100.85	106.33
24	8	607	CHL	C2D-C1D-ND	7.71	115.79	110.10
24	p	607	CHL	CMD-C2D-C1D	7.71	138.31	124.71
24	7	607	CHL	C1D-ND-C4D	-7.71	100.86	106.33
24	y	608	CHL	C2D-C1D-ND	7.70	115.78	110.10
24	9	609	CHL	CHD-C1D-ND	-7.70	117.38	124.45
24	0	607	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
35	a	412	SQD	O8-S-C6	7.69	118.00	105.74
27	0	1622	XAT	C36-C21-C22	7.69	122.35	108.98
24	0	606	CHL	C1D-ND-C4D	-7.69	100.87	106.33
35	A	412	SQD	O8-S-C6	7.69	118.00	105.74
24	g	607	CHL	C1D-ND-C4D	-7.69	100.88	106.33
24	3	606	CHL	C2B-C1B-NB	7.68	115.38	110.23
24	5	606	CHL	C2B-C1B-NB	7.68	115.38	110.23
24	7	609	CHL	C2C-C3C-C4C	-7.68	101.02	106.49
24	8	608	CHL	C1D-ND-C4D	-7.68	100.88	106.33
24	Y	608	CHL	C2D-C1D-ND	7.67	115.75	110.10
24	g	608	CHL	C1D-ND-C4D	-7.66	100.89	106.33
24	N	609	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
24	1	601	CHL	CHD-C1D-ND	-7.65	117.43	124.45
24	1	609	CHL	C1D-ND-C4D	-7.64	100.91	106.33
24	3	607	CHL	C2D-C1D-ND	7.64	115.73	110.10
24	3	608	CHL	C1D-ND-C4D	-7.63	100.91	106.33
24	1	609	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
24	g	605	CHL	C1D-ND-C4D	-7.62	100.92	106.33
24	2	609	CHL	C1D-ND-C4D	-7.61	100.93	106.33
24	5	609	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
24	R	606	CHL	C1D-ND-C4D	-7.60	100.93	106.33
24	r	606	CHL	C1D-ND-C4D	-7.60	100.93	106.33
24	7	601	CHL	CHD-C1D-ND	-7.60	117.47	124.45
24	R	608	CHL	C1D-ND-C4D	-7.60	100.94	106.33
24	q	608	CHL	C2B-C1B-NB	7.60	115.32	110.23
24	2	606	CHL	C2C-C3C-C4C	-7.60	101.08	106.49
24	3	607	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
24	n	606	CHL	C2C-C3C-C4C	-7.58	101.09	106.49
33	a	408	PHO	C4D-CHA-CBD	-7.57	105.09	108.52
24	5	605	CHL	C2C-C3C-C4C	-7.57	101.09	106.49
24	0	605	CHL	C2C-C3C-C4C	-7.56	101.10	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	601	CHL	C1D-ND-C4D	-7.56	100.97	106.33
24	1	606	CHL	C1D-ND-C4D	-7.55	100.97	106.33
24	4	601	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
24	4	601	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	s	608	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	S	608	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	9	606	CHL	C2B-C1B-NB	7.53	115.28	110.23
24	s	607	CHL	C2B-C1B-NB	7.53	115.28	110.23
24	1	607	CHL	C1D-ND-C4D	-7.53	100.99	106.33
24	1	608	CHL	C2D-C1D-ND	7.53	115.65	110.10
33	A	408	PHO	C4D-CHA-CBD	-7.52	105.11	108.52
24	2	609	CHL	CHD-C1D-ND	-7.52	117.54	124.45
24	3	608	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
24	8	608	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	q	607	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	p	608	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	Y	606	CHL	C1D-ND-C4D	-7.50	101.00	106.33
24	G	609	CHL	C2B-C1B-NB	7.50	115.26	110.23
24	G	605	CHL	C1D-ND-C4D	-7.50	101.01	106.33
24	R	607	CHL	C1D-ND-C4D	-7.50	101.01	106.33
24	0	608	CHL	C1D-ND-C4D	-7.49	101.01	106.33
24	s	607	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
24	5	609	CHL	CHD-C1D-ND	-7.49	117.57	124.45
24	s	601	CHL	C1D-ND-C4D	-7.49	101.01	106.33
24	r	607	CHL	C1D-ND-C4D	-7.49	101.02	106.33
24	1	606	CHL	C2C-C3C-C4C	-7.48	101.15	106.49
24	y	606	CHL	C1D-ND-C4D	-7.48	101.02	106.33
24	9	606	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	r	608	CHL	C1D-ND-C4D	-7.48	101.02	106.33
24	4	607	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	S	607	CHL	C2B-C1B-NB	7.47	115.24	110.23
24	p	606	CHL	C2B-C1B-NB	7.47	115.24	110.23
24	Y	605	CHL	C2C-C3C-C4C	-7.47	101.17	106.49
24	8	605	CHL	C2B-C1B-NB	7.47	115.24	110.23
24	g	606	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
24	S	607	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
24	G	606	CHL	C2C-C3C-C4C	-7.45	101.18	106.49
24	8	607	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
24	y	605	CHL	C2C-C3C-C4C	-7.42	101.20	106.49
24	4	608	CHL	CHD-C1D-ND	-7.41	117.64	124.45
24	7	606	CHL	C2C-C3C-C4C	-7.41	101.20	106.49
24	5	608	CHL	C2C-C3C-C4C	-7.41	101.21	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	509	CLA	C4A-NA-C1A	7.40	110.03	106.71
24	0	601	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
24	6	607	CHL	C1D-ND-C4D	-7.39	101.08	106.33
25	C	509	CLA	C4A-NA-C1A	7.39	110.03	106.71
24	7	608	CHL	C2D-C1D-ND	7.38	115.55	110.10
24	3	605	CHL	C2B-C1B-NB	7.38	115.18	110.23
24	7	607	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
24	0	609	CHL	CHD-C1D-ND	-7.37	117.68	124.45
24	N	607	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
24	p	605	CHL	C1D-ND-C4D	-7.36	101.11	106.33
24	6	605	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
24	6	608	CHL	C1D-ND-C4D	-7.36	101.11	106.33
24	N	606	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
24	G	605	CHL	C2C-C3C-C4C	-7.34	101.25	106.49
24	G	608	CHL	C1D-ND-C4D	-7.34	101.12	106.33
24	p	609	CHL	CHD-C1D-ND	-7.34	117.71	124.45
24	q	605	CHL	C1D-ND-C4D	-7.33	101.12	106.33
24	g	609	CHL	CHD-C1D-ND	-7.32	117.72	124.45
24	8	606	CHL	CHD-C1D-ND	-7.31	117.73	124.45
24	4	608	CHL	C1D-ND-C4D	-7.31	101.14	106.33
24	0	608	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
24	g	609	CHL	C2B-C1B-NB	7.30	115.13	110.23
24	p	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
24	G	609	CHL	CHD-C1D-ND	-7.29	117.76	124.45
24	3	606	CHL	CHD-C1D-ND	-7.28	117.76	124.45
27	Y	1622	XAT	O24-C25-C24	7.28	118.85	113.38
24	n	605	CHL	C1D-ND-C4D	-7.27	101.17	106.33
24	g	605	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
24	4	609	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
24	5	606	CHL	C1D-ND-C4D	-7.25	101.18	106.33
24	5	606	CHL	C2C-C3C-C4C	-7.23	101.33	106.49
24	p	607	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
25	B	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	b	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	5	601	CHL	CHD-C1D-ND	-7.22	117.82	124.45
25	5	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	9	608	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
27	y	1622	XAT	O24-C25-C24	7.21	118.80	113.38
24	n	607	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
24	0	601	CHL	CMD-C2D-C1D	7.20	137.40	124.71
24	q	601	CHL	C2C-C3C-C4C	-7.19	101.37	106.49
24	5	608	CHL	C2D-C1D-ND	7.18	115.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	606	CHL	C1D-ND-C4D	-7.18	101.23	106.33
24	q	605	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
24	N	609	CHL	C1D-ND-C4D	-7.15	101.25	106.33
24	2	608	CHL	C2C-C3C-C4C	-7.14	101.40	106.49
24	N	605	CHL	C1D-ND-C4D	-7.14	101.26	106.33
24	y	605	CHL	C1D-ND-C4D	-7.14	101.26	106.33
24	0	607	CHL	C2D-C1D-ND	7.13	115.36	110.10
24	n	609	CHL	CHD-C1D-ND	-7.13	117.91	124.45
24	6	601	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
24	p	608	CHL	C2D-C1D-ND	7.12	115.35	110.10
24	y	609	CHL	C2D-C1D-ND	7.12	115.35	110.10
24	1	607	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
24	Y	607	CHL	C2D-C1D-ND	7.11	115.34	110.10
24	g	608	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
24	n	609	CHL	C1D-ND-C4D	-7.10	101.29	106.33
24	8	609	CHL	C2D-C1D-ND	7.10	115.33	110.10
24	y	601	CHL	CHD-C1D-ND	-7.09	117.94	124.45
24	G	608	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
24	p	609	CHL	C1D-ND-C4D	-7.08	101.31	106.33
24	S	601	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
24	Y	605	CHL	C1D-ND-C4D	-7.07	101.31	106.33
24	2	607	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
24	0	605	CHL	C1D-ND-C4D	-7.05	101.32	106.33
24	2	605	CHL	C1D-ND-C4D	-7.05	101.33	106.33
24	Y	609	CHL	C2D-C1D-ND	7.04	115.29	110.10
24	y	607	CHL	C2D-C1D-ND	7.04	115.29	110.10
24	6	606	CHL	C2C-C3C-C4C	-7.04	101.47	106.49
24	2	606	CHL	C1D-ND-C4D	-7.02	101.35	106.33
24	4	606	CHL	C2C-C3C-C4C	-7.02	101.49	106.49
24	s	601	CHL	CHD-C1D-ND	-7.00	118.02	124.45
27	r	622	XAT	O4-C5-C4	7.00	118.64	113.38
24	9	601	CHL	CHD-C1D-ND	-7.00	118.03	124.45
24	n	608	CHL	C2D-C1D-ND	6.99	115.26	110.10
24	9	606	CHL	C1D-ND-C4D	-6.99	101.37	106.33
25	C	506	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	9	605	CHL	C1D-ND-C4D	-6.99	101.37	106.33
24	9	607	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
24	5	607	CHL	C2C-C3C-C4C	-6.98	101.52	106.49
24	9	609	CHL	C1D-ND-C4D	-6.97	101.38	106.33
24	3	609	CHL	C2D-C1D-ND	6.97	115.24	110.10
25	c	506	CLA	C4A-NA-C1A	6.97	109.84	106.71
24	S	601	CHL	CHD-C1D-ND	-6.97	118.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	601	CHL	C2C-C3C-C4C	-6.97	101.52	106.49
27	q	1622	XAT	O24-C25-C24	6.96	118.61	113.38
24	n	607	CHL	C2D-C1D-ND	6.95	115.23	110.10
27	R	622	XAT	O4-C5-C4	6.95	118.61	113.38
24	Y	601	CHL	CHD-C1D-ND	-6.95	118.06	124.45
24	n	609	CHL	C2C-C3C-C4C	-6.95	101.54	106.49
24	4	605	CHL	C1D-ND-C4D	-6.94	101.40	106.33
24	9	607	CHL	C1D-ND-C4D	-6.94	101.40	106.33
24	s	601	CHL	C2C-C3C-C4C	-6.94	101.54	106.49
25	n	613	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	4	607	CHL	C1D-ND-C4D	-6.93	101.41	106.33
24	N	608	CHL	C2D-C1D-ND	6.92	115.21	110.10
24	4	605	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
24	3	609	CHL	CMD-C2D-C1D	6.92	136.90	124.71
24	6	601	CHL	C2D-C1D-ND	6.91	115.19	110.10
24	9	601	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
24	4	607	CHL	CHD-C1D-ND	-6.90	118.11	124.45
24	5	609	CHL	C1D-ND-C4D	-6.89	101.44	106.33
24	q	609	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
24	q	606	CHL	C2C-C3C-C4C	-6.88	101.58	106.49
24	2	605	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
24	N	607	CHL	C2D-C1D-ND	6.87	115.17	110.10
24	n	606	CHL	C2D-C1D-ND	6.86	115.16	110.10
24	9	607	CHL	CHD-C1D-ND	-6.85	118.16	124.45
24	0	606	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
24	9	605	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
24	6	609	CHL	C1D-ND-C4D	-6.84	101.48	106.33
24	5	607	CHL	C2D-C1D-ND	6.84	115.14	110.10
25	r	601	CLA	C4A-NA-C1A	6.83	109.78	106.71
24	2	607	CHL	CHD-C1D-ND	-6.83	118.17	124.45
24	q	607	CHL	CHD-C1D-ND	-6.83	118.18	124.45
24	7	609	CHL	C2D-C1D-ND	6.83	115.14	110.10
24	1	605	CHL	C1D-ND-C4D	-6.83	101.48	106.33
25	r	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	6	609	CHL	CHD-C1D-ND	-6.82	118.18	124.45
24	N	609	CHL	CHD-C1D-ND	-6.82	118.18	124.45
25	R	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	8	609	CHL	CMD-C2D-C1D	6.81	136.71	124.71
24	7	605	CHL	CHD-C1D-ND	-6.81	118.20	124.45
24	4	609	CHL	C2B-C1B-NB	6.81	114.80	110.23
24	q	606	CHL	CHD-C1D-ND	-6.80	118.20	124.45
24	2	607	CHL	C1D-ND-C4D	-6.80	101.51	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	608	CHL	CHD-C1D-ND	-6.78	118.23	124.45
24	p	601	CHL	C2D-C1D-ND	6.77	115.09	110.10
24	r	607	CHL	C2D-C1D-ND	6.76	115.08	110.10
25	8	613	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	N	613	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	1	605	CHL	CHD-C1D-ND	-6.75	118.25	124.45
24	p	601	CHL	CHD-C1D-ND	-6.75	118.25	124.45
24	7	605	CHL	C1D-ND-C4D	-6.74	101.55	106.33
28	7	1623	NEX	O24-C25-C24	6.74	118.44	113.38
24	N	606	CHL	C2D-C1D-ND	6.72	115.05	110.10
24	2	608	CHL	C2D-C1D-ND	6.72	115.05	110.10
24	9	608	CHL	C2D-C1D-ND	6.72	115.05	110.10
24	R	607	CHL	C2D-C1D-ND	6.70	115.04	110.10
24	4	606	CHL	C1D-ND-C4D	-6.69	101.58	106.33
24	Y	606	CHL	C2D-C1D-ND	6.69	115.03	110.10
25	R	601	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	3	606	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
24	n	607	CHL	CHD-C1D-ND	-6.68	118.32	124.45
24	G	607	CHL	C2D-C1D-ND	6.67	115.02	110.10
24	p	601	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
24	8	606	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
24	0	601	CHL	C2D-C1D-ND	6.66	115.01	110.10
24	s	607	CHL	C1D-ND-C4D	-6.65	101.61	106.33
24	8	601	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
24	p	606	CHL	CHD-C1D-ND	-6.64	118.35	124.45
24	8	606	CHL	C1D-ND-C4D	-6.63	101.62	106.33
24	y	606	CHL	C2D-C1D-ND	6.63	114.99	110.10
24	5	601	CHL	C2C-C3C-C4C	-6.63	101.76	106.49
25	r	602	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	y	1622	XAT	O4-C5-C4	6.62	118.35	113.38
24	G	601	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
24	Y	601	CHL	C2C-C3C-C4C	-6.61	101.77	106.49
24	S	607	CHL	C1D-ND-C4D	-6.61	101.64	106.33
27	p	1622	XAT	O4-C5-C4	6.61	118.34	113.38
24	s	608	CHL	C2D-C1D-ND	6.60	114.97	110.10
24	1	609	CHL	C2D-C1D-ND	6.60	114.97	110.10
25	R	602	CLA	C4A-NA-C1A	6.60	109.67	106.71
27	Y	1622	XAT	O4-C5-C4	6.59	118.33	113.38
24	3	601	CHL	CHD-C1D-ND	-6.58	118.40	124.45
24	2	601	CHL	CHD-C1D-ND	-6.57	118.42	124.45
24	0	609	CHL	C1D-ND-C4D	-6.57	101.67	106.33
24	n	601	CHL	CHD-C1D-ND	-6.56	118.43	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	605	CHL	C2D-C1D-ND	6.56	114.94	110.10
24	G	609	CHL	C1D-ND-C4D	-6.55	101.68	106.33
25	3	613	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	R	608	CHL	C2D-C1D-ND	6.55	114.93	110.10
24	N	607	CHL	CHD-C1D-ND	-6.55	118.44	124.45
24	S	608	CHL	C2D-C1D-ND	6.54	114.93	110.10
24	g	601	CHL	C2C-C3C-C4C	-6.54	101.83	106.49
24	s	608	CHL	CHD-C1D-ND	-6.53	118.45	124.45
24	S	608	CHL	CHD-C1D-ND	-6.53	118.45	124.45
24	r	608	CHL	C2D-C1D-ND	6.53	114.91	110.10
24	6	605	CHL	C1D-ND-C4D	-6.52	101.70	106.33
24	S	606	CHL	C2D-C1D-ND	6.52	114.91	110.10
24	9	606	CHL	CHD-C1D-ND	-6.52	118.46	124.45
27	g	1622	XAT	O24-C25-C24	6.51	118.28	113.38
24	g	606	CHL	C2D-C1D-ND	6.51	114.90	110.10
25	B	611	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	0	601	CHL	CHD-C1D-ND	-6.50	118.48	124.45
24	8	601	CHL	C2D-C1D-ND	6.50	114.89	110.10
24	g	609	CHL	C1D-ND-C4D	-6.49	101.72	106.33
24	q	609	CHL	C2B-C1B-NB	6.49	114.58	110.23
24	2	606	CHL	CHD-C1D-ND	-6.48	118.50	124.45
25	c	512	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	6	608	CHL	CHD-C1D-ND	-6.48	118.50	124.45
24	y	601	CHL	C2C-C3C-C4C	-6.48	101.87	106.49
24	3	606	CHL	C1D-ND-C4D	-6.48	101.73	106.33
24	G	606	CHL	C2D-C1D-ND	6.47	114.88	110.10
24	0	605	CHL	C2D-C1D-ND	6.46	114.87	110.10
25	C	512	CLA	C4A-NA-C1A	6.46	109.61	106.71
24	6	601	CHL	CHD-C1D-ND	-6.45	118.52	124.45
24	g	605	CHL	C2D-C1D-ND	6.45	114.86	110.10
24	g	608	CHL	C2D-C1D-ND	6.45	114.86	110.10
24	p	606	CHL	C2C-C3C-C4C	-6.44	101.90	106.49
24	g	607	CHL	CHD-C1D-ND	-6.44	118.54	124.45
27	G	1622	XAT	O24-C25-C24	6.43	118.21	113.38
27	3	1622	XAT	O4-C5-C4	6.42	118.21	113.38
24	s	606	CHL	C2D-C1D-ND	6.42	114.84	110.10
24	g	609	CHL	C2C-C3C-C4C	-6.42	101.91	106.49
24	4	606	CHL	CHD-C1D-ND	-6.42	118.55	124.45
24	N	601	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
24	G	609	CHL	C2C-C3C-C4C	-6.40	101.92	106.49
24	0	606	CHL	CHD-C1D-ND	-6.39	118.58	124.45
24	8	601	CHL	CHD-C1D-ND	-6.39	118.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	606	CHL	CHD-C1D-ND	-6.39	118.58	124.45
27	4	1622	XAT	O24-C25-C24	6.39	118.18	113.38
24	8	605	CHL	C1D-ND-C4D	-6.38	101.80	106.33
24	3	601	CHL	C2D-C1D-ND	6.38	114.80	110.10
25	b	611	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	2	601	CHL	C1D-ND-C4D	-6.37	101.81	106.33
24	n	601	CHL	C2D-C1D-ND	6.37	114.80	110.10
24	g	607	CHL	C2D-C1D-ND	6.35	114.78	110.10
24	p	606	CHL	C1D-ND-C4D	-6.35	101.82	106.33
27	8	1622	XAT	O4-C5-C4	6.35	118.15	113.38
24	q	606	CHL	C1D-ND-C4D	-6.35	101.82	106.33
24	8	608	CHL	C2D-C1D-ND	6.34	114.78	110.10
24	5	601	CHL	C2D-C1D-ND	6.32	114.76	110.10
24	6	607	CHL	C2D-C1D-ND	6.31	114.76	110.10
24	q	608	CHL	CHB-C1B-NB	-6.31	117.58	124.26
24	G	605	CHL	C2D-C1D-ND	6.31	114.75	110.10
24	1	606	CHL	CHD-C1D-ND	-6.31	118.66	124.45
24	3	608	CHL	C2D-C1D-ND	6.30	114.75	110.10
24	q	608	CHL	C1D-ND-C4D	-6.29	101.87	106.33
24	6	608	CHL	C2D-C1D-ND	6.29	114.74	110.10
24	N	601	CHL	CHD-C1D-ND	-6.29	118.68	124.45
25	1	613	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	N	605	CHL	C2C-C3C-C4C	-6.28	102.01	106.49
27	N	1622	XAT	O4-C5-C4	6.28	118.10	113.38
24	G	607	CHL	CHD-C1D-ND	-6.28	118.69	124.45
24	3	605	CHL	C1D-ND-C4D	-6.28	101.88	106.33
24	p	607	CHL	C2D-C1D-ND	6.27	114.72	110.10
24	7	607	CHL	C2D-C1D-ND	6.26	114.72	110.10
24	q	601	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	y	605	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	0	608	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	q	601	CHL	CHD-C1D-ND	-6.25	118.71	124.45
25	7	613	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	n	605	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
24	4	601	CHL	C2D-C1D-ND	6.23	114.69	110.10
24	y	608	CHL	CHD-C1D-ND	-6.23	118.73	124.45
24	Y	608	CHL	CHD-C1D-ND	-6.22	118.73	124.45
24	Y	605	CHL	C2D-C1D-ND	6.22	114.69	110.10
24	5	608	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	6	607	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	2	608	CHL	CHD-C1D-ND	-6.19	118.77	124.45
27	7	1622	XAT	O24-C25-C38	6.16	122.44	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	603	CLA	C4A-NA-C1A	6.15	109.47	106.71
27	6	1622	XAT	C38-C25-C26	-6.15	111.95	122.26
24	p	607	CHL	CHD-C1D-ND	-6.15	118.80	124.45
24	R	606	CHL	C2D-C1D-ND	6.15	114.64	110.10
24	3	601	CHL	C2C-C3C-C4C	-6.15	102.11	106.49
24	q	607	CHL	C1D-ND-C4D	-6.15	101.97	106.33
24	r	606	CHL	C2D-C1D-ND	6.14	114.63	110.10
24	6	606	CHL	CHD-C1D-ND	-6.14	118.81	124.45
24	6	609	CHL	C2D-C1D-ND	6.13	114.62	110.10
27	n	1622	XAT	O4-C5-C4	6.12	117.98	113.38
24	q	609	CHL	C1D-ND-C4D	-6.12	101.99	106.33
25	2	603	CLA	C4A-NA-C1A	6.11	109.45	106.71
24	9	608	CHL	CHD-C1D-ND	-6.11	118.84	124.45
25	1	611	CLA	C4A-NA-C1A	6.10	109.45	106.71
24	g	605	CHL	CHD-C1D-ND	-6.08	118.87	124.45
25	R	610	CLA	C4A-NA-C1A	6.07	109.44	106.71
25	0	614	CLA	C4A-NA-C1A	6.07	109.43	106.71
25	r	612	CLA	C4A-NA-C1A	6.06	109.43	106.71
24	9	605	CHL	C2D-C1D-ND	6.06	114.57	110.10
24	N	601	CHL	C2D-C1D-ND	6.05	114.56	110.10
24	G	605	CHL	CHD-C1D-ND	-6.04	118.90	124.45
24	4	608	CHL	C2D-C1D-ND	6.04	114.56	110.10
24	G	608	CHL	C2D-C1D-ND	6.03	114.55	110.10
25	p	613	CLA	C4A-NA-C1A	6.03	109.42	106.71
24	s	607	CHL	CHD-C1D-ND	-6.03	118.92	124.45
24	9	601	CHL	C3B-C2B-C1B	-6.03	99.89	107.16
24	S	607	CHL	CHD-C1D-ND	-6.03	118.92	124.45
34	D	404	BCR	C7-C8-C9	-6.02	117.13	126.23
24	2	609	CHL	C2D-C1D-ND	6.02	114.54	110.10
34	d	404	BCR	C7-C8-C9	-6.02	117.14	126.23
24	1	607	CHL	C2D-C1D-ND	6.01	114.54	110.10
24	y	601	CHL	C2D-C1D-ND	6.01	114.53	110.10
24	p	608	CHL	CHD-C1D-ND	-6.01	118.93	124.45
24	4	601	CHL	CHD-C1D-ND	-6.01	118.93	124.45
24	y	607	CHL	C3B-C2B-C1B	-6.01	99.91	107.16
24	y	608	CHL	C3C-C4C-NC	6.01	117.31	110.57
25	r	610	CLA	C4A-NA-C1A	6.01	109.41	106.71
24	3	609	CHL	C3C-C4C-NC	6.00	117.31	110.57
24	2	605	CHL	C2D-C1D-ND	6.00	114.53	110.10
25	G	603	CLA	C4A-NA-C1A	6.00	109.40	106.71
25	N	603	CLA	C4A-NA-C1A	6.00	109.40	106.71
25	g	603	CLA	C4A-NA-C1A	6.00	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	607	CHL	CHD-C1D-ND	-6.00	118.94	124.45
24	y	606	CHL	CHD-C1D-ND	-5.99	118.95	124.45
24	Y	606	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	7	609	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	1	609	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	p	605	CHL	O2D-CGD-CBD	5.97	121.88	111.27
24	g	601	CHL	CHD-C1D-ND	-5.97	118.96	124.45
25	G	611	CLA	C4A-NA-C1A	5.97	109.39	106.71
24	9	605	CHL	CHD-C1D-ND	-5.97	118.97	124.45
24	Y	601	CHL	C2D-C1D-ND	5.97	114.50	110.10
25	7	611	CLA	C4A-NA-C1A	5.96	109.39	106.71
27	q	1622	XAT	C18-C5-C6	-5.96	112.27	122.26
24	R	606	CHL	CHD-C1D-ND	-5.96	118.98	124.45
24	Y	607	CHL	C3B-C2B-C1B	-5.96	99.97	107.16
25	R	612	CLA	C4A-NA-C1A	5.95	109.38	106.71
24	y	606	CHL	C3C-C4C-NC	5.95	117.25	110.57
24	R	606	CHL	CAC-C3C-C4C	5.95	132.53	124.81
25	C	511	CLA	C4A-NA-C1A	5.94	109.38	106.71
25	n	603	CLA	C4A-NA-C1A	5.94	109.38	106.71
24	3	607	CHL	CHD-C1D-ND	-5.94	119.00	124.45
24	Y	608	CHL	C3C-C4C-NC	5.93	117.22	110.57
24	r	606	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	2	605	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	Y	607	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	g	601	CHL	C2D-C1D-ND	5.91	114.46	110.10
24	S	606	CHL	CHD-C1D-ND	-5.91	119.03	124.45
24	Y	606	CHL	C3C-C4C-NC	5.91	117.19	110.57
24	r	607	CHL	C3B-C2B-C1B	-5.91	100.03	107.16
24	5	605	CHL	O2D-CGD-CBD	5.90	121.76	111.27
24	g	606	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	Y	609	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	y	607	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	R	607	CHL	C3B-C2B-C1B	-5.89	100.05	107.16
24	5	607	CHL	CHD-C1D-ND	-5.89	119.04	124.45
24	n	606	CHL	CHD-C1D-ND	-5.89	119.04	124.45
24	q	605	CHL	C2D-C1D-ND	5.89	114.44	110.10
27	1	1622	XAT	O24-C25-C38	5.89	122.11	115.06
24	r	606	CHL	CAC-C3C-C4C	5.89	132.45	124.81
24	N	606	CHL	CHD-C1D-ND	-5.89	119.05	124.45
24	n	601	CHL	C2C-C3C-C4C	-5.88	102.30	106.49
24	7	601	CHL	C2D-C1D-ND	5.88	114.44	110.10
24	G	601	CHL	CHD-C1D-ND	-5.88	119.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	611	CLA	C4A-NA-C1A	5.88	109.35	106.71
24	6	606	CHL	C2D-C1D-ND	5.88	114.44	110.10
27	5	1622	XAT	O4-C5-C4	5.87	117.80	113.38
24	N	609	CHL	C3B-C2B-C1B	-5.87	100.07	107.16
24	1	606	CHL	C2D-C1D-ND	5.87	114.43	110.10
24	6	605	CHL	C2D-C1D-ND	5.87	114.43	110.10
27	q	1622	XAT	O4-C5-C18	5.87	122.09	115.06
24	n	601	CHL	C3B-C2B-C1B	-5.87	100.07	107.16
25	c	511	CLA	C4A-NA-C1A	5.87	109.35	106.71
27	r	622	XAT	O24-C25-C24	5.87	117.79	113.38
24	s	606	CHL	CHD-C1D-ND	-5.87	119.06	124.45
24	0	609	CHL	CHB-C1B-NB	-5.86	118.06	124.26
24	7	608	CHL	C3C-C4C-NC	5.86	117.14	110.57
24	n	609	CHL	C3B-C2B-C1B	-5.86	100.09	107.16
24	Y	605	CHL	CHD-C1D-ND	-5.85	119.08	124.45
24	5	606	CHL	CHD-C1D-ND	-5.85	119.08	124.45
24	8	609	CHL	C3C-C4C-NC	5.85	117.13	110.57
24	q	608	CHL	C2D-C1D-ND	5.84	114.41	110.10
27	9	1622	XAT	C38-C25-C26	-5.84	112.47	122.26
27	0	1622	XAT	C38-C25-C26	-5.84	112.48	122.26
27	R	622	XAT	O24-C25-C24	5.83	117.77	113.38
24	y	605	CHL	CHD-C1D-ND	-5.83	119.09	124.45
25	q	613	CLA	C4A-NA-C1A	5.83	109.33	106.71
34	H	101	BCR	C7-C8-C9	-5.83	117.43	126.23
25	2	612	CLA	C4A-NA-C1A	5.83	109.33	106.71
24	1	601	CHL	C2D-C1D-ND	5.82	114.39	110.10
24	y	601	CHL	O2D-CGD-CBD	5.82	121.61	111.27
24	8	605	CHL	CHB-C1B-NB	-5.81	118.10	124.26
34	h	101	BCR	C7-C8-C9	-5.81	117.45	126.23
24	G	608	CHL	CHD-C1D-ND	-5.81	119.11	124.45
24	G	606	CHL	CHD-C1D-ND	-5.80	119.12	124.45
24	0	607	CHL	CHD-C1D-ND	-5.80	119.13	124.45
24	Y	605	CHL	C3B-C2B-C1B	-5.79	100.17	107.16
24	R	608	CHL	CHD-C1D-ND	-5.79	119.13	124.45
24	1	608	CHL	C3C-C4C-NC	5.79	117.06	110.57
24	9	607	CHL	C2D-C1D-ND	5.79	114.37	110.10
24	N	609	CHL	C2D-C1D-ND	5.78	114.37	110.10
24	N	605	CHL	C2D-C1D-ND	5.78	114.36	110.10
24	q	607	CHL	CHB-C1B-NB	-5.78	118.14	124.26
24	8	608	CHL	CHD-C1D-ND	-5.77	119.15	124.45
24	9	601	CHL	C1D-ND-C4D	-5.77	102.23	106.33
24	y	605	CHL	C3B-C2B-C1B	-5.76	100.20	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	q	611	CLA	C4A-NA-C1A	5.76	109.30	106.71
24	n	605	CHL	C2D-C1D-ND	5.76	114.35	110.10
24	g	608	CHL	CHD-C1D-ND	-5.76	119.16	124.45
25	Y	611	CLA	C4A-NA-C1A	5.75	109.29	106.71
24	N	601	CHL	C3B-C2B-C1B	-5.75	100.22	107.16
24	N	605	CHL	CHD-C1D-ND	-5.74	119.17	124.45
27	7	1622	XAT	C38-C25-C26	-5.74	112.63	122.26
24	2	607	CHL	C2D-C1D-ND	5.74	114.34	110.10
24	Y	608	CHL	C3D-C2D-C1D	-5.74	98.00	105.83
24	4	605	CHL	CHB-C1B-NB	-5.74	118.18	124.26
24	y	606	CHL	C3B-C2B-C1B	-5.74	100.24	107.16
24	3	605	CHL	CHB-C1B-NB	-5.73	118.19	124.26
24	3	607	CHL	C3C-C4C-NC	5.73	117.00	110.57
25	8	603	CLA	C4A-NA-C1A	5.73	109.28	106.71
27	1	1622	XAT	C38-C25-C26	-5.73	112.66	122.26
24	7	601	CHL	C2C-C3C-C4C	-5.73	102.41	106.49
24	y	608	CHL	C3D-C2D-C1D	-5.72	98.02	105.83
24	0	609	CHL	C2D-C1D-ND	5.72	114.32	110.10
24	Y	606	CHL	C3B-C2B-C1B	-5.72	100.26	107.16
24	3	608	CHL	CHD-C1D-ND	-5.72	119.20	124.45
27	4	1622	XAT	C18-C5-C6	-5.72	112.68	122.26
24	6	605	CHL	CHD-C1D-ND	-5.72	119.20	124.45
24	S	601	CHL	C2D-C1D-ND	5.71	114.31	110.10
24	1	605	CHL	C2D-C1D-ND	5.71	114.31	110.10
24	r	608	CHL	CHD-C1D-ND	-5.71	119.21	124.45
27	5	1622	XAT	C18-C5-C6	-5.71	112.69	122.26
27	2	1622	XAT	C38-C25-C26	-5.71	112.69	122.26
24	8	605	CHL	C2D-C1D-ND	5.70	114.31	110.10
24	y	609	CHL	C3D-C2D-C1D	-5.70	98.05	105.83
24	0	605	CHL	CHD-C1D-ND	-5.70	119.21	124.45
24	N	607	CHL	C3C-C4C-NC	5.70	116.97	110.57
24	1	601	CHL	C2C-C3C-C4C	-5.70	102.43	106.49
27	6	1622	XAT	O24-C25-C38	5.70	121.89	115.06
24	9	606	CHL	C2D-C1D-ND	5.70	114.30	110.10
24	N	608	CHL	CHD-C1D-ND	-5.70	119.22	124.45
24	5	601	CHL	C3B-C2B-C1B	-5.69	100.29	107.16
24	n	605	CHL	CHD-C1D-ND	-5.69	119.22	124.45
27	y	1622	XAT	C38-C25-C26	-5.69	112.72	122.26
24	4	607	CHL	C2D-C1D-ND	5.69	114.30	110.10
24	y	609	CHL	CHD-C1D-ND	-5.69	119.23	124.45
25	y	611	CLA	C4A-NA-C1A	5.68	109.26	106.71
24	N	601	CHL	O2D-CGD-CBD	5.68	121.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	609	CHL	C2D-C1D-ND	5.68	114.29	110.10
27	Y	1622	XAT	C38-C25-C26	-5.68	112.75	122.26
27	4	1622	XAT	C38-C25-C26	-5.68	112.75	122.26
24	n	609	CHL	C2D-C1D-ND	5.68	114.29	110.10
24	R	608	CHL	O2D-CGD-CBD	5.67	121.35	111.27
24	2	601	CHL	C3B-C2B-C1B	-5.67	100.31	107.16
24	n	608	CHL	C3C-C4C-NC	5.67	116.93	110.57
24	p	601	CHL	C3B-C2B-C1B	-5.67	100.32	107.16
24	r	608	CHL	O2D-CGD-CBD	5.67	121.33	111.27
24	8	607	CHL	C3C-C4C-NC	5.66	116.92	110.57
25	2	613	CLA	C4A-NA-C1A	5.66	109.25	106.71
24	Y	609	CHL	C3D-C2D-C1D	-5.66	98.11	105.83
25	6	611	CLA	C4A-NA-C1A	5.66	109.25	106.71
24	n	606	CHL	C3C-C4C-NC	5.65	116.91	110.57
25	9	612	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	p	603	CLA	C4A-NA-C1A	5.65	109.25	106.71
24	7	606	CHL	C2D-C1D-ND	5.65	114.27	110.10
24	5	606	CHL	C2D-C1D-ND	5.64	114.26	110.10
24	y	609	CHL	C3C-C4C-NC	5.64	116.89	110.57
24	3	605	CHL	C2D-C1D-ND	5.64	114.26	110.10
24	n	601	CHL	O2D-CGD-CBD	5.63	121.27	111.27
24	R	606	CHL	C3B-C2B-C1B	-5.63	100.37	107.16
28	5	1623	NEX	C27-C28-C29	-5.63	116.80	125.53
24	4	605	CHL	C2D-C1D-ND	5.62	114.25	110.10
24	g	607	CHL	C3B-C2B-C1B	-5.62	100.37	107.16
25	6	613	CLA	C4A-NA-C1A	5.62	109.23	106.71
24	G	607	CHL	C3B-C2B-C1B	-5.62	100.38	107.16
24	4	606	CHL	C2D-C1D-ND	5.62	114.24	110.10
27	2	1622	XAT	O24-C25-C24	5.61	117.60	113.38
24	r	607	CHL	O2D-CGD-CBD	5.61	121.23	111.27
24	7	608	CHL	C3D-C2D-C1D	-5.60	98.18	105.83
24	4	609	CHL	CHB-C1B-NB	-5.60	118.33	124.26
25	4	603	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	6	614	CLA	C4A-NA-C1A	5.59	109.22	106.71
24	3	606	CHL	O2D-CGD-CBD	5.59	121.20	111.27
24	s	601	CHL	C2D-C1D-ND	5.59	114.22	110.10
24	2	606	CHL	C2D-C1D-ND	5.59	114.22	110.10
24	4	601	CHL	O2D-CGD-CBD	5.58	121.19	111.27
24	r	606	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
24	Y	607	CHL	C3C-C4C-NC	5.58	116.83	110.57
24	Y	601	CHL	O2D-CGD-CBD	5.58	121.17	111.27
24	R	607	CHL	O2D-CGD-CBD	5.57	121.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	608	CHL	C3C-C4C-NC	5.57	116.82	110.57
24	y	607	CHL	C3C-C4C-NC	5.57	116.82	110.57
24	1	608	CHL	C3D-C2D-C1D	-5.57	98.23	105.83
24	6	609	CHL	C3B-C2B-C1B	-5.56	100.45	107.16
25	C	504	CLA	C4A-NA-C1A	5.56	109.20	106.71
24	0	609	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
24	6	605	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
24	N	606	CHL	C3C-C4C-NC	5.55	116.79	110.57
24	6	607	CHL	C3B-C2B-C1B	-5.55	100.47	107.16
24	q	601	CHL	O2D-CGD-CBD	5.55	121.12	111.27
25	q	603	CLA	C4A-NA-C1A	5.54	109.20	106.71
24	Y	609	CHL	C3C-C4C-NC	5.54	116.78	110.57
24	8	601	CHL	C3B-C2B-C1B	-5.54	100.48	107.16
24	G	601	CHL	C2D-C1D-ND	5.54	114.18	110.10
24	0	605	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
24	3	601	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
38	D	401	BCT	O2-C-O1	5.52	133.87	119.55
24	R	608	CHL	C3C-C4C-NC	5.52	116.76	110.57
24	r	608	CHL	C3C-C4C-NC	5.52	116.76	110.57
25	5	603	CLA	C4A-NA-C1A	5.52	109.19	106.71
24	8	609	CHL	O2D-CGD-CBD	5.51	121.07	111.27
38	d	401	BCT	O2-C-O1	5.51	133.83	119.55
24	n	607	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
27	g	1622	XAT	O4-C5-C4	5.50	117.52	113.38
24	n	607	CHL	C3C-C4C-NC	5.50	116.74	110.57
24	9	609	CHL	C2D-C1D-ND	5.50	114.16	110.10
25	3	603	CLA	C4A-NA-C1A	5.49	109.18	106.71
25	c	504	CLA	C4A-NA-C1A	5.49	109.17	106.71
24	1	607	CHL	C3B-C2B-C1B	-5.49	100.53	107.16
25	4	611	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	0	611	CLA	C4A-NA-C1A	5.49	109.17	106.71
27	7	1622	XAT	C18-C5-C6	-5.48	113.07	122.26
24	N	607	CHL	C3B-C2B-C1B	-5.48	100.55	107.16
24	3	609	CHL	O2D-CGD-CBD	5.48	121.01	111.27
24	S	601	CHL	C3B-C2B-C1B	-5.48	100.55	107.16
24	7	607	CHL	C3B-C2B-C1B	-5.48	100.55	107.16
24	9	605	CHL	CHB-C1B-NB	-5.47	118.46	124.26
24	2	608	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
24	R	607	CHL	C3C-C4C-NC	5.47	116.70	110.57
24	5	609	CHL	C2D-C1D-ND	5.47	114.13	110.10
34	B	618	BCR	C28-C27-C26	-5.47	104.32	114.08
24	7	609	CHL	C3C-C4C-NC	5.47	116.70	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	607	CHL	C3C-C4C-NC	5.47	116.70	110.57
34	b	618	BCR	C28-C27-C26	-5.46	104.33	114.08
25	4	613	CLA	C4A-NA-C1A	5.46	109.16	106.71
27	1	1622	XAT	C18-C5-C6	-5.46	113.12	122.26
24	9	609	CHL	C3B-C2B-C1B	-5.46	100.58	107.16
27	4	1622	XAT	O4-C5-C18	5.45	121.59	115.06
24	3	609	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
24	8	606	CHL	O2D-CGD-CBD	5.45	120.96	111.27
24	s	608	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
24	q	606	CHL	C3B-C2B-C1B	-5.45	100.59	107.16
24	0	606	CHL	C2D-C1D-ND	5.45	114.12	110.10
24	7	609	CHL	C3D-C2D-C1D	-5.44	98.40	105.83
27	9	1622	XAT	O24-C25-C38	5.44	121.58	115.06
24	S	608	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
24	9	601	CHL	CHB-C1B-NB	-5.44	118.50	124.26
28	Y	1623	NEX	C38-C25-C26	-5.44	113.14	122.26
28	y	1623	NEX	C38-C25-C26	-5.44	113.15	122.26
24	p	605	CHL	C2D-C1D-ND	5.44	114.11	110.10
27	9	1622	XAT	O24-C25-C24	5.44	117.47	113.38
24	q	605	CHL	CHB-C1B-NB	-5.43	118.50	124.26
27	g	1622	XAT	C38-C25-C26	-5.43	113.16	122.26
24	y	601	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
27	G	1622	XAT	O4-C5-C4	5.43	117.46	113.38
24	s	606	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
25	s	613	CLA	C4A-NA-C1A	5.42	109.14	106.71
24	s	607	CHL	C2D-C1D-ND	5.42	114.10	110.10
24	s	608	CHL	C3D-C2D-C1D	-5.42	98.43	105.83
25	0	603	CLA	C4A-NA-C1A	5.42	109.14	106.71
24	n	608	CHL	C3D-C2D-C1D	-5.42	98.44	105.83
24	2	605	CHL	CHB-C1B-NB	-5.42	118.52	124.26
24	9	607	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	8	609	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
24	7	605	CHL	C2D-C1D-ND	5.41	114.09	110.10
25	R	613	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	b	617	CLA	C4A-NA-C1A	5.41	109.14	106.71
24	s	601	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	2	607	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
24	n	608	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
25	B	617	CLA	C4A-NA-C1A	5.40	109.13	106.71
25	9	613	CLA	C4A-NA-C1A	5.40	109.13	106.71
24	q	607	CHL	C3B-C2B-C1B	-5.40	100.65	107.16
24	N	605	CHL	O2D-CGD-CBD	5.39	120.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1622	XAT	O4-C5-C18	5.39	121.51	115.06
24	6	608	CHL	C3C-C4C-NC	5.39	116.61	110.57
24	1	605	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	S	606	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
24	S	606	CHL	O2D-CGD-CBD	5.39	120.84	111.27
27	q	1622	XAT	C38-C25-C26	-5.39	113.23	122.26
24	S	607	CHL	C2D-C1D-ND	5.38	114.07	110.10
24	2	609	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
24	8	606	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
25	b	616	CLA	C4A-NA-C1A	5.38	109.12	106.71
24	n	605	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
24	3	606	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
27	7	1622	XAT	O4-C5-C18	5.37	121.50	115.06
24	6	608	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
25	r	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	S	608	CHL	C3D-C2D-C1D	-5.37	98.50	105.83
24	N	605	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
25	S	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	N	608	CHL	C3D-C2D-C1D	-5.37	98.50	105.83
24	1	605	CHL	C3C-C4C-NC	5.37	116.59	110.57
27	0	1622	XAT	O24-C25-C24	5.37	117.42	113.38
27	G	1622	XAT	C38-C25-C26	-5.37	113.27	122.26
24	4	607	CHL	CHB-C1B-NB	-5.37	118.58	124.26
27	p	1622	XAT	C18-C5-C6	-5.36	113.27	122.26
27	4	1622	XAT	O4-C5-C4	5.36	117.41	113.38
24	9	608	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
27	2	1622	XAT	O24-C25-C38	5.36	121.48	115.06
24	s	606	CHL	O2D-CGD-CBD	5.36	120.79	111.27
27	5	1622	XAT	O4-C5-C18	5.35	121.47	115.06
24	4	606	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
24	7	601	CHL	O2D-CGD-CBD	5.35	120.78	111.27
25	R	616	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	r	622	XAT	C6-C7-C8	-5.35	114.69	125.99
25	N	604	CLA	C4A-NA-C1A	5.34	109.11	106.71
27	R	622	XAT	C6-C7-C8	-5.34	114.69	125.99
24	N	608	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
24	g	605	CHL	O2D-CGD-CBD	5.34	120.76	111.27
24	5	608	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	7	607	CHL	CHD-C1D-ND	-5.34	119.55	124.45
24	y	601	CHL	C4A-NA-C1A	-5.33	104.31	106.71
24	Y	606	CHL	C3D-C2D-C1D	-5.33	98.55	105.83
24	Y	601	CHL	C3B-C2B-C1B	-5.33	100.73	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	601	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
24	7	601	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
24	Y	607	CHL	C3D-C2D-C1D	-5.32	98.56	105.83
24	n	608	CHL	CHD-C1D-ND	-5.32	119.56	124.45
28	S	1623	NEX	C15-C14-C13	-5.32	119.71	127.31
24	7	605	CHL	C3C-C4C-NC	5.32	116.54	110.57
24	n	609	CHL	O2D-CGD-CBD	5.32	120.72	111.27
24	8	607	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	1	609	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	4	607	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
24	y	607	CHL	C3D-C2D-C1D	-5.32	98.58	105.83
28	7	1623	NEX	C38-C25-C26	-5.32	113.35	122.26
25	R	609	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	r	609	CLA	C4A-NA-C1A	5.32	109.10	106.71
24	6	608	CHL	C3D-C2D-C1D	-5.31	98.58	105.83
24	G	606	CHL	C3C-C4C-NC	5.31	116.53	110.57
28	N	1623	NEX	C38-C25-C26	-5.31	113.36	122.26
24	7	605	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
24	s	606	CHL	C3C-C4C-NC	5.30	116.52	110.57
24	3	607	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
24	y	606	CHL	C3D-C2D-C1D	-5.30	98.59	105.83
24	S	606	CHL	C3C-C4C-NC	5.30	116.52	110.57
24	p	608	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
24	5	609	CHL	O2D-CGD-CBD	5.29	120.67	111.27
24	q	601	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
25	r	616	CLA	C4A-NA-C1A	5.29	109.08	106.71
24	p	608	CHL	C3C-C4C-NC	5.29	116.50	110.57
24	3	601	CHL	O2D-CGD-CBD	5.29	120.66	111.27
24	7	601	CHL	C3D-C4D-ND	5.29	118.79	110.24
28	n	1623	NEX	C38-C25-C26	-5.28	113.40	122.26
24	2	601	CHL	C2D-C1D-ND	5.28	114.00	110.10
24	1	606	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
24	p	605	CHL	CHB-C1B-NB	-5.28	118.67	124.26
25	S	603	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	p	611	CLA	C4A-NA-C1A	5.28	109.08	106.71
24	1	601	CHL	O2D-CGD-CBD	5.28	120.64	111.27
24	G	607	CHL	C3C-C4C-NC	5.28	116.49	110.57
25	n	604	CLA	C4A-NA-C1A	5.27	109.08	106.71
24	g	606	CHL	C3C-C4C-NC	5.27	116.48	110.57
24	6	609	CHL	C3D-C2D-C1D	-5.27	98.64	105.83
24	2	605	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
24	p	607	CHL	C3B-C2B-C1B	-5.27	100.80	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	1622	XAT	C31-C30-C29	-5.27	119.79	127.31
25	6	603	CLA	C4A-NA-C1A	5.26	109.07	106.71
27	p	1622	XAT	C38-C25-C26	-5.26	113.44	122.26
24	1	601	CHL	C3D-C4D-ND	5.26	118.75	110.24
34	C	517	BCR	C20-C21-C22	-5.26	119.80	127.31
24	p	601	CHL	O2D-CGD-CBD	5.26	120.62	111.27
25	c	501	CLA	C4A-NA-C1A	5.26	109.07	106.71
24	g	601	CHL	O2D-CGD-CBD	5.26	120.61	111.27
24	2	608	CHL	O2D-CGD-CBD	5.26	120.61	111.27
24	5	608	CHL	C3C-C4C-NC	5.25	116.46	110.57
24	G	605	CHL	O2D-CGD-CBD	5.25	120.60	111.27
24	1	609	CHL	C3C-C4C-NC	5.25	116.46	110.57
24	3	607	CHL	C3D-C2D-C1D	-5.24	98.67	105.83
24	3	608	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
25	d	402	CLA	C4A-NA-C1A	5.24	109.06	106.71
24	9	608	CHL	C3D-C2D-C1D	-5.24	98.68	105.83
24	7	608	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
24	r	608	CHL	C3D-C2D-C1D	-5.24	98.69	105.83
24	2	609	CHL	C3C-C4C-NC	5.23	116.44	110.57
24	8	608	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
24	Y	601	CHL	C4A-NA-C1A	-5.23	104.35	106.71
24	5	607	CHL	C3C-C4C-NC	5.23	116.44	110.57
24	0	601	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
27	6	1622	XAT	C18-C5-C6	-5.23	113.50	122.26
24	q	605	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
24	2	608	CHL	C3D-C2D-C1D	-5.23	98.70	105.83
34	c	517	BCR	C20-C21-C22	-5.23	119.85	127.31
24	5	605	CHL	C3D-C4D-ND	5.23	118.69	110.24
24	4	605	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
24	9	608	CHL	C3C-C4C-NC	5.22	116.43	110.57
25	s	603	CLA	C4A-NA-C1A	5.22	109.05	106.71
24	2	608	CHL	C3C-C4C-NC	5.22	116.42	110.57
24	7	609	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
24	p	609	CHL	O2D-CGD-CBD	5.22	120.53	111.27
25	8	611	CLA	C4A-NA-C1A	5.21	109.05	106.71
24	2	607	CHL	CHB-C1B-NB	-5.21	118.74	124.26
24	q	606	CHL	C2D-C1D-ND	5.21	113.94	110.10
24	2	607	CHL	O2D-CGD-CBD	5.20	120.52	111.27
24	9	605	CHL	C3B-C2B-C1B	-5.20	100.88	107.16
24	R	608	CHL	C3D-C2D-C1D	-5.20	98.73	105.83
24	1	607	CHL	CHD-C1D-ND	-5.20	119.67	124.45
24	q	607	CHL	C2D-C1D-ND	5.20	113.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	607	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
24	6	606	CHL	O2D-CGD-CBD	5.20	120.50	111.27
24	p	605	CHL	C3D-C4D-ND	5.20	118.64	110.24
24	0	608	CHL	C3D-C2D-C1D	-5.20	98.74	105.83
24	1	609	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
27	G	1622	XAT	C18-C5-C6	-5.19	113.56	122.26
24	5	601	CHL	O2D-CGD-CBD	5.19	120.49	111.27
28	Y	1623	NEX	O24-C25-C38	5.19	121.27	115.06
24	9	609	CHL	C3C-C4C-NC	5.19	116.39	110.57
24	n	607	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
24	G	607	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
27	R	622	XAT	C38-C25-C26	-5.18	113.57	122.26
24	5	608	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
27	y	1622	XAT	C6-C7-C8	-5.18	115.04	125.99
24	G	605	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
25	c	508	CLA	C4A-NA-C1A	5.18	109.03	106.71
27	8	1622	XAT	C18-C5-C6	-5.18	113.58	122.26
25	s	611	CLA	C4A-NA-C1A	5.18	109.03	106.71
24	4	608	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
24	g	607	CHL	C3C-C4C-NC	5.17	116.37	110.57
24	p	608	CHL	C3D-C2D-C1D	-5.17	98.77	105.83
27	7	1622	XAT	C37-C21-C26	-5.17	96.08	110.05
24	Y	605	CHL	C3C-C4C-NC	5.17	116.37	110.57
24	n	609	CHL	CHB-C1B-NB	-5.17	118.78	124.26
24	q	601	CHL	C3D-C2D-C1D	-5.17	98.78	105.83
25	N	614	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	b	608	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	3	611	CLA	C4A-NA-C1A	5.16	109.03	106.71
25	S	602	CLA	C4A-NA-C1A	5.16	109.03	106.71
24	Y	605	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
24	y	605	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
24	S	608	CHL	C3C-C4C-NC	5.16	116.36	110.57
27	Y	1622	XAT	C6-C7-C8	-5.16	115.08	125.99
27	r	622	XAT	C38-C25-C26	-5.16	113.61	122.26
24	y	605	CHL	C3C-C4C-NC	5.16	116.36	110.57
24	0	607	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
27	N	1622	XAT	C6-C7-C8	-5.16	115.09	125.99
24	2	606	CHL	C3C-C4C-NC	5.16	116.36	110.57
27	3	1622	XAT	C18-C5-C6	-5.16	113.62	122.26
27	g	1622	XAT	C18-C5-C6	-5.16	113.62	122.26
25	B	614	CLA	C4A-NA-C1A	5.16	109.02	106.71
24	p	605	CHL	C3B-C2B-C1B	-5.15	100.94	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	607	CHL	C3D-C2D-C1D	-5.15	98.80	105.83
25	D	402	CLA	C4A-NA-C1A	5.15	109.02	106.71
24	R	607	CHL	C3D-C2D-C1D	-5.15	98.80	105.83
24	5	605	CHL	C3B-C2B-C1B	-5.15	100.95	107.16
28	y	1623	NEX	O24-C25-C38	5.15	121.22	115.06
25	B	616	CLA	C4A-NA-C1A	5.14	109.02	106.71
27	1	1622	XAT	C37-C21-C26	-5.14	96.15	110.05
24	s	608	CHL	C3C-C4C-NC	5.14	116.34	110.57
24	3	606	CHL	CHB-C1B-NB	-5.13	118.82	124.26
27	y	1622	XAT	C15-C14-C13	-5.13	119.98	127.31
24	0	609	CHL	C3C-C4C-NC	5.13	116.33	110.57
25	C	508	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	N	609	CHL	O2D-CGD-CBD	5.13	120.39	111.27
24	7	606	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
24	r	607	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
24	n	606	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
24	g	609	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
25	s	602	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	G	609	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
28	G	1623	NEX	C38-C25-C26	-5.13	113.67	122.26
25	5	612	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	N	607	CHL	C3D-C2D-C1D	-5.13	98.84	105.83
24	5	609	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
24	0	601	CHL	C3C-C4C-NC	5.12	116.31	110.57
25	r	611	CLA	C4A-NA-C1A	5.12	109.01	106.71
27	n	1622	XAT	C6-C7-C8	-5.12	115.17	125.99
27	Y	1622	XAT	C15-C14-C13	-5.11	120.01	127.31
24	N	606	CHL	C3D-C2D-C1D	-5.11	98.85	105.83
24	8	601	CHL	C3D-C4D-ND	5.11	118.51	110.24
24	p	609	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
27	1	1622	XAT	O24-C25-C24	5.11	117.22	113.38
24	0	606	CHL	C3D-C4D-ND	5.11	118.51	110.24
24	0	608	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
25	C	501	CLA	C4A-NA-C1A	5.11	109.00	106.71
24	r	606	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
24	Y	609	CHL	C3B-C2B-C1B	-5.11	101.00	107.16
24	0	605	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
25	3	612	CLA	C4A-NA-C1A	5.10	109.00	106.71
28	1	1623	NEX	C11-C10-C9	-5.10	120.03	127.31
24	q	608	CHL	C3B-C2B-C1B	-5.10	101.00	107.16
27	8	1622	XAT	O4-C5-C18	5.10	121.17	115.06
28	s	1623	NEX	C15-C14-C13	-5.10	120.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	606	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
27	8	1622	XAT	C38-C25-C26	-5.10	113.72	122.26
24	g	605	CHL	C3B-C2B-C1B	-5.10	101.01	107.16
24	0	607	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	G	613	CLA	C4A-NA-C1A	5.09	109.00	106.71
28	7	1623	NEX	C15-C14-C13	-5.09	120.04	127.31
24	8	608	CHL	C3C-C4C-NC	5.09	116.28	110.57
24	6	601	CHL	C3C-C4C-NC	5.09	116.28	110.57
24	9	606	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	b	607	CLA	C4A-NA-C1A	5.09	109.00	106.71
24	5	605	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	6	604	CLA	C4A-NA-C1A	5.09	108.99	106.71
24	p	601	CHL	C3D-C2D-C1D	-5.08	98.89	105.83
24	S	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
24	R	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
24	7	608	CHL	CHD-C1D-ND	-5.08	119.78	124.45
24	g	606	CHL	C3B-C2B-C1B	-5.08	101.03	107.16
24	1	609	CHL	O2D-CGD-CBD	5.08	120.29	111.27
24	3	608	CHL	C3C-C4C-NC	5.08	116.26	110.57
27	3	1622	XAT	C38-C25-C26	-5.07	113.75	122.26
24	y	609	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
24	G	601	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
24	0	607	CHL	C3D-C2D-C1D	-5.07	98.91	105.83
25	q	614	CLA	C4A-NA-C1A	5.07	108.98	106.71
24	G	601	CHL	O2D-CGD-CBD	5.07	120.27	111.27
28	g	1623	NEX	C38-C25-C26	-5.07	113.77	122.26
28	4	1623	NEX	C11-C10-C9	-5.07	120.08	127.31
27	0	1622	XAT	O24-C25-C38	5.06	121.12	115.06
25	g	613	CLA	C4A-NA-C1A	5.06	108.98	106.71
24	8	601	CHL	O2D-CGD-CBD	5.06	120.26	111.27
25	q	604	CLA	C4A-NA-C1A	5.06	108.98	106.71
24	3	601	CHL	C3D-C4D-ND	5.06	118.42	110.24
24	6	609	CHL	C3C-C4C-NC	5.06	116.25	110.57
24	6	601	CHL	C3B-C2B-C1B	-5.06	101.06	107.16
24	6	601	CHL	C3D-C4D-ND	5.06	118.42	110.24
24	p	606	CHL	CHB-C1B-NB	-5.06	118.90	124.26
27	3	1622	XAT	O4-C5-C18	5.06	121.11	115.06
24	0	609	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
24	1	608	CHL	CHD-C1D-ND	-5.05	119.81	124.45
24	9	607	CHL	CHB-C1B-NB	-5.05	118.91	124.26
25	Y	603	CLA	C4A-NA-C1A	5.05	108.98	106.71
25	b	614	CLA	C4A-NA-C1A	5.05	108.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R	623	NEX	C27-C28-C29	-5.05	117.70	125.53
24	g	601	CHL	C3B-C2B-C1B	-5.05	101.07	107.16
24	N	605	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
24	4	601	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
24	9	609	CHL	CHB-C1B-NB	-5.04	118.92	124.26
24	y	601	CHL	C3D-C4D-ND	5.04	118.39	110.24
24	q	608	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
27	4	1622	XAT	O24-C25-C38	5.03	121.09	115.06
24	q	606	CHL	CHB-C1B-NB	-5.03	118.93	124.26
24	G	606	CHL	C3D-C2D-C1D	-5.03	98.96	105.83
24	6	606	CHL	C3D-C4D-ND	5.03	118.38	110.24
24	G	606	CHL	C3B-C2B-C1B	-5.03	101.09	107.16
27	2	1622	XAT	C31-C30-C29	-5.03	120.13	127.31
24	7	609	CHL	O2D-CGD-CBD	5.03	120.20	111.27
24	0	605	CHL	C3C-C4C-NC	5.03	116.21	110.57
24	4	601	CHL	C3B-C2B-C1B	-5.02	101.10	107.16
28	r	623	NEX	C27-C28-C29	-5.02	117.73	125.53
24	N	601	CHL	C3D-C4D-ND	5.02	118.36	110.24
24	0	608	CHL	C3C-C4C-NC	5.02	116.20	110.57
25	R	611	CLA	C4A-NA-C1A	5.02	108.96	106.71
24	4	608	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	9	607	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	s	606	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
24	N	609	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
24	Y	605	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	y	605	CHL	O2D-CGD-CBD	5.01	120.17	111.27
28	1	1623	NEX	C38-C25-C26	-5.01	113.87	122.26
24	N	607	CHL	CHD-C4C-C3C	-5.01	117.48	124.84
24	q	609	CHL	O2D-CGD-CBD	5.01	120.16	111.27
25	c	510	CLA	C4A-NA-C1A	5.00	108.96	106.71
34	c	517	BCR	C24-C23-C22	-5.00	118.67	126.23
27	1	1622	XAT	O4-C5-C4	5.00	117.14	113.38
28	4	1623	NEX	C15-C14-C13	-5.00	120.17	127.31
24	n	601	CHL	C3D-C4D-ND	5.00	118.33	110.24
24	g	605	CHL	C3C-C4C-NC	5.00	116.18	110.57
24	6	601	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
25	B	608	CLA	C4A-NA-C1A	5.00	108.95	106.71
24	Y	601	CHL	C3D-C4D-ND	4.99	118.32	110.24
25	8	612	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	g	608	CHL	C3C-C4C-NC	4.99	116.17	110.57
24	8	605	CHL	C3B-C2B-C1B	-4.99	101.14	107.16
25	S	611	CLA	C4A-NA-C1A	4.99	108.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
25	y	603	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	5	605	CHL	C3D-C2D-C1D	-4.99	99.03	105.83
24	S	601	CHL	C3D-C4D-ND	4.98	118.30	110.24
24	R	606	CHL	C3C-C4C-NC	4.98	116.16	110.57
24	p	609	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
25	B	607	CLA	C4A-NA-C1A	4.98	108.94	106.71
24	q	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
24	2	606	CHL	C3B-C2B-C1B	-4.97	101.16	107.16
24	0	606	CHL	O2D-CGD-CBD	4.97	120.11	111.27
24	0	607	CHL	O2D-CGD-CBD	4.97	120.11	111.27
24	2	609	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
24	g	605	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
34	C	517	BCR	C24-C23-C22	-4.97	118.73	126.23
24	8	605	CHL	C3D-C2D-C1D	-4.97	99.06	105.83
24	n	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	n	609	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	6	607	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
25	n	614	CLA	C4A-NA-C1A	4.96	108.94	106.71
24	N	607	CHL	C3D-C4D-ND	4.96	118.27	110.24
24	Y	609	CHL	O2D-CGD-CBD	4.96	120.08	111.27
24	G	609	CHL	C2D-C1D-ND	4.96	113.76	110.10
24	1	605	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	n	606	CHL	C3B-C2B-C1B	-4.96	101.18	107.16
27	7	1622	XAT	O4-C5-C4	4.96	117.11	113.38
24	3	605	CHL	C3B-C2B-C1B	-4.96	101.18	107.16
24	q	609	CHL	C3D-C4D-ND	4.96	118.26	110.24
24	9	605	CHL	O2D-CGD-CBD	4.95	120.07	111.27
28	p	1623	NEX	C27-C28-C29	-4.95	117.85	125.53
25	9	604	CLA	C4A-NA-C1A	4.95	108.93	106.71
24	3	605	CHL	C3D-C2D-C1D	-4.95	99.07	105.83
24	n	607	CHL	C3D-C4D-ND	4.95	118.25	110.24
24	8	608	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
27	5	1622	XAT	C38-C25-C26	-4.95	113.97	122.26
24	n	605	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
24	p	609	CHL	C3C-C4C-NC	4.95	116.12	110.57
24	6	605	CHL	CHB-C1B-NB	-4.94	119.02	124.26
24	5	601	CHL	C3D-C2D-C1D	-4.94	99.08	105.83
24	s	607	CHL	C3B-C2B-C1B	-4.94	101.20	107.16
24	3	608	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	6	606	CHL	C3C-C4C-NC	4.94	116.11	110.57
24	4	608	CHL	C3D-C2D-C1D	-4.94	99.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	605	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
28	G	1623	NEX	C15-C14-C13	-4.94	120.27	127.31
24	N	609	CHL	CHB-C1B-NB	-4.94	119.03	124.26
24	g	609	CHL	C2D-C1D-ND	4.93	113.74	110.10
24	Y	601	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
24	G	605	CHL	C3C-C4C-NC	4.93	116.10	110.57
24	y	601	CHL	C3D-C2D-C1D	-4.93	99.11	105.83
25	A	407	CLA	C4A-NA-C1A	4.93	108.92	106.71
24	8	607	CHL	C3D-C4D-ND	4.92	118.20	110.24
25	a	407	CLA	C4A-NA-C1A	4.92	108.92	106.71
24	5	609	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
24	0	601	CHL	CHB-C1B-NB	-4.92	119.05	124.26
24	3	607	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
24	3	601	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
24	s	601	CHL	C3D-C4D-ND	4.92	118.19	110.24
24	7	605	CHL	O2D-CGD-CBD	4.92	120.00	111.27
24	3	607	CHL	C3D-C4D-ND	4.91	118.19	110.24
27	6	1622	XAT	C37-C21-C26	-4.91	96.78	110.05
24	8	609	CHL	C3D-C4D-ND	4.91	118.18	110.24
25	a	405	CLA	C4A-NA-C1A	4.91	108.91	106.71
24	5	607	CHL	C3B-C2B-C1B	-4.91	101.23	107.16
27	G	1622	XAT	O4-C5-C18	4.91	120.94	115.06
24	2	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
24	g	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
24	S	607	CHL	C3B-C2B-C1B	-4.91	101.24	107.16
24	s	606	CHL	C3D-C4D-ND	4.91	118.17	110.24
28	0	1623	NEX	C27-C28-C29	-4.90	117.92	125.53
28	6	1623	NEX	C27-C28-C29	-4.90	117.92	125.53
28	6	1623	NEX	C38-C25-C26	-4.90	114.04	122.26
24	9	606	CHL	C3B-C2B-C1B	-4.90	101.25	107.16
24	n	605	CHL	O2D-CGD-CBD	4.90	119.98	111.27
24	6	605	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
24	2	605	CHL	O2D-CGD-CBD	4.90	119.97	111.27
28	q	1623	NEX	C15-C14-C13	-4.90	120.32	127.31
24	r	606	CHL	C3C-C4C-NC	4.89	116.06	110.57
24	8	601	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
24	2	609	CHL	C3D-C4D-ND	4.89	118.15	110.24
24	p	607	CHL	C3D-C4D-ND	4.89	118.15	110.24
24	6	605	CHL	O2D-CGD-CBD	4.89	119.96	111.27
24	1	606	CHL	C3C-C4C-NC	4.89	116.06	110.57
25	n	611	CLA	C4A-NA-C1A	4.89	108.90	106.71
24	S	606	CHL	C3D-C4D-ND	4.89	118.14	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	606	CHL	O2D-CGD-CBD	4.88	119.95	111.27
27	g	1622	XAT	O4-C5-C18	4.88	120.91	115.06
24	4	605	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
24	1	608	CHL	C3B-C2B-C1B	-4.88	101.27	107.16
24	3	609	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
24	0	608	CHL	O2D-CGD-CBD	4.88	119.94	111.27
26	8	1620	LUT	C35-C34-C33	-4.88	120.35	127.31
27	0	1622	XAT	C37-C21-C26	-4.88	96.87	110.05
28	9	1623	NEX	C11-C10-C9	-4.88	120.35	127.31
25	C	507	CLA	C4A-NA-C1A	4.88	108.90	106.71
28	5	1623	NEX	C15-C14-C13	-4.88	120.35	127.31
27	y	1622	XAT	C18-C5-C6	-4.88	114.09	122.26
24	5	606	CHL	C3B-C2B-C1B	-4.87	101.28	107.16
34	D	404	BCR	C11-C10-C9	-4.87	120.35	127.31
24	q	609	CHL	CHB-C1B-NB	-4.87	119.10	124.26
24	5	605	CHL	CHB-C1B-NB	-4.87	119.10	124.26
24	4	601	CHL	C3D-C4D-ND	4.87	118.12	110.24
24	7	606	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
24	n	607	CHL	CHD-C4C-C3C	-4.87	117.68	124.84
24	q	609	CHL	C2D-C1D-ND	4.87	113.69	110.10
24	6	607	CHL	C3C-C4C-NC	4.87	116.03	110.57
27	r	622	XAT	C18-C5-C6	-4.87	114.11	122.26
34	h	101	BCR	C28-C27-C26	-4.87	105.39	114.08
24	4	607	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
24	G	606	CHL	C3D-C4D-ND	4.86	118.11	110.24
24	1	606	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
24	6	608	CHL	O2D-CGD-CBD	4.86	119.91	111.27
24	0	607	CHL	C3D-C4D-ND	4.86	118.10	110.24
24	9	609	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
27	R	622	XAT	C18-C5-C6	-4.86	114.12	122.26
24	1	606	CHL	C3D-C4D-ND	4.86	118.10	110.24
27	Y	1622	XAT	C18-C5-C6	-4.86	114.12	122.26
24	p	601	CHL	C3D-C4D-ND	4.85	118.09	110.24
24	g	606	CHL	C3D-C4D-ND	4.85	118.09	110.24
24	S	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
34	H	101	BCR	C28-C27-C26	-4.85	105.41	114.08
24	s	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
24	N	601	CHL	C3C-C4C-NC	4.85	116.01	110.57
24	n	607	CHL	O2D-CGD-CBD	4.85	119.89	111.27
27	9	1622	XAT	C18-C5-C6	-4.85	114.13	122.26
24	7	605	CHL	C3D-C2D-C1D	-4.85	99.22	105.83
25	A	410	CLA	C4A-NA-C1A	4.84	108.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	609	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
25	b	603	CLA	C4A-NA-C1A	4.84	108.88	106.71
28	4	1623	NEX	C38-C25-C26	-4.84	114.14	122.26
24	5	607	CHL	C3D-C4D-ND	4.84	118.07	110.24
24	9	605	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
27	p	1622	XAT	O4-C5-C18	4.84	120.85	115.06
28	3	1623	NEX	C38-C25-C26	-4.84	114.15	122.26
24	n	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
24	9	601	CHL	C2D-C1D-ND	4.84	113.67	110.10
24	8	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
24	1	601	CHL	C3D-C2D-C1D	-4.83	99.23	105.83
24	0	601	CHL	C3D-C4D-ND	4.83	118.06	110.24
24	0	601	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
24	1	605	CHL	O2D-CGD-CBD	4.83	119.85	111.27
25	C	510	CLA	C4A-NA-C1A	4.83	108.88	106.71
24	7	601	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
24	7	607	CHL	C3C-C4C-NC	4.83	115.99	110.57
28	5	1623	NEX	C11-C10-C9	-4.83	120.42	127.31
24	7	606	CHL	C3C-C4C-NC	4.83	115.98	110.57
24	3	606	CHL	C3D-C4D-ND	4.83	118.04	110.24
24	9	607	CHL	C3D-C2D-C1D	-4.83	99.25	105.83
34	d	404	BCR	C11-C10-C9	-4.82	120.42	127.31
24	4	601	CHL	C3C-C4C-NC	4.82	115.98	110.57
27	N	1622	XAT	C38-C25-C26	-4.82	114.18	122.26
24	5	608	CHL	C3D-C4D-ND	4.82	118.04	110.24
24	G	608	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
34	C	515	BCR	C7-C8-C9	-4.82	118.95	126.23
24	p	601	CHL	C3C-C4C-NC	4.82	115.97	110.57
27	n	1622	XAT	C38-C25-C26	-4.82	114.19	122.26
28	8	1623	NEX	C38-C25-C26	-4.82	114.19	122.26
24	9	609	CHL	C3D-C4D-ND	4.82	118.03	110.24
24	5	607	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	N	601	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	4	609	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	q	605	CHL	C3D-C4D-ND	4.81	118.03	110.24
24	G	608	CHL	C3C-C4C-NC	4.81	115.97	110.57
24	4	609	CHL	C3B-C2B-C1B	-4.81	101.35	107.16
27	q	1622	XAT	O24-C25-C38	4.81	120.82	115.06
27	2	1622	XAT	C18-C5-C6	-4.81	114.20	122.26
24	5	601	CHL	C3D-C4D-ND	4.81	118.02	110.24
25	q	612	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	8	606	CHL	C2D-C1D-ND	4.81	113.65	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	1622	XAT	C15-C14-C13	-4.81	120.45	127.31
24	q	609	CHL	C3D-C2D-C1D	-4.80	99.27	105.83
24	s	607	CHL	C3D-C2D-C1D	-4.80	99.27	105.83
24	N	606	CHL	C3D-C4D-ND	4.80	118.01	110.24
24	2	605	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
27	0	1622	XAT	C18-C5-C6	-4.80	114.22	122.26
24	2	607	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
34	c	515	BCR	C7-C8-C9	-4.80	118.98	126.23
28	3	1623	NEX	C27-C28-C29	-4.80	118.08	125.53
25	r	604	CLA	C4A-NA-C1A	4.80	108.86	106.71
24	8	607	CHL	CHD-C4C-C3C	-4.80	117.79	124.84
24	2	606	CHL	O2D-CGD-CBD	4.80	119.79	111.27
24	3	609	CHL	C3D-C4D-ND	4.80	118.00	110.24
24	Y	607	CHL	O2D-CGD-CBD	4.79	119.79	111.27
24	4	606	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
24	q	609	CHL	C3B-C2B-C1B	-4.79	101.37	107.16
25	B	609	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	b	609	CLA	C4A-NA-C1A	4.79	108.86	106.71
24	q	601	CHL	C3D-C4D-ND	4.79	117.99	110.24
24	0	606	CHL	C3B-C2B-C1B	-4.79	101.38	107.16
25	N	611	CLA	C4A-NA-C1A	4.79	108.86	106.71
28	q	1623	NEX	C38-C25-C26	-4.79	114.24	122.26
24	7	607	CHL	C3D-C4D-ND	4.79	117.98	110.24
24	S	607	CHL	C3D-C2D-C1D	-4.78	99.30	105.83
24	5	606	CHL	C3C-C4C-NC	4.78	115.94	110.57
24	2	606	CHL	C3D-C4D-ND	4.78	117.97	110.24
24	6	606	CHL	C3B-C2B-C1B	-4.78	101.40	107.16
24	5	606	CHL	C3D-C4D-ND	4.78	117.96	110.24
24	8	609	CHL	CHD-C1D-ND	-4.78	120.06	124.45
24	s	607	CHL	O2D-CGD-CBD	4.77	119.75	111.27
25	R	604	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	S	607	CHL	O2D-CGD-CBD	4.77	119.75	111.27
24	p	608	CHL	C3D-C4D-ND	4.77	117.96	110.24
25	A	405	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	a	410	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	y	608	CHL	CHD-C4C-C3C	-4.77	117.83	124.84
24	y	607	CHL	O2D-CGD-CBD	4.76	119.73	111.27
24	n	606	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
27	n	1622	XAT	C18-C5-C6	-4.75	114.29	122.26
24	y	606	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
25	c	507	CLA	C4A-NA-C1A	4.75	108.84	106.71
24	4	608	CHL	C3C-C4C-NC	4.75	115.90	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	606	CHL	CHB-C1B-NB	-4.75	119.23	124.26
28	0	1623	NEX	C38-C25-C26	-4.75	114.30	122.26
24	S	601	CHL	O2D-CGD-CBD	4.74	119.70	111.27
24	p	605	CHL	C3C-C4C-NC	4.74	115.89	110.57
24	G	609	CHL	C3B-C2B-C1B	-4.74	101.44	107.16
24	p	607	CHL	C3C-C4C-NC	4.74	115.89	110.57
24	N	606	CHL	C3B-C2B-C1B	-4.74	101.44	107.16
24	y	609	CHL	O2D-CGD-CBD	4.74	119.69	111.27
24	9	606	CHL	C3D-C4D-ND	4.74	117.90	110.24
24	9	601	CHL	C3D-C2D-C1D	-4.74	99.37	105.83
24	G	601	CHL	C3D-C4D-ND	4.74	117.90	110.24
24	1	607	CHL	O2D-CGD-CBD	4.74	119.68	111.27
24	g	601	CHL	C3D-C4D-ND	4.74	117.90	110.24
27	9	1622	XAT	C31-C30-C29	-4.73	120.55	127.31
27	N	1622	XAT	C18-C5-C6	-4.73	114.33	122.26
28	p	1623	NEX	C38-C25-C26	-4.73	114.33	122.26
24	p	606	CHL	C3D-C4D-ND	4.73	117.89	110.24
25	4	614	CLA	C4A-NA-C1A	4.73	108.83	106.71
24	7	606	CHL	C3D-C4D-ND	4.73	117.89	110.24
24	4	608	CHL	C3D-C4D-ND	4.73	117.88	110.24
28	q	1623	NEX	C11-C10-C9	-4.73	120.56	127.31
24	1	607	CHL	C3D-C4D-ND	4.72	117.88	110.24
24	0	605	CHL	O2D-CGD-CBD	4.72	119.66	111.27
24	3	605	CHL	C3C-C4C-NC	4.72	115.87	110.57
25	p	612	CLA	C4A-NA-C1A	4.72	108.83	106.71
28	g	1623	NEX	C15-C14-C13	-4.72	120.57	127.31
24	s	607	CHL	C3D-C4D-ND	4.72	117.87	110.24
24	4	606	CHL	CHB-C1B-NB	-4.72	119.26	124.26
24	Y	607	CHL	C3D-C4D-ND	4.72	117.87	110.24
24	q	607	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
24	2	609	CHL	O2D-CGD-CBD	4.71	119.64	111.27
24	s	601	CHL	O2D-CGD-CBD	4.71	119.64	111.27
24	y	607	CHL	C3D-C4D-ND	4.71	117.86	110.24
24	5	609	CHL	C3C-C4C-NC	4.71	115.85	110.57
24	8	605	CHL	C3C-C4C-NC	4.71	115.85	110.57
24	G	607	CHL	C3D-C4D-ND	4.71	117.85	110.24
26	3	1620	LUT	C35-C34-C33	-4.71	120.59	127.31
24	7	607	CHL	O2D-CGD-CBD	4.71	119.63	111.27
24	q	605	CHL	C3C-C4C-NC	4.70	115.85	110.57
25	5	604	CLA	C4A-NA-C1A	4.70	108.82	106.71
26	p	1620	LUT	C31-C30-C29	-4.70	120.60	127.31
24	S	607	CHL	C3D-C4D-ND	4.70	117.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	606	CHL	O2D-CGD-CBD	4.70	119.62	111.27
24	4	605	CHL	C3D-C4D-ND	4.70	117.84	110.24
24	6	605	CHL	C3C-C4C-NC	4.70	115.84	110.57
25	B	603	CLA	C4A-NA-C1A	4.70	108.82	106.71
24	Y	606	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
29	d	410	LHG	O7-C7-C8	4.70	121.62	111.50
24	8	601	CHL	C3C-C4C-NC	4.70	115.84	110.57
24	G	607	CHL	O2D-CGD-CBD	4.70	119.61	111.27
24	N	609	CHL	C3D-C4D-ND	4.70	117.83	110.24
29	D	410	LHG	O7-C7-C8	4.69	121.62	111.50
24	p	606	CHL	C3B-C2B-C1B	-4.69	101.50	107.16
24	4	605	CHL	O2D-CGD-CBD	4.69	119.61	111.27
24	G	601	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
27	7	1622	XAT	O24-C25-C24	4.69	116.91	113.38
24	g	607	CHL	C3D-C4D-ND	4.69	117.82	110.24
24	5	601	CHL	C3C-C4C-NC	4.69	115.83	110.57
24	4	609	CHL	C1D-ND-C4D	-4.68	103.01	106.33
24	6	607	CHL	O2D-CGD-CBD	4.68	119.59	111.27
24	n	609	CHL	C3D-C4D-ND	4.68	117.81	110.24
24	N	605	CHL	C3C-C4C-NC	4.68	115.82	110.57
24	4	608	CHL	CHB-C1B-NB	-4.68	119.30	124.26
26	2	1621	LUT	C35-C34-C33	-4.68	120.63	127.31
24	6	607	CHL	C3D-C4D-ND	4.68	117.80	110.24
24	N	607	CHL	O2D-CGD-CBD	4.67	119.57	111.27
24	R	608	CHL	C3B-C2B-C1B	-4.67	101.52	107.16
27	y	1622	XAT	C37-C21-C26	-4.67	97.43	110.05
24	9	606	CHL	O2D-CGD-CBD	4.66	119.56	111.27
24	g	608	CHL	C3D-C4D-ND	4.66	117.78	110.24
24	1	607	CHL	C3C-C4C-NC	4.66	115.80	110.57
27	Y	1622	XAT	C37-C21-C26	-4.66	97.46	110.05
24	N	608	CHL	O2D-CGD-CBD	4.66	119.55	111.27
24	2	607	CHL	C3C-C4C-NC	4.66	115.80	110.57
24	p	605	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
24	R	606	CHL	C3D-C4D-ND	4.66	117.77	110.24
28	y	1623	NEX	C35-C34-C33	-4.66	120.66	127.31
24	G	605	CHL	CHB-C1B-NB	-4.65	119.33	124.26
25	5	611	CLA	C4A-NA-C1A	4.65	108.80	106.71
24	p	606	CHL	C2D-C1D-ND	4.65	113.53	110.10
24	r	608	CHL	C3B-C2B-C1B	-4.65	101.55	107.16
24	5	607	CHL	O2D-CGD-CBD	4.65	119.53	111.27
24	g	609	CHL	O2D-CGD-CBD	4.65	119.53	111.27
25	G	602	CLA	C4A-NA-C1A	4.65	108.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	606	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
24	5	609	CHL	C3D-C4D-ND	4.64	117.75	110.24
24	p	609	CHL	C3D-C4D-ND	4.64	117.75	110.24
34	c	515	BCR	C15-C14-C13	-4.64	120.68	127.31
28	N	1623	NEX	C27-C28-C29	-4.64	118.33	125.53
24	n	605	CHL	C3C-C4C-NC	4.64	115.78	110.57
25	N	612	CLA	C4A-NA-C1A	4.64	108.79	106.71
24	7	607	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
24	N	606	CHL	O2D-CGD-CBD	4.64	119.51	111.27
24	r	606	CHL	C3D-C4D-ND	4.64	117.74	110.24
24	g	609	CHL	C3B-C2B-C1B	-4.64	101.56	107.16
24	0	606	CHL	C3C-C4C-NC	4.64	115.77	110.57
24	1	606	CHL	O2D-CGD-CBD	4.64	119.51	111.27
24	0	608	CHL	C3D-C4D-ND	4.63	117.73	110.24
24	4	605	CHL	C3C-C4C-NC	4.63	115.76	110.57
24	r	606	CHL	O2D-CGD-CBD	4.63	119.50	111.27
24	r	607	CHL	CHD-C1D-ND	-4.63	120.20	124.45
24	G	608	CHL	C3D-C4D-ND	4.63	117.73	110.24
25	g	602	CLA	C4A-NA-C1A	4.63	108.79	106.71
24	3	606	CHL	C2D-C1D-ND	4.63	113.52	110.10
24	0	605	CHL	CHB-C1B-NB	-4.63	119.36	124.26
34	c	516	BCR	C16-C17-C18	-4.63	120.71	127.31
27	g	1622	XAT	O24-C25-C38	4.62	120.60	115.06
24	Y	608	CHL	CHD-C4C-C3C	-4.62	118.04	124.84
24	R	606	CHL	O2D-CGD-CBD	4.62	119.48	111.27
25	B	605	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	q	606	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
25	2	602	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	7	605	CHL	C3D-C4D-ND	4.62	117.70	110.24
25	5	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	9	607	CHL	C3C-C4C-NC	4.62	115.75	110.57
24	q	605	CHL	O2D-CGD-CBD	4.61	119.47	111.27
28	Y	1623	NEX	C35-C34-C33	-4.61	120.73	127.31
24	5	606	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
24	5	609	CHL	CHB-C1B-NB	-4.61	119.38	124.26
24	0	601	CHL	O2D-CGD-CBD	4.61	119.46	111.27
27	G	1622	XAT	O24-C25-C38	4.61	120.58	115.06
34	C	516	BCR	C16-C17-C18	-4.60	120.74	127.31
24	1	609	CHL	C3D-C4D-ND	4.60	117.68	110.24
25	4	612	CLA	C4A-NA-C1A	4.60	108.77	106.71
28	n	1623	NEX	C35-C34-C33	-4.60	120.75	127.31
24	g	605	CHL	C3D-C4D-ND	4.60	117.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	606	CHL	C3D-C4D-ND	4.59	117.67	110.24
24	Y	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	9	607	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	s	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
28	n	1623	NEX	C27-C28-C29	-4.59	118.41	125.53
24	G	605	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	y	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	G	601	CHL	C3C-C4C-NC	4.59	115.71	110.57
24	p	607	CHL	C3D-C2D-C1D	-4.58	99.57	105.83
24	2	606	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
24	8	608	CHL	C3D-C4D-ND	4.58	117.65	110.24
34	C	515	BCR	C15-C14-C13	-4.58	120.77	127.31
27	0	1622	XAT	C31-C30-C29	-4.58	120.77	127.31
24	q	601	CHL	C3C-C4C-NC	4.58	115.70	110.57
26	r	620	LUT	C15-C14-C13	-4.57	120.78	127.31
24	6	606	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
34	b	619	BCR	C15-C14-C13	-4.57	120.79	127.31
27	q	1622	XAT	C6-C7-C8	-4.57	116.34	125.99
24	s	607	CHL	CHB-C1B-NB	-4.57	119.42	124.26
24	N	609	CHL	CAC-C3C-C4C	4.57	130.73	124.81
24	9	608	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	3	608	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	1	605	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	7	608	CHL	CHD-C4C-C3C	-4.56	118.13	124.84
24	4	607	CHL	C3D-C4D-ND	4.56	117.61	110.24
24	Y	608	CHL	C3B-C2B-C1B	-4.56	101.66	107.16
33	a	408	PHO	C2B-C1B-NB	-4.56	106.38	109.53
24	g	601	CHL	C3C-C4C-NC	4.56	115.68	110.57
24	y	608	CHL	C3B-C2B-C1B	-4.56	101.66	107.16
26	R	620	LUT	C15-C14-C13	-4.56	120.81	127.31
24	9	606	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
25	2	611	CLA	C4A-NA-C1A	4.55	108.75	106.71
34	B	619	BCR	C15-C14-C13	-4.55	120.81	127.31
24	4	609	CHL	O2D-CGD-CBD	4.55	119.36	111.27
24	S	608	CHL	C3D-C4D-ND	4.55	117.60	110.24
28	g	1623	NEX	C27-C28-C29	-4.55	118.47	125.53
25	b	605	CLA	C4A-NA-C1A	4.55	108.75	106.71
24	1	607	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
24	5	607	CHL	CHD-C4C-C3C	-4.55	118.16	124.84
28	9	1623	NEX	C38-C25-C26	-4.55	114.64	122.26
24	g	605	CHL	CHB-C1B-NB	-4.55	119.44	124.26
24	6	609	CHL	CHB-C1B-NB	-4.55	119.44	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	C3D-C4D-ND	4.54	117.59	110.24
29	q	2630	LHG	O7-C7-C8	4.54	121.29	111.50
24	S	607	CHL	CHB-C1B-NB	-4.54	119.45	124.26
27	R	622	XAT	O4-C5-C18	4.54	120.49	115.06
24	R	608	CHL	C3D-C4D-ND	4.53	117.57	110.24
24	Y	609	CHL	C3D-C4D-ND	4.53	117.57	110.24
24	R	607	CHL	CHD-C1D-ND	-4.53	120.29	124.45
26	5	1620	LUT	C31-C30-C29	-4.53	120.84	127.31
28	r	623	NEX	C38-C25-C26	-4.53	114.67	122.26
24	G	609	CHL	O2D-CGD-CBD	4.53	119.32	111.27
29	9	2630	LHG	O7-C7-C8	4.53	121.26	111.50
27	r	622	XAT	O4-C5-C18	4.53	120.48	115.06
25	B	610	CLA	C4A-NA-C1A	4.53	108.74	106.71
25	b	610	CLA	C4A-NA-C1A	4.53	108.74	106.71
24	8	606	CHL	C3D-C2D-C1D	-4.53	99.66	105.83
24	1	607	CHL	CHB-C1B-NB	-4.52	119.47	124.26
28	5	1623	NEX	C38-C25-C26	-4.52	114.68	122.26
24	y	606	CHL	O2D-CGD-CBD	4.52	119.30	111.27
26	5	1620	LUT	C15-C14-C13	-4.52	120.86	127.31
24	G	609	CHL	C3D-C4D-ND	4.52	117.55	110.24
24	n	601	CHL	C3C-C4C-NC	4.52	115.64	110.57
24	r	608	CHL	C3D-C4D-ND	4.51	117.54	110.24
24	1	608	CHL	CHD-C4C-C3C	-4.51	118.20	124.84
24	2	608	CHL	C3D-C4D-ND	4.51	117.54	110.24
24	4	606	CHL	C3D-C4D-ND	4.51	117.54	110.24
33	a	409	PHO	C2B-C1B-NB	-4.51	106.41	109.53
26	p	1620	LUT	C15-C14-C13	-4.51	120.87	127.31
25	7	603	CLA	C4A-NA-C1A	4.51	108.73	106.71
33	A	409	PHO	C2B-C1B-NB	-4.51	106.41	109.53
24	7	609	CHL	C3D-C4D-ND	4.51	117.53	110.24
28	R	623	NEX	C38-C25-C26	-4.51	114.71	122.26
27	4	1622	XAT	C26-C27-C28	-4.50	116.47	125.99
34	H	101	BCR	C11-C10-C9	-4.50	120.89	127.31
27	R	622	XAT	O24-C25-C38	4.50	120.45	115.06
33	A	408	PHO	C2B-C1B-NB	-4.50	106.42	109.53
25	1	603	CLA	C4A-NA-C1A	4.50	108.73	106.71
24	Y	606	CHL	O2D-CGD-CBD	4.50	119.26	111.27
24	4	601	CHL	CHC-C4B-NB	-4.50	119.49	124.26
24	3	609	CHL	CHD-C1D-ND	-4.50	120.32	124.45
27	N	1622	XAT	C15-C14-C13	-4.49	120.89	127.31
24	q	608	CHL	C3D-C4D-ND	4.49	117.51	110.24
25	2	604	CLA	C4A-NA-C1A	4.49	108.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	p	604	CLA	C4A-NA-C1A	4.49	108.72	106.71
27	r	622	XAT	O24-C25-C38	4.49	120.43	115.06
24	9	609	CHL	O2D-CGD-CBD	4.48	119.23	111.27
24	y	609	CHL	C3D-C4D-ND	4.48	117.48	110.24
25	B	612	CLA	C4A-NA-C1A	4.48	108.72	106.71
25	b	612	CLA	C4A-NA-C1A	4.48	108.72	106.71
26	5	1621	LUT	C35-C34-C33	-4.48	120.92	127.31
24	N	608	CHL	C3D-C4D-ND	4.47	117.48	110.24
24	3	606	CHL	C3D-C2D-C1D	-4.47	99.72	105.83
27	p	1622	XAT	C15-C14-C13	-4.47	120.92	127.31
28	p	1623	NEX	C15-C14-C13	-4.47	120.93	127.31
24	y	607	CHL	CHD-C4C-C3C	-4.47	118.27	124.84
24	6	608	CHL	C3D-C4D-ND	4.47	117.46	110.24
28	N	1623	NEX	O24-C25-C38	4.47	120.41	115.06
28	7	1623	NEX	O24-C25-C38	4.47	120.41	115.06
34	h	101	BCR	C11-C10-C9	-4.47	120.94	127.31
24	0	606	CHL	C3D-C2D-C1D	-4.46	99.74	105.83
24	Y	607	CHL	CHD-C4C-C3C	-4.46	118.28	124.84
24	n	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
28	S	1623	NEX	C38-C25-C26	-4.45	114.79	122.26
24	8	605	CHL	C3D-C4D-ND	4.45	117.44	110.24
24	y	605	CHL	C3D-C4D-ND	4.45	117.44	110.24
24	Y	608	CHL	O2D-CGD-CBD	4.45	119.17	111.27
24	n	605	CHL	C3D-C4D-ND	4.44	117.41	110.24
28	2	1623	NEX	C38-C25-C26	-4.43	114.83	122.26
24	G	608	CHL	O2D-CGD-CBD	4.43	119.14	111.27
24	3	605	CHL	C3D-C4D-ND	4.43	117.40	110.24
24	5	601	CHL	CHB-C1B-NB	-4.43	119.57	124.26
24	2	601	CHL	C3C-C4C-NC	4.43	115.53	110.57
24	5	608	CHL	O2D-CGD-CBD	4.42	119.13	111.27
28	g	1623	NEX	C11-C10-C9	-4.42	121.00	127.31
27	7	1622	XAT	C6-C7-C8	-4.42	116.64	125.99
24	p	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27
24	n	608	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
24	g	609	CHL	C3D-C4D-ND	4.42	117.38	110.24
25	4	604	CLA	C4A-NA-C1A	4.42	108.69	106.71
24	7	607	CHL	CHB-C1B-NB	-4.42	119.58	124.26
24	4	606	CHL	C3C-C4C-NC	4.41	115.52	110.57
24	s	608	CHL	CHB-C1B-NB	-4.41	119.59	124.26
24	2	605	CHL	C3D-C4D-ND	4.41	117.37	110.24
24	Y	605	CHL	C3D-C4D-ND	4.41	117.37	110.24
27	R	622	XAT	C26-C27-C28	-4.41	116.68	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	602	CLA	C4A-NA-C1A	4.40	108.69	106.71
24	q	608	CHL	C3C-C4C-NC	4.40	115.51	110.57
24	q	608	CHL	CHC-C4B-NB	-4.40	119.60	124.26
28	s	1623	NEX	C38-C25-C26	-4.40	114.89	122.26
28	2	1623	NEX	C11-C10-C9	-4.40	121.03	127.31
24	Y	606	CHL	C3D-C4D-ND	4.40	117.35	110.24
24	4	607	CHL	CAC-C3C-C4C	4.40	130.51	124.81
27	6	1622	XAT	O24-C25-C24	4.40	116.69	113.38
24	N	609	CHL	C3C-C4C-NC	4.40	115.50	110.57
28	8	1623	NEX	C27-C28-C29	-4.40	118.71	125.53
24	1	605	CHL	CHB-C1B-NB	-4.40	119.60	124.26
24	y	608	CHL	O2D-CGD-CBD	4.39	119.08	111.27
26	s	1621	LUT	C35-C34-C33	-4.39	121.04	127.31
25	9	611	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	r	622	XAT	C26-C27-C28	-4.39	116.71	125.99
25	D	403	CLA	C4A-NA-C1A	4.39	108.68	106.71
26	S	1621	LUT	C35-C34-C33	-4.39	121.05	127.31
24	2	605	CHL	C3C-C4C-NC	4.39	115.49	110.57
24	G	609	CHL	C3C-C4C-NC	4.39	115.49	110.57
25	n	612	CLA	C4A-NA-C1A	4.39	108.68	106.71
26	G	1621	LUT	C15-C14-C13	-4.39	121.05	127.31
26	9	1620	LUT	C35-C34-C33	-4.38	121.05	127.31
24	0	609	CHL	C3D-C4D-ND	4.38	117.33	110.24
24	S	608	CHL	CHB-C1B-NB	-4.38	119.62	124.26
24	y	606	CHL	C3D-C4D-ND	4.38	117.33	110.24
28	n	1623	NEX	O24-C25-C38	4.38	120.31	115.06
25	1	602	CLA	C4A-NA-C1A	4.38	108.68	106.71
24	9	605	CHL	C3C-C4C-NC	4.38	115.48	110.57
24	G	608	CHL	C3B-C2B-C1B	-4.38	101.88	107.16
24	g	609	CHL	C3C-C4C-NC	4.37	115.48	110.57
26	p	1620	LUT	C35-C34-C33	-4.37	121.07	127.31
24	s	607	CHL	C3C-C4C-NC	4.37	115.48	110.57
24	3	608	CHL	O2D-CGD-CBD	4.37	119.04	111.27
28	1	1623	NEX	C35-C34-C33	-4.37	121.07	127.31
28	y	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
28	N	1623	NEX	C35-C34-C33	-4.37	121.07	127.31
24	q	607	CHL	CAC-C3C-C4C	4.37	130.48	124.81
24	R	607	CHL	C3D-C4D-ND	4.37	117.31	110.24
28	Y	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
24	9	605	CHL	C3D-C4D-ND	4.37	117.30	110.24
27	n	1622	XAT	C15-C14-C13	-4.36	121.08	127.31
24	N	605	CHL	C3D-C4D-ND	4.36	117.29	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	O2D-CGD-CBD	4.36	119.02	111.27
25	y	602	CLA	C4A-NA-C1A	4.36	108.67	106.71
26	p	1621	LUT	C35-C34-C33	-4.36	121.09	127.31
39	d	405	PL9	C7-C3-C4	4.36	120.42	116.88
24	N	608	CHL	CHD-C4C-C3C	-4.36	118.44	124.84
27	q	1622	XAT	C15-C14-C13	-4.35	121.10	127.31
24	6	609	CHL	C3D-C4D-ND	4.35	117.28	110.24
24	6	601	CHL	O2D-CGD-CBD	4.35	119.00	111.27
26	G	1621	LUT	C35-C34-C33	-4.35	121.10	127.31
28	G	1623	NEX	C27-C28-C29	-4.35	118.78	125.53
25	0	613	CLA	C4A-NA-C1A	4.35	108.66	106.71
24	g	608	CHL	C3B-C2B-C1B	-4.35	101.91	107.16
24	8	608	CHL	O2D-CGD-CBD	4.35	118.99	111.27
24	3	601	CHL	C3C-C4C-NC	4.34	115.44	110.57
24	q	607	CHL	C3C-C4C-NC	4.34	115.44	110.57
36	s	2631	LMG	O7-C10-C11	4.34	120.85	111.50
24	4	606	CHL	O2D-CGD-CBD	4.33	118.97	111.27
24	y	607	CHL	CHB-C4A-NA	4.33	130.50	124.51
34	B	619	BCR	C1-C6-C5	-4.33	116.51	122.61
27	N	1622	XAT	C27-C28-C29	-4.33	118.82	125.53
29	2	2630	LHG	O7-C7-C8	4.32	120.82	111.50
24	1	601	CHL	CMD-C2D-C3D	-4.32	117.67	127.61
26	2	1620	LUT	C35-C34-C33	-4.32	121.14	127.31
36	D	411	LMG	O7-C10-C11	4.32	120.82	111.50
24	S	607	CHL	C3C-C4C-NC	4.32	115.42	110.57
24	3	601	CHL	CHB-C1B-NB	-4.32	119.69	124.26
24	6	607	CHL	CHB-C1B-NB	-4.31	119.69	124.26
24	Y	607	CHL	CHB-C4A-NA	4.31	130.47	124.51
25	d	403	CLA	C4A-NA-C1A	4.31	108.64	106.71
24	0	609	CHL	O2D-CGD-CBD	4.31	118.93	111.27
24	p	608	CHL	O2D-CGD-CBD	4.31	118.92	111.27
24	r	607	CHL	C3D-C4D-ND	4.31	117.20	110.24
24	7	605	CHL	CHB-C1B-NB	-4.31	119.70	124.26
24	4	607	CHL	C3C-C4C-NC	4.30	115.40	110.57
24	p	606	CHL	C3D-C2D-C1D	-4.30	99.96	105.83
34	b	619	BCR	C1-C6-C5	-4.30	116.55	122.61
36	d	411	LMG	O7-C10-C11	4.30	120.77	111.50
27	N	1622	XAT	C31-C30-C29	-4.30	121.17	127.31
27	1	1622	XAT	C6-C7-C8	-4.30	116.90	125.99
24	4	609	CHL	C3D-C4D-ND	4.30	117.19	110.24
34	b	618	BCR	C15-C14-C13	-4.29	121.18	127.31
24	6	609	CHL	O2D-CGD-CBD	4.29	118.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	608	CHL	C3D-C4D-ND	4.29	117.18	110.24
26	q	1621	LUT	C15-C14-C13	-4.29	121.19	127.31
24	1	608	CHL	O2D-CGD-CBD	4.29	118.88	111.27
24	n	608	CHL	C3D-C4D-ND	4.28	117.16	110.24
39	D	405	PL9	C7-C3-C4	4.28	120.36	116.88
27	p	1622	XAT	O24-C25-C38	4.28	120.18	115.06
26	q	1621	LUT	C35-C34-C33	-4.28	121.20	127.31
24	3	601	CHL	C3B-C4B-NB	4.28	114.48	110.52
24	q	607	CHL	C3D-C4D-ND	4.28	117.16	110.24
25	Y	602	CLA	C4A-NA-C1A	4.28	108.63	106.71
29	s	2630	LHG	O7-C7-C8	4.27	120.71	111.50
29	5	2630	LHG	O7-C7-C8	4.27	120.71	111.50
29	4	2630	LHG	O7-C7-C8	4.27	120.70	111.50
26	5	1620	LUT	C35-C34-C33	-4.27	121.22	127.31
24	7	601	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
24	Y	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
34	d	404	BCR	C24-C23-C22	-4.26	119.79	126.23
24	G	601	CHL	CMD-C2D-C3D	-4.26	117.80	127.61
28	1	1623	NEX	C15-C14-C13	-4.26	121.23	127.31
34	D	404	BCR	C24-C23-C22	-4.26	119.80	126.23
34	B	618	BCR	C15-C14-C13	-4.26	121.23	127.31
26	g	1621	LUT	C15-C14-C13	-4.25	121.24	127.31
24	G	608	CHL	CHC-C4B-NB	-4.25	119.76	124.26
36	S	2631	LMG	O7-C10-C11	4.25	120.66	111.50
29	S	2630	LHG	O7-C7-C8	4.25	120.66	111.50
24	n	609	CHL	C3C-C4C-NC	4.25	115.34	110.57
25	c	503	CLA	C4A-NA-C1A	4.25	108.62	106.71
28	s	1623	NEX	C35-C34-C33	-4.25	121.25	127.31
24	3	609	CHL	CHD-C4C-C3C	-4.24	118.60	124.84
24	5	606	CHL	CHB-C1B-NB	-4.24	119.77	124.26
24	2	601	CHL	C3D-C4D-ND	4.24	117.10	110.24
27	0	1622	XAT	O4-C5-C18	4.24	120.13	115.06
24	3	605	CHL	O2D-CGD-CBD	4.23	118.79	111.27
34	B	620	BCR	C24-C23-C22	-4.23	119.84	126.23
24	6	607	CHL	CAC-C3C-C4C	4.23	130.30	124.81
24	g	606	CHL	O2D-CGD-CBD	4.23	118.78	111.27
27	8	1622	XAT	C6-C7-C8	-4.23	117.06	125.99
24	p	606	CHL	O2D-CGD-CBD	4.23	118.78	111.27
24	0	605	CHL	C3D-C4D-ND	4.23	117.07	110.24
24	5	606	CHL	O2D-CGD-CBD	4.22	118.77	111.27
29	y	2630	LHG	O7-C7-C8	4.22	120.60	111.50
28	1	1623	NEX	C39-C29-C30	-4.22	117.02	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	413	LMG	O7-C10-C11	4.22	120.59	111.50
24	7	608	CHL	C3D-C4D-ND	4.22	117.06	110.24
24	g	608	CHL	CHB-C1B-NB	-4.21	119.80	124.26
28	r	623	NEX	C11-C10-C9	-4.21	121.30	127.31
24	5	608	CHL	CHD-C4C-C3C	-4.21	118.65	124.84
28	6	1623	NEX	O24-C25-C38	4.21	120.10	115.06
24	y	609	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
24	n	609	CHL	CAC-C3C-C4C	4.20	130.26	124.81
36	a	413	LMG	O7-C10-C11	4.20	120.55	111.50
24	G	608	CHL	CHB-C1B-NB	-4.20	119.81	124.26
34	H	101	BCR	C15-C14-C13	-4.20	121.32	127.31
27	2	1622	XAT	C15-C14-C13	-4.19	121.33	127.31
35	b	623	SQD	O47-C7-C8	4.19	120.53	111.50
27	g	1622	XAT	C26-C27-C28	-4.19	117.14	125.99
27	G	1622	XAT	C26-C27-C28	-4.19	117.14	125.99
24	N	605	CHL	CHB-C1B-NB	-4.18	119.83	124.26
35	B	623	SQD	O47-C7-C8	4.18	120.52	111.50
24	g	608	CHL	CHC-C4B-NB	-4.18	119.83	124.26
34	b	620	BCR	C24-C23-C22	-4.18	119.92	126.23
25	b	602	CLA	C4A-NA-C1A	4.18	108.59	106.71
24	q	605	CHL	CAC-C3C-C4C	4.18	130.23	124.81
36	h	102	LMG	O7-C10-C11	4.18	120.51	111.50
25	y	613	CLA	C4A-NA-C1A	4.18	108.58	106.71
27	5	1622	XAT	O24-C25-C38	4.17	120.06	115.06
24	g	607	CHL	O2D-CGD-CBD	4.17	118.68	111.27
24	Y	605	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
26	9	1621	LUT	C35-C34-C33	-4.17	121.36	127.31
34	h	101	BCR	C15-C14-C13	-4.17	121.36	127.31
24	8	605	CHL	O2D-CGD-CBD	4.17	118.67	111.27
24	g	607	CHL	CAC-C3C-C4C	4.16	130.21	124.81
24	6	605	CHL	C3D-C4D-ND	4.16	116.97	110.24
24	7	608	CHL	O2D-CGD-CBD	4.16	118.66	111.27
24	G	606	CHL	O2D-CGD-CBD	4.16	118.66	111.27
34	b	619	BCR	C28-C27-C26	-4.16	106.65	114.08
36	H	102	LMG	O7-C10-C11	4.16	120.47	111.50
24	R	607	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
27	n	1622	XAT	C27-C28-C29	-4.15	119.09	125.53
24	y	605	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
24	9	601	CHL	C3D-C4D-ND	4.15	116.95	110.24
24	4	609	CHL	C2D-C1D-ND	4.15	113.16	110.10
34	B	619	BCR	C28-C27-C26	-4.14	106.68	114.08
25	r	601	CLA	C2A-C1A-CHA	4.14	131.10	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	2630	LHG	O7-C7-C8	4.14	120.42	111.50
24	q	601	CHL	CHC-C4B-NB	-4.14	119.88	124.26
27	q	1622	XAT	O4-C5-C4	4.14	116.49	113.38
25	p	614	CLA	C4A-NA-C1A	4.14	108.57	106.71
27	n	1622	XAT	C31-C30-C29	-4.13	121.41	127.31
24	r	607	CHL	CHD-C4C-C3C	-4.13	118.76	124.84
24	6	601	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	Y	609	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	y	601	CHL	C3C-C4C-NC	4.13	115.20	110.57
24	p	606	CHL	CHC-C4B-NB	-4.13	119.89	124.26
29	R	2630	LHG	O7-C7-C8	4.12	120.39	111.50
27	3	1622	XAT	C6-C7-C8	-4.12	117.27	125.99
24	q	606	CHL	C3C-C4C-NC	4.12	115.20	110.57
24	8	609	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
28	S	1623	NEX	C27-C28-C29	-4.12	119.14	125.53
25	R	601	CLA	C2A-C1A-CHA	4.12	131.06	123.86
27	q	1622	XAT	C26-C27-C28	-4.12	117.29	125.99
24	9	606	CHL	CHB-C1B-NB	-4.12	119.90	124.26
24	p	609	CHL	CHB-C1B-NB	-4.12	119.90	124.26
26	6	1620	LUT	C15-C14-C13	-4.11	121.44	127.31
24	9	608	CHL	O2D-CGD-CBD	4.11	118.58	111.27
29	r	2630	LHG	O7-C7-C8	4.11	120.36	111.50
35	a	412	SQD	O47-C7-C8	4.11	120.36	111.50
28	s	1623	NEX	C2-C1-C6	4.11	113.21	109.21
28	N	1623	NEX	C15-C14-C13	-4.11	121.44	127.31
25	G	604	CLA	C4A-NA-C1A	4.11	108.55	106.71
27	G	1622	XAT	C6-C7-C8	-4.11	117.31	125.99
25	7	604	CLA	CAC-C3C-C4C	4.11	130.14	124.81
34	c	516	BCR	C24-C23-C22	-4.11	120.03	126.23
27	g	1622	XAT	C6-C7-C8	-4.11	117.31	125.99
24	p	606	CHL	CAC-C3C-C4C	4.11	130.14	124.81
24	S	606	CHL	CAC-C3C-C4C	4.10	130.13	124.81
28	S	1623	NEX	C35-C34-C33	-4.10	121.45	127.31
24	s	608	CHL	O2D-CGD-CBD	4.10	118.56	111.27
34	D	404	BCR	C16-C15-C14	-4.10	115.07	123.47
24	g	606	CHL	CAC-C3C-C4C	4.10	130.13	124.81
29	Y	2630	LHG	O7-C7-C8	4.10	120.34	111.50
25	Y	613	CLA	C4A-NA-C1A	4.10	108.55	106.71
26	n	1621	LUT	C35-C34-C33	-4.10	121.46	127.31
35	A	412	SQD	O47-C7-C8	4.10	120.34	111.50
24	G	606	CHL	CHD-C4C-C3C	-4.10	118.82	124.84
27	6	1622	XAT	O4-C5-C18	4.09	119.96	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	d	404	BCR	C16-C15-C14	-4.09	115.09	123.47
28	s	1623	NEX	C27-C28-C29	-4.09	119.18	125.53
25	B	602	CLA	C4A-NA-C1A	4.09	108.55	106.71
26	g	1621	LUT	C35-C34-C33	-4.09	121.47	127.31
36	B	622	LMG	O7-C10-C11	4.09	120.32	111.50
24	p	608	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
29	1	2630	LHG	O7-C7-C8	4.09	120.32	111.50
24	9	601	CHL	C3C-C4C-NC	4.09	115.16	110.57
27	6	1622	XAT	C6-C7-C8	-4.09	117.35	125.99
27	1	1622	XAT	C15-C14-C13	-4.09	121.48	127.31
24	S	607	CHL	CHC-C4B-NB	-4.09	119.93	124.26
27	7	1622	XAT	C15-C14-C13	-4.08	121.48	127.31
34	C	516	BCR	C24-C23-C22	-4.08	120.06	126.23
24	G	607	CHL	CAC-C3C-C4C	4.08	130.11	124.81
27	G	1622	XAT	C31-C30-C29	-4.08	121.49	127.31
29	g	2630	LHG	O7-C7-C8	4.08	120.29	111.50
24	q	608	CHL	O2D-CGD-CBD	4.08	118.51	111.27
28	S	1623	NEX	C31-C30-C29	-4.07	121.50	127.31
25	b	611	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
36	b	622	LMG	O7-C10-C11	4.07	120.28	111.50
26	9	1621	LUT	C15-C14-C13	-4.07	121.50	127.31
37	c	523	DGD	O2G-C1B-C2B	4.07	120.28	111.50
24	G	606	CHL	CAC-C3C-C4C	4.07	130.09	124.81
24	s	606	CHL	CAC-C3C-C4C	4.07	130.09	124.81
27	6	1622	XAT	C27-C28-C29	-4.07	119.22	125.53
24	S	608	CHL	O2D-CGD-CBD	4.07	118.50	111.27
25	C	503	CLA	C4A-NA-C1A	4.07	108.53	106.71
25	S	614	CLA	C4A-NA-C1A	4.07	108.53	106.71
29	G	2630	LHG	O7-C7-C8	4.06	120.26	111.50
24	r	608	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
25	B	611	CLA	CAA-C2A-C3A	-4.06	101.66	112.78
25	7	602	CLA	C4A-NA-C1A	4.06	108.53	106.71
37	C	523	DGD	O2G-C1B-C2B	4.05	120.24	111.50
27	4	1622	XAT	C11-C10-C9	-4.05	121.53	127.31
24	R	608	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
24	8	601	CHL	C3B-C4B-NB	4.05	114.27	110.52
28	R	623	NEX	C11-C10-C9	-4.05	121.53	127.31
27	9	1622	XAT	C15-C14-C13	-4.05	121.53	127.31
24	p	601	CHL	CHB-C1B-NB	-4.05	119.97	124.26
26	2	1621	LUT	C15-C14-C13	-4.04	121.54	127.31
24	2	609	CHL	C3B-C4B-NB	4.04	114.27	110.52
34	c	517	BCR	C7-C8-C9	-4.04	120.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	607	CHL	CAC-C3C-C4C	4.04	130.05	124.81
27	4	1622	XAT	C15-C14-C13	-4.04	121.55	127.31
34	B	620	BCR	C7-C8-C9	-4.03	120.14	126.23
24	s	607	CHL	CHC-C4B-NB	-4.03	119.99	124.26
27	8	1622	XAT	C15-C14-C13	-4.03	121.55	127.31
25	g	604	CLA	C4A-NA-C1A	4.03	108.52	106.71
34	b	620	BCR	C7-C8-C9	-4.03	120.14	126.23
35	B	623	SQD	O9-S-C6	4.03	111.73	106.94
25	7	614	CLA	C4A-NA-C1A	4.03	108.52	106.71
25	1	604	CLA	C4A-NA-C1A	4.02	108.51	106.71
24	5	609	CHL	CAC-C3C-C4C	4.02	130.02	124.81
34	C	514	BCR	C16-C17-C18	-4.02	121.58	127.31
24	q	606	CHL	CAC-C3C-C4C	4.02	130.02	124.81
24	p	606	CHL	C3C-C4C-NC	4.02	115.08	110.57
26	N	1621	LUT	C35-C34-C33	-4.01	121.58	127.31
24	2	601	CHL	C3B-C4B-NB	4.01	114.24	110.52
24	g	606	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
24	3	607	CHL	O2D-CGD-CBD	4.01	118.39	111.27
24	7	609	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
24	r	607	CHL	CAC-C3C-C4C	4.01	130.01	124.81
24	9	609	CHL	C3B-C4B-NB	4.01	114.23	110.52
27	y	1622	XAT	C31-C30-C29	-4.01	121.59	127.31
28	0	1623	NEX	C39-C29-C30	-4.01	117.31	122.92
24	p	609	CHL	CAC-C3C-C4C	4.00	130.01	124.81
24	S	601	CHL	C3C-C4C-NC	4.00	115.06	110.57
25	s	614	CLA	C4A-NA-C1A	4.00	108.51	106.71
34	c	514	BCR	C16-C17-C18	-4.00	121.60	127.31
34	C	517	BCR	C7-C8-C9	-4.00	120.19	126.23
37	C	520	DGD	O2G-C1B-C2B	4.00	120.13	111.50
25	Y	604	CLA	C4A-NA-C1A	4.00	108.50	106.71
28	n	1623	NEX	C15-C14-C13	-4.00	121.60	127.31
25	s	612	CLA	C4A-NA-C1A	4.00	108.50	106.71
24	3	607	CHL	CHB-C4A-NA	4.00	130.04	124.51
24	2	601	CHL	CHB-C1B-NB	-4.00	120.02	124.26
24	6	608	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
27	q	1622	XAT	C11-C10-C9	-3.99	121.61	127.31
29	n	2630	LHG	O7-C7-C8	3.99	120.10	111.50
25	3	610	CLA	C4A-NA-C1A	3.99	108.50	106.71
24	9	608	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
28	8	1623	NEX	C11-C10-C9	-3.98	121.63	127.31
37	c	520	DGD	O2G-C1B-C2B	3.98	120.08	111.50
27	3	1622	XAT	C15-C14-C13	-3.98	121.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	608	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
24	q	608	CHL	C4A-NA-C1A	3.98	108.50	106.71
25	q	610	CLA	C4A-NA-C1A	3.98	108.50	106.71
24	7	601	CHL	C3C-C4C-NC	3.98	115.03	110.57
27	9	1622	XAT	O4-C5-C18	3.98	119.82	115.06
24	1	609	CHL	CAC-C3C-C4C	3.98	129.97	124.81
29	p	2630	LHG	O7-C7-C8	3.98	120.07	111.50
24	G	607	CHL	O2A-CGA-CBA	3.97	124.38	111.91
24	8	607	CHL	O2D-CGD-CBD	3.97	118.33	111.27
35	b	623	SQD	O9-S-C6	3.97	111.66	106.94
28	Y	1623	NEX	C15-C14-C13	-3.97	121.64	127.31
24	8	607	CHL	CHB-C4A-NA	3.97	130.00	124.51
24	5	606	CHL	CAC-C3C-C4C	3.97	129.96	124.81
24	n	601	CHL	CHD-C4C-C3C	-3.96	119.01	124.84
24	4	605	CHL	CAC-C3C-C4C	3.96	129.95	124.81
24	s	601	CHL	C3C-C4C-NC	3.96	115.02	110.57
25	c	513	CLA	C4A-NA-C1A	3.96	108.49	106.71
24	N	601	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
25	S	612	CLA	C4A-NA-C1A	3.96	108.48	106.71
27	Y	1622	XAT	C31-C30-C29	-3.96	121.66	127.31
24	p	601	CHL	CHD-C4C-C3C	-3.96	119.03	124.84
27	7	1622	XAT	C26-C27-C28	-3.95	117.63	125.99
29	N	2630	LHG	O7-C7-C8	3.95	120.02	111.50
24	4	607	CHL	O2D-CGD-CBD	3.95	118.29	111.27
34	D	404	BCR	C16-C17-C18	-3.95	121.67	127.31
25	s	604	CLA	C4A-NA-C1A	3.95	108.48	106.71
25	s	603	CLA	CAA-C2A-C3A	-3.95	104.39	114.26
34	a	411	BCR	C7-C8-C9	-3.95	120.27	126.23
26	1	1620	LUT	C15-C14-C13	-3.95	121.68	127.31
25	S	603	CLA	CAA-C2A-C3A	-3.94	104.41	114.26
25	1	614	CLA	C4A-NA-C1A	3.94	108.48	106.71
24	1	601	CHL	C3C-C4C-NC	3.94	114.99	110.57
25	b	606	CLA	C4A-NA-C1A	3.94	108.48	106.71
34	d	404	BCR	C16-C17-C18	-3.94	121.69	127.31
29	l	101	LHG	O7-C7-C8	3.93	119.98	111.50
24	p	601	CHL	C3B-C4B-NB	3.93	114.16	110.52
24	2	601	CHL	O2D-CGD-CBD	3.93	118.25	111.27
25	4	610	CLA	C4A-NA-C1A	3.93	108.47	106.71
29	L	101	LHG	O7-C7-C8	3.92	119.96	111.50
34	A	411	BCR	C7-C8-C9	-3.92	120.31	126.23
36	d	412	LMG	O7-C10-C11	3.92	119.95	111.50
27	7	1622	XAT	C35-C34-C33	-3.92	121.72	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	1621	LUT	C35-C34-C33	-3.92	121.72	127.31
26	0	1620	LUT	C15-C14-C13	-3.92	121.72	127.31
36	D	412	LMG	O7-C10-C11	3.91	119.94	111.50
24	g	605	CHL	C3B-C4B-NB	3.91	114.14	110.52
24	2	609	CHL	CHB-C1B-NB	-3.91	120.12	124.26
24	N	609	CHL	OMC-CMC-C2C	-3.91	116.85	125.69
24	9	601	CHL	O2D-CGD-CBD	3.91	118.21	111.27
26	3	1621	LUT	C35-C34-C33	-3.91	121.73	127.31
24	2	606	CHL	CHB-C1B-NB	-3.91	120.12	124.26
25	q	604	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
27	1	1622	XAT	C35-C34-C33	-3.90	121.74	127.31
24	g	607	CHL	O2A-CGA-CBA	3.90	124.13	111.91
27	Y	1622	XAT	O4-C5-C18	3.89	119.72	115.06
27	r	622	XAT	C4-C3-C2	-3.89	103.27	110.77
25	B	615	CLA	C4A-NA-C1A	3.88	108.45	106.71
24	p	609	CHL	C3B-C4B-NB	3.88	114.12	110.52
28	6	1623	NEX	C39-C29-C30	-3.88	117.49	122.92
24	G	601	CHL	C3B-C4B-NB	3.88	114.11	110.52
28	0	1623	NEX	C35-C34-C33	-3.88	121.78	127.31
34	c	514	BCR	C15-C14-C13	-3.88	121.78	127.31
25	B	606	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	y	614	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	4	602	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	S	609	CLA	C4A-NA-C1A	3.87	108.45	106.71
24	4	606	CHL	CAC-C3C-C4C	3.87	129.83	124.81
24	0	601	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
24	g	601	CHL	C3B-C4B-NB	3.87	114.11	110.52
24	4	608	CHL	CAC-C3C-C4C	3.87	129.83	124.81
37	C	519	DGD	O2G-C1B-C2B	3.87	119.84	111.50
27	2	1622	XAT	O4-C5-C18	3.87	119.69	115.06
29	D	408	LHG	O7-C7-C8	3.86	119.83	111.50
26	7	1621	LUT	C15-C14-C13	-3.86	121.80	127.31
26	7	1620	LUT	C15-C14-C13	-3.86	121.80	127.31
37	c	519	DGD	O2G-C1B-C2B	3.86	119.81	111.50
27	R	622	XAT	C4-C3-C2	-3.86	103.33	110.77
28	6	1623	NEX	C15-C14-C13	-3.85	121.81	127.31
28	5	1623	NEX	C35-C34-C33	-3.85	121.81	127.31
24	5	601	CHL	C3B-C4B-NB	3.85	114.09	110.52
24	3	606	CHL	CAC-C3C-C4C	3.85	129.81	124.81
28	3	1623	NEX	C39-C29-C30	-3.85	117.53	122.92
25	y	604	CLA	C4A-NA-C1A	3.85	108.44	106.71
27	1	1622	XAT	C27-C28-C29	-3.85	119.56	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y	1622	XAT	O4-C5-C18	3.85	119.67	115.06
34	C	517	BCR	C15-C14-C13	-3.85	121.82	127.31
24	G	607	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
25	3	604	CLA	C4A-NA-C1A	3.84	108.43	106.71
24	4	609	CHL	C3C-C4C-NC	3.84	114.88	110.57
27	g	1622	XAT	C31-C30-C29	-3.84	121.83	127.31
27	4	1622	XAT	C31-C30-C29	-3.84	121.83	127.31
24	6	606	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
28	Y	1623	NEX	C24-C23-C22	-3.83	103.37	110.77
28	y	1623	NEX	C24-C23-C22	-3.83	103.37	110.77
25	0	612	CLA	C4A-NA-C1A	3.83	108.43	106.71
24	N	607	CHL	CAA-C2A-C3A	-3.83	102.29	112.78
24	R	607	CHL	CHB-C4A-NA	3.83	129.81	124.51
24	8	608	CHL	CHD-C4C-C3C	-3.83	119.22	124.84
25	Y	614	CLA	C4A-NA-C1A	3.83	108.43	106.71
29	d	408	LHG	O7-C7-C8	3.82	119.74	111.50
25	S	604	CLA	C4A-NA-C1A	3.82	108.42	106.71
25	b	615	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	0	607	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
27	8	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
24	g	601	CHL	CMD-C2D-C3D	-3.82	118.83	127.61
28	1	1623	NEX	C27-C28-C29	-3.82	119.61	125.53
26	g	1620	LUT	C35-C34-C33	-3.82	121.86	127.31
24	4	601	CHL	CHB-C1B-NB	-3.82	120.22	124.26
24	3	608	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
24	7	609	CHL	CAC-C3C-C4C	3.81	129.76	124.81
26	7	1621	LUT	C35-C34-C33	-3.81	121.87	127.31
24	9	601	CHL	C3B-C4B-NB	3.81	114.05	110.52
26	y	1621	LUT	C15-C14-C13	-3.81	121.87	127.31
34	C	514	BCR	C15-C14-C13	-3.81	121.87	127.31
34	A	411	BCR	C16-C17-C18	-3.81	121.88	127.31
34	a	411	BCR	C16-C17-C18	-3.81	121.88	127.31
25	8	604	CLA	C4A-NA-C1A	3.81	108.42	106.71
26	0	1621	LUT	C35-C34-C33	-3.81	121.88	127.31
34	c	517	BCR	C15-C14-C13	-3.81	121.88	127.31
28	p	1623	NEX	C11-C10-C9	-3.80	121.88	127.31
24	8	606	CHL	C3C-C4C-NC	3.80	114.84	110.57
26	9	1620	LUT	C7-C8-C9	-3.80	120.49	126.23
24	q	606	CHL	O2D-CGD-CBD	3.80	118.02	111.27
24	9	608	CHL	CHB-C1B-NB	-3.80	120.23	124.26
28	7	1623	NEX	C27-C28-C29	-3.80	119.63	125.53
24	G	605	CHL	C3B-C4B-NB	3.80	114.04	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	1620	LUT	C35-C34-C33	-3.80	121.89	127.31
26	G	1620	LUT	C35-C34-C33	-3.80	121.89	127.31
24	n	608	CHL	CAC-C3C-C4C	3.79	129.73	124.81
27	n	1622	XAT	O4-C5-C18	3.79	119.60	115.06
25	b	613	CLA	CHB-C4A-NA	3.79	129.76	124.51
24	6	609	CHL	CAC-C3C-C4C	3.79	129.73	124.81
24	1	606	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
24	1	609	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
26	y	1620	LUT	C35-C34-C33	-3.79	121.90	127.31
25	g	610	CLA	C4A-NA-C1A	3.79	108.41	106.71
26	0	1620	LUT	C35-C34-C33	-3.79	121.90	127.31
24	r	607	CHL	CHB-C4A-NA	3.79	129.75	124.51
24	8	601	CHL	CHB-C1B-NB	-3.78	120.25	124.26
28	s	1623	NEX	C31-C30-C29	-3.78	121.91	127.31
28	s	1623	NEX	C11-C10-C9	-3.78	121.91	127.31
24	8	606	CHL	CAC-C3C-C4C	3.78	129.72	124.81
26	n	1621	LUT	C15-C14-C13	-3.78	121.92	127.31
24	s	608	CHL	CAC-C3C-C4C	3.78	129.71	124.81
24	g	607	CHL	CHB-C1B-NB	-3.78	120.26	124.26
28	g	1623	NEX	O24-C25-C38	3.78	119.58	115.06
34	B	620	BCR	C33-C5-C6	-3.77	120.29	124.53
27	8	1622	XAT	O24-C25-C38	3.77	119.58	115.06
24	G	607	CHL	CHB-C1B-NB	-3.77	120.27	124.26
24	R	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	3	604	CLA	CMB-C2B-C1B	-3.77	119.63	125.37
24	1	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
34	b	620	BCR	C33-C5-C6	-3.77	120.30	124.53
28	G	1623	NEX	O24-C25-C38	3.76	119.56	115.06
25	3	614	CLA	C4A-NA-C1A	3.76	108.40	106.71
28	G	1623	NEX	C11-C10-C9	-3.76	121.94	127.31
26	Y	1620	LUT	C35-C34-C33	-3.76	121.94	127.31
25	G	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
25	g	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
25	B	613	CLA	CHB-C4A-NA	3.76	129.71	124.51
24	S	608	CHL	CAC-C3C-C4C	3.76	129.69	124.81
25	C	513	CLA	C4A-NA-C1A	3.76	108.39	106.71
24	r	608	CHL	CAC-C3C-C4C	3.76	129.68	124.81
27	5	1622	XAT	C27-C28-C29	-3.75	119.70	125.53
24	0	608	CHL	CHD-C4C-C3C	-3.75	119.32	124.84
26	Y	1621	LUT	C15-C14-C13	-3.75	121.96	127.31
24	0	607	CHL	CAC-C3C-C4C	3.75	129.68	124.81
28	7	1623	NEX	C39-C29-C30	-3.75	117.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	1620	LUT	C15-C14-C13	-3.75	121.96	127.31
25	G	610	CLA	C4A-NA-C1A	3.75	108.39	106.71
26	G	1620	LUT	C15-C14-C13	-3.75	121.96	127.31
25	7	612	CLA	C4A-NA-C1A	3.75	108.39	106.71
24	g	607	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
24	s	606	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	2	610	CLA	C4A-NA-C1A	3.74	108.39	106.71
24	S	606	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	8	610	CLA	C4A-NA-C1A	3.74	108.39	106.71
26	8	1621	LUT	C35-C34-C33	-3.74	121.97	127.31
24	0	607	CHL	C3B-C4B-NB	3.74	113.98	110.52
24	N	608	CHL	CAC-C3C-C4C	3.73	129.66	124.81
24	1	607	CHL	CAC-C3C-C4C	3.73	129.66	124.81
25	Y	604	CLA	CHB-C1B-NB	3.73	128.21	124.26
24	N	606	CHL	CAC-C3C-C4C	3.73	129.65	124.81
24	7	608	CHL	CAC-C3C-C4C	3.73	129.65	124.81
24	q	609	CHL	C3C-C4C-NC	3.73	114.75	110.57
37	c	518	DGD	O2G-C1B-C2B	3.73	119.53	111.50
27	3	1622	XAT	O24-C25-C38	3.73	119.52	115.06
27	6	1622	XAT	C15-C14-C13	-3.73	121.99	127.31
27	4	1622	XAT	C6-C7-C8	-3.72	118.12	125.99
24	1	605	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
27	9	1622	XAT	C11-C10-C9	-3.72	122.00	127.31
34	b	619	BCR	C11-C10-C9	-3.72	122.00	127.31
28	G	1623	NEX	C2-C1-C6	3.72	112.82	109.21
24	4	606	CHL	CHC-C4B-NB	-3.72	120.32	124.26
25	s	609	CLA	C4A-NA-C1A	3.72	108.38	106.71
24	0	605	CHL	CHD-C4C-C3C	-3.72	119.38	124.84
24	q	607	CHL	O2D-CGD-CBD	3.71	117.87	111.27
25	B	604	CLA	C4A-NA-C1A	3.71	108.38	106.71
24	n	605	CHL	C1C-C2C-C3C	-3.71	104.17	107.11
34	A	411	BCR	C15-C14-C13	-3.71	122.01	127.31
25	y	604	CLA	CHB-C1B-NB	3.71	128.19	124.26
24	6	606	CHL	C4-C3-C5	3.71	121.51	115.27
24	2	608	CHL	CHB-C1B-NB	-3.71	120.33	124.26
34	B	619	BCR	C11-C10-C9	-3.71	122.02	127.31
26	8	1621	LUT	C7-C8-C9	-3.70	120.64	126.23
33	A	409	PHO	CMB-C2B-C3B	3.70	131.61	124.68
24	N	605	CHL	CHD-C4C-C3C	-3.70	119.40	124.84
37	C	518	DGD	O2G-C1B-C2B	3.70	119.47	111.50
33	a	409	PHO	CMB-C2B-C3B	3.70	131.60	124.68
27	1	1622	XAT	C11-C10-C9	-3.70	122.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	101	BCR	C16-C17-C18	-3.70	122.04	127.31
34	a	411	BCR	C15-C14-C13	-3.70	122.04	127.31
35	b	621	SQD	O47-C7-C8	3.69	119.46	111.50
34	h	101	BCR	C16-C17-C18	-3.69	122.04	127.31
28	Y	1623	NEX	C39-C29-C30	-3.69	117.75	122.92
28	y	1623	NEX	C39-C29-C30	-3.69	117.75	122.92
24	0	606	CHL	CHC-C4B-NB	-3.69	120.35	124.26
28	y	1623	NEX	C15-C14-C13	-3.69	122.04	127.31
24	0	606	CHL	C4-C3-C5	3.69	121.48	115.27
28	7	1623	NEX	C11-C10-C9	-3.69	122.05	127.31
25	Y	612	CLA	C4A-NA-C1A	3.69	108.36	106.71
25	8	604	CLA	CMB-C2B-C1B	-3.68	119.76	125.37
24	3	606	CHL	C3C-C4C-NC	3.68	114.70	110.57
24	y	607	CHL	C1-O2A-CGA	3.68	126.11	116.44
24	n	607	CHL	CAA-C2A-C3A	-3.68	102.69	112.78
24	Y	601	CHL	CAC-C3C-C4C	3.68	129.59	124.81
27	N	1622	XAT	O4-C5-C18	3.68	119.47	115.06
24	8	608	CHL	CAC-C3C-C4C	3.67	129.58	124.81
24	8	601	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
24	4	609	CHL	CAC-C3C-C4C	3.67	129.57	124.81
25	8	602	CLA	C4A-NA-C1A	3.67	108.35	106.71
24	n	605	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
27	N	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
25	p	610	CLA	C4A-NA-C1A	3.66	108.35	106.71
26	N	1621	LUT	C15-C14-C13	-3.66	122.08	127.31
24	q	606	CHL	CHC-C4B-NB	-3.66	120.38	124.26
35	B	621	SQD	O47-C7-C8	3.66	119.39	111.50
26	S	1621	LUT	C7-C8-C9	-3.66	120.71	126.23
25	0	604	CLA	C4A-NA-C1A	3.66	108.35	106.71
27	2	1622	XAT	C11-C10-C9	-3.66	122.09	127.31
24	5	609	CHL	C3B-C4B-NB	3.66	113.91	110.52
34	C	515	BCR	C24-C23-C22	-3.65	120.72	126.23
34	c	515	BCR	C24-C23-C22	-3.65	120.72	126.23
24	0	606	CHL	CAC-C3C-C4C	3.65	129.55	124.81
25	8	614	CLA	C4A-NA-C1A	3.65	108.35	106.71
25	c	505	CLA	C4A-NA-C1A	3.65	108.35	106.71
27	7	1622	XAT	C11-C10-C9	-3.65	122.10	127.31
27	n	1622	XAT	C11-C10-C9	-3.65	122.10	127.31
27	q	1622	XAT	C31-C30-C29	-3.65	122.10	127.31
35	b	623	SQD	O7-S-C6	3.65	111.27	106.94
24	5	601	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
24	6	601	CHL	C3B-C4B-NB	3.64	113.90	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	0	1623	NEX	O24-C25-C38	3.64	119.42	115.06
24	N	601	CHL	C3B-C4B-NB	3.64	113.89	110.52
27	y	1622	XAT	O24-C25-C38	3.64	119.42	115.06
24	1	601	CHL	CAC-C3C-C4C	3.64	129.53	124.81
24	y	601	CHL	CAC-C3C-C4C	3.64	129.53	124.81
24	7	608	CHL	C3B-C4B-NB	3.64	113.89	110.52
26	7	1620	LUT	C35-C34-C33	-3.63	122.12	127.31
24	S	606	CHL	CMB-C2B-C1B	3.63	130.90	125.37
24	S	601	CHL	CHB-C1B-NB	-3.63	120.41	124.26
28	8	1623	NEX	C15-C14-C13	-3.63	122.13	127.31
26	s	1621	LUT	C7-C8-C9	-3.63	120.75	126.23
25	6	612	CLA	C4A-NA-C1A	3.63	108.34	106.71
27	3	1622	XAT	C26-C27-C28	-3.63	118.32	125.99
24	3	608	CHL	CAC-C3C-C4C	3.63	129.52	124.81
34	B	619	BCR	C33-C5-C6	-3.62	120.46	124.53
24	s	606	CHL	CMB-C2B-C1B	3.62	130.89	125.37
28	6	1623	NEX	C35-C34-C33	-3.62	122.14	127.31
24	2	605	CHL	CAC-C3C-C4C	3.62	129.51	124.81
34	b	618	BCR	C24-C23-C22	-3.62	120.76	126.23
25	q	602	CLA	C4A-NA-C1A	3.62	108.33	106.71
36	c	521	LMG	O7-C10-C11	3.62	119.30	111.50
24	N	605	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
27	N	1622	XAT	C35-C34-C33	-3.62	122.15	127.31
27	Y	1622	XAT	O24-C25-C38	3.62	119.39	115.06
26	4	1620	LUT	C35-C34-C33	-3.62	122.15	127.31
25	y	612	CLA	C4A-NA-C1A	3.61	108.33	106.71
24	7	607	CHL	CAC-C3C-C4C	3.61	129.50	124.81
28	4	1623	NEX	C31-C30-C29	-3.61	122.15	127.31
24	N	601	CHL	CHB-C1B-NB	-3.61	120.43	124.26
25	b	616	CLA	CHC-C4B-NB	3.61	128.08	124.26
25	3	602	CLA	C4A-NA-C1A	3.61	108.33	106.71
34	b	619	BCR	C33-C5-C6	-3.61	120.47	124.53
24	4	609	CHL	CHC-C4B-NB	-3.61	120.44	124.26
24	n	608	CHL	CHB-C1B-NB	-3.60	120.44	124.26
29	6	2630	LHG	O7-C7-C8	3.60	119.27	111.50
34	B	618	BCR	C24-C23-C22	-3.60	120.79	126.23
36	C	521	LMG	O7-C10-C11	3.60	119.27	111.50
28	S	1623	NEX	C11-C10-C9	-3.60	122.17	127.31
24	2	601	CHL	CAC-C3C-C4C	3.60	129.48	124.81
25	p	602	CLA	C4A-NA-C1A	3.60	108.32	106.71
27	r	622	XAT	C15-C14-C13	-3.60	122.17	127.31
28	3	1623	NEX	C15-C14-C13	-3.60	122.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	608	CHL	CHC-C4B-NB	-3.60	120.45	124.26
24	1	601	CHL	C4A-NA-C1A	-3.60	105.09	106.71
25	B	616	CLA	CHC-C4B-NB	3.59	128.06	124.26
28	8	1623	NEX	C39-C29-C30	-3.59	117.89	122.92
24	N	601	CHL	CMD-C2D-C3D	-3.59	119.36	127.61
28	7	1623	NEX	C35-C34-C33	-3.59	122.19	127.31
27	9	1622	XAT	C6-C7-C8	-3.59	118.41	125.99
24	g	608	CHL	CHD-C4C-C3C	-3.59	119.57	124.84
29	0	2630	LHG	O7-C7-C8	3.59	119.23	111.50
24	Y	607	CHL	C1-O2A-CGA	3.59	125.85	116.44
24	3	608	CHL	CHB-C1B-NB	-3.59	120.46	124.26
28	q	1623	NEX	C31-C30-C29	-3.58	122.20	127.31
25	b	604	CLA	C4A-NA-C1A	3.58	108.31	106.71
35	B	623	SQD	O7-S-C6	3.58	111.19	106.94
29	d	409	LHG	O7-C7-C8	3.58	119.21	111.50
24	1	601	CHL	C3B-C4B-NB	3.57	113.83	110.52
24	y	607	CHL	C6-C5-C3	-3.57	104.08	113.45
24	n	606	CHL	CAC-C3C-C4C	3.57	129.44	124.81
27	R	622	XAT	C15-C14-C13	-3.57	122.21	127.31
29	D	409	LHG	O7-C7-C8	3.57	119.19	111.50
24	7	606	CHL	CHB-C1B-NB	-3.57	120.48	124.26
27	9	1622	XAT	C26-C27-C28	-3.57	118.45	125.99
27	2	1622	XAT	C6-C7-C8	-3.57	118.45	125.99
24	9	601	CHL	CAC-C3C-C4C	3.57	129.44	124.81
25	C	510	CLA	CMB-C2B-C1B	-3.57	119.94	125.37
26	5	1621	LUT	C35-C15-C14	-3.57	116.17	123.47
26	3	1620	LUT	C15-C14-C13	-3.57	122.22	127.31
24	N	605	CHL	C3B-C4B-NB	3.56	113.82	110.52
24	r	606	CHL	CAA-C2A-C3A	-3.56	103.02	112.78
24	y	606	CHL	CAA-C2A-C3A	-3.56	103.02	112.78
25	C	502	CLA	CMC-C2C-C1C	-3.56	119.61	125.04
24	7	605	CHL	CHD-C4C-C3C	-3.56	119.60	124.84
24	7	601	CHL	CAC-C3C-C4C	3.56	129.43	124.81
24	2	605	CHL	CHC-C4B-NB	-3.56	120.49	124.26
24	G	601	CHL	CAC-C3C-C4C	3.56	129.43	124.81
24	Y	609	CHL	C3B-C4B-NB	3.56	113.82	110.52
24	7	601	CHL	C3B-C4B-NB	3.56	113.82	110.52
24	Y	607	CHL	C6-C5-C3	-3.56	104.12	113.45
24	R	606	CHL	CAA-C2A-C3A	-3.56	103.03	112.78
26	3	1621	LUT	C7-C8-C9	-3.55	120.86	126.23
24	G	605	CHL	CAC-C3C-C4C	3.55	129.42	124.81
24	S	606	CHL	CHB-C1B-NB	-3.55	120.50	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	502	CLA	CMC-C2C-C1C	-3.55	119.64	125.04
34	b	619	BCR	C24-C23-C22	-3.55	120.88	126.23
34	c	517	BCR	C11-C10-C9	-3.54	122.25	127.31
24	Y	606	CHL	CAA-C2A-C3A	-3.54	103.08	112.78
24	n	601	CHL	CHB-C1B-NB	-3.54	120.51	124.26
24	s	606	CHL	CHB-C1B-NB	-3.54	120.51	124.26
28	9	1623	NEX	C15-C14-C13	-3.53	122.27	127.31
28	1	1623	NEX	O24-C25-C38	3.53	119.29	115.06
28	3	1623	NEX	O24-C25-C38	3.53	119.29	115.06
24	4	608	CHL	CHC-C4B-NB	-3.53	120.52	124.26
24	y	605	CHL	C3B-C4B-NB	3.53	113.79	110.52
24	s	601	CHL	CHB-C1B-NB	-3.53	120.52	124.26
28	9	1623	NEX	C35-C34-C33	-3.53	122.28	127.31
24	n	605	CHL	CHB-C1B-NB	-3.53	120.53	124.26
24	y	609	CHL	C3B-C4B-NB	3.52	113.78	110.52
24	q	608	CHL	CAC-C3C-C4C	3.52	129.38	124.81
24	7	606	CHL	CHC-C4B-NB	-3.52	120.53	124.26
25	1	612	CLA	C4A-NA-C1A	3.52	108.29	106.71
24	7	608	CHL	CHB-C1B-NB	-3.52	120.53	124.26
24	1	609	CHL	CHB-C1B-NB	-3.52	120.53	124.26
24	n	601	CHL	C3B-C4B-NB	3.52	113.78	110.52
25	c	510	CLA	CMB-C2B-C1B	-3.52	120.01	125.37
24	9	605	CHL	CAC-C3C-C4C	3.52	129.38	124.81
24	g	609	CHL	CMD-C2D-C3D	-3.52	119.52	127.61
34	B	619	BCR	C24-C23-C22	-3.52	120.92	126.23
24	0	609	CHL	CHC-C4B-NB	-3.52	120.53	124.26
27	0	1622	XAT	C27-C28-C29	-3.52	120.08	125.53
24	7	606	CHL	CAC-C3C-C4C	3.52	129.37	124.81
26	r	620	LUT	C18-C5-C6	-3.51	120.58	124.53
24	N	608	CHL	CHB-C1B-NB	-3.51	120.54	124.26
24	Y	606	CHL	CHB-C1B-NB	-3.51	120.54	124.26
24	8	608	CHL	CHB-C1B-NB	-3.51	120.54	124.26
34	a	411	BCR	C33-C5-C6	-3.51	120.59	124.53
24	n	607	CHL	CHB-C4A-NA	3.51	129.37	124.51
28	N	1623	NEX	C39-C29-C30	-3.51	118.01	122.92
37	C	523	DGD	O6D-C5D-C6D	3.51	113.75	106.67
24	G	609	CHL	CMD-C2D-C3D	-3.51	119.54	127.61
26	Y	1621	LUT	C35-C34-C33	-3.51	122.30	127.31
24	0	605	CHL	C3B-C4B-NB	3.51	113.77	110.52
34	C	517	BCR	C11-C10-C9	-3.51	122.31	127.31
24	n	605	CHL	C3B-C4B-NB	3.51	113.77	110.52
26	y	1621	LUT	C35-C34-C33	-3.50	122.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	409	PHO	C2D-C1D-ND	-3.50	107.11	109.53
24	4	609	CHL	C4A-NA-C1A	3.50	108.28	106.71
27	N	1622	XAT	C4-C3-C2	-3.50	104.02	110.77
24	g	601	CHL	CAC-C3C-C4C	3.50	129.35	124.81
34	b	618	BCR	C7-C8-C9	-3.50	120.95	126.23
24	g	605	CHL	CAC-C3C-C4C	3.49	129.34	124.81
27	0	1622	XAT	C11-C10-C9	-3.49	122.32	127.31
24	y	606	CHL	CHB-C1B-NB	-3.49	120.56	124.26
34	B	618	BCR	C7-C8-C9	-3.49	120.96	126.23
25	a	410	CLA	CHB-C1B-NB	3.49	127.95	124.26
24	0	606	CHL	CHD-C4C-C3C	-3.49	119.72	124.84
24	7	601	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
37	c	523	DGD	O6D-C5D-C6D	3.48	113.70	106.67
24	2	608	CHL	C3B-C4B-NB	3.48	113.75	110.52
24	9	605	CHL	CHC-C4B-NB	-3.48	120.57	124.26
26	1	1620	LUT	C35-C34-C33	-3.48	122.34	127.31
34	b	618	BCR	C16-C17-C18	-3.48	122.34	127.31
27	5	1622	XAT	C6-C7-C8	-3.48	118.63	125.99
34	A	411	BCR	C33-C5-C6	-3.48	120.62	124.53
26	R	620	LUT	C18-C5-C6	-3.48	120.62	124.53
26	2	1620	LUT	C35-C15-C14	-3.47	116.36	123.47
34	B	618	BCR	C16-C17-C18	-3.47	122.35	127.31
24	6	601	CHL	CHB-C1B-NB	-3.47	120.58	124.26
24	7	609	CHL	CHB-C1B-NB	-3.47	120.58	124.26
24	3	601	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
24	N	607	CHL	CHB-C4A-NA	3.47	129.31	124.51
25	A	410	CLA	CHB-C1B-NB	3.47	127.93	124.26
24	4	601	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
25	5	602	CLA	C4A-NA-C1A	3.46	108.26	106.71
28	R	623	NEX	C15-C14-C13	-3.46	122.37	127.31
24	y	607	CHL	CMB-C2B-C1B	3.46	130.64	125.37
24	n	601	CHL	CMD-C2D-C3D	-3.46	119.66	127.61
34	h	101	BCR	C27-C26-C25	-3.46	117.71	122.73
24	7	601	CHL	C4A-NA-C1A	-3.46	105.15	106.71
28	8	1623	NEX	O24-C25-C38	3.46	119.20	115.06
27	g	1622	XAT	C24-C23-C22	-3.46	104.10	110.77
28	2	1623	NEX	C35-C34-C33	-3.46	122.38	127.31
34	H	101	BCR	C27-C26-C25	-3.45	117.72	122.73
26	2	1620	LUT	C7-C8-C9	-3.45	121.02	126.23
24	Y	605	CHL	C3B-C4B-NB	3.45	113.72	110.52
27	n	1622	XAT	C4-C3-C2	-3.45	104.11	110.77
25	c	507	CLA	O2D-CGD-O1D	-3.45	117.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	607	CHL	CMB-C2B-C1B	3.45	130.62	125.37
33	a	409	PHO	C2D-C1D-ND	-3.44	107.15	109.53
37	c	524	DGD	O2G-C1B-C2B	3.44	118.92	111.50
34	B	618	BCR	C20-C21-C22	-3.44	122.40	127.31
27	G	1622	XAT	C24-C23-C22	-3.44	104.12	110.77
24	q	609	CHL	CHC-C4B-NB	-3.44	120.61	124.26
24	7	606	CHL	CHD-C4C-C3C	-3.44	119.78	124.84
28	1	1623	NEX	C17-C1-C6	-3.44	107.39	110.47
24	2	606	CHL	CAC-C3C-C4C	3.44	129.27	124.81
25	5	610	CLA	C4A-NA-C1A	3.44	108.25	106.71
28	n	1623	NEX	C39-C29-C30	-3.44	118.11	122.92
27	2	1622	XAT	C27-C28-C29	-3.44	120.20	125.53
24	n	608	CHL	C3B-C4B-NB	3.44	113.70	110.52
24	q	609	CHL	CAC-C3C-C4C	3.44	129.27	124.81
34	a	411	BCR	C24-C23-C22	-3.43	121.05	126.23
24	6	606	CHL	CAC-C3C-C4C	3.43	129.26	124.81
37	C	524	DGD	C2G-O2G-C1B	-3.43	109.34	117.79
25	N	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
25	N	613	CLA	CHB-C4A-NA	3.43	129.26	124.51
24	2	606	CHL	CHD-C4C-C3C	-3.43	119.80	124.84
25	n	613	CLA	CHB-C4A-NA	3.43	129.25	124.51
24	p	607	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
27	4	1622	XAT	C35-C34-C33	-3.42	122.42	127.31
34	A	411	BCR	C24-C23-C22	-3.42	121.06	126.23
34	h	101	BCR	C24-C23-C22	-3.42	121.06	126.23
24	p	608	CHL	CAC-C3C-C4C	3.42	129.25	124.81
26	R	620	LUT	C35-C34-C33	-3.42	122.43	127.31
24	0	609	CHL	CAC-C3C-C4C	3.42	129.25	124.81
25	n	603	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
25	2	614	CLA	C4A-NA-C1A	3.42	108.24	106.71
26	1	1621	LUT	C35-C34-C33	-3.42	122.44	127.31
34	b	618	BCR	C20-C21-C22	-3.42	122.44	127.31
24	q	609	CHL	C1D-CHD-C4C	-3.41	118.69	126.06
34	H	101	BCR	C24-C23-C22	-3.41	121.08	126.23
34	b	619	BCR	C7-C8-C9	-3.41	121.09	126.23
28	8	1623	NEX	C24-C23-C22	-3.41	104.20	110.77
25	C	505	CLA	C4A-NA-C1A	3.41	108.24	106.71
24	1	601	CHL	C1C-C2C-C3C	-3.40	104.41	107.11
24	G	609	CHL	CHB-C1B-NB	-3.40	120.65	124.26
27	G	1622	XAT	C4-C3-C2	-3.40	104.20	110.77
37	C	524	DGD	O2G-C1B-C2B	3.40	118.83	111.50
24	n	609	CHL	C3B-C4B-NB	3.40	113.67	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	524	DGD	C2G-O2G-C1B	-3.40	109.42	117.79
24	r	607	CHL	C3B-C4B-NB	3.40	113.67	110.52
24	6	606	CHL	CHC-C4B-NB	-3.40	120.66	124.26
26	6	1621	LUT	C15-C14-C13	-3.40	122.46	127.31
24	7	607	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
26	r	620	LUT	C35-C34-C33	-3.40	122.46	127.31
24	Y	607	CHL	CAC-C3C-C4C	3.40	129.22	124.81
24	y	606	CHL	CMB-C2B-C1B	3.39	130.54	125.37
28	6	1623	NEX	C11-C10-C9	-3.39	122.47	127.31
24	1	608	CHL	CHB-C1B-NB	-3.39	120.67	124.26
26	n	1620	LUT	C35-C34-C33	-3.39	122.47	127.31
27	g	1622	XAT	C15-C14-C13	-3.39	122.47	127.31
24	p	608	CHL	C3B-C4B-NB	3.39	113.66	110.52
28	4	1623	NEX	C26-C27-C28	-3.39	118.83	125.99
28	G	1623	NEX	C39-C29-C30	-3.39	118.18	122.92
24	9	608	CHL	C3B-C4B-NB	3.39	113.66	110.52
34	B	619	BCR	C7-C8-C9	-3.39	121.12	126.23
37	c	519	DGD	C3G-O3G-C1D	-3.39	107.12	113.74
25	0	610	CLA	C4A-NA-C1A	3.39	108.23	106.71
25	5	613	CLA	CHB-C4A-NA	3.38	129.19	124.51
24	3	601	CHL	CMB-C2B-C1B	3.38	130.52	125.37
27	N	1622	XAT	C15-C35-C34	-3.38	116.54	123.47
24	7	601	CHL	C1C-C2C-C3C	-3.38	104.43	107.11
25	N	603	CLA	CAA-C2A-C3A	-3.38	103.52	112.78
24	4	609	CHL	C1D-CHD-C4C	-3.38	118.76	126.06
24	g	606	CHL	C3B-C4B-NB	3.38	113.65	110.52
24	q	601	CHL	CAC-C3C-C4C	3.38	129.20	124.81
28	3	1623	NEX	C24-C23-C22	-3.38	104.25	110.77
24	Y	605	CHL	CHB-C1B-NB	-3.38	120.68	124.26
24	s	601	CHL	CHC-C4B-NB	-3.38	120.68	124.26
24	r	607	CHL	CHB-C1B-NB	-3.38	120.68	124.26
24	n	608	CHL	CMB-C2B-C1B	3.38	130.51	125.37
24	6	608	CHL	CHB-C1B-NB	-3.38	120.68	124.26
24	N	606	CHL	CHC-C4B-NB	-3.37	120.69	124.26
24	q	607	CHL	CHC-C4B-NB	-3.37	120.69	124.26
25	C	513	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
28	5	1623	NEX	O24-C25-C38	3.37	119.09	115.06
25	9	614	CLA	C4A-NA-C1A	3.37	108.22	106.71
27	1	1622	XAT	C31-C30-C29	-3.37	122.50	127.31
33	a	408	PHO	C2D-C1D-ND	-3.37	107.20	109.53
24	6	607	CHL	CHD-C4C-C3C	-3.37	119.89	124.84
26	q	1620	LUT	C31-C30-C29	-3.36	122.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	514	BCR	C20-C21-C22	-3.36	122.51	127.31
24	1	609	CHL	C3B-C4B-NB	3.36	113.63	110.52
24	Y	601	CHL	CMB-C2B-C1B	3.36	130.49	125.37
24	g	601	CHL	CHD-C4C-C3C	-3.36	119.90	124.84
26	q	1620	LUT	C35-C34-C33	-3.36	122.52	127.31
25	4	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
25	q	613	CLA	CHB-C4A-NA	3.36	129.16	124.51
24	G	601	CHL	CHD-C4C-C3C	-3.36	119.90	124.84
25	B	610	CLA	CMB-C2B-C1B	-3.36	120.26	125.37
24	4	601	CHL	CAC-C3C-C4C	3.36	129.16	124.81
34	D	404	BCR	C33-C5-C6	-3.36	120.76	124.53
24	1	601	CHL	CHD-C4C-C3C	-3.36	119.91	124.84
34	c	516	BCR	C20-C21-C22	-3.35	122.52	127.31
24	G	606	CHL	C3B-C4B-NB	3.35	113.63	110.52
24	q	601	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
28	0	1623	NEX	C15-C14-C13	-3.35	122.53	127.31
24	9	606	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
24	y	601	CHL	CMB-C2B-C1B	3.35	130.47	125.37
24	r	606	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
24	y	607	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	R	607	CHL	C3B-C4B-NB	3.35	113.62	110.52
24	R	606	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
24	S	608	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
24	Y	606	CHL	CMB-C2B-C1B	3.35	130.47	125.37
25	r	601	CLA	CHB-C4A-NA	3.35	129.14	124.51
26	N	1620	LUT	C35-C34-C33	-3.35	122.53	127.31
24	N	601	CHL	C1C-C2C-C3C	-3.35	104.46	107.11
27	g	1622	XAT	C4-C3-C2	-3.35	104.31	110.77
34	B	620	BCR	C20-C21-C22	-3.35	122.53	127.31
24	1	607	CHL	CHD-C4C-C3C	-3.34	119.92	124.84
24	Y	601	CHL	CHD-C4C-C3C	-3.34	119.93	124.84
27	y	1622	XAT	C4-C3-C2	-3.34	104.32	110.77
25	b	617	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
24	3	601	CHL	C1C-C2C-C3C	-3.34	104.46	107.11
24	N	607	CHL	CAC-C3C-C4C	3.34	129.15	124.81
25	5	612	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
24	S	601	CHL	CHC-C4B-NB	-3.34	120.72	124.26
39	D	405	PL9	C7-C8-C9	-3.34	121.24	126.79
27	Y	1622	XAT	C4-C3-C2	-3.34	104.33	110.77
26	1	1621	LUT	C15-C14-C13	-3.33	122.55	127.31
25	7	604	CLA	C4A-NA-C1A	3.33	108.20	106.71
27	R	622	XAT	C24-C23-C22	-3.33	104.33	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	610	CLA	CMB-C2B-C1B	-3.33	120.29	125.37
28	p	1623	NEX	C35-C34-C33	-3.33	122.55	127.31
28	r	623	NEX	C15-C14-C13	-3.33	122.55	127.31
24	R	607	CHL	CHB-C1B-NB	-3.33	120.73	124.26
24	5	606	CHL	CHC-C4B-NB	-3.33	120.73	124.26
25	N	602	CLA	C4A-NA-C1A	3.33	108.20	106.71
24	n	601	CHL	C1C-C2C-C3C	-3.33	104.47	107.11
28	Y	1623	NEX	C28-C29-C30	3.33	124.05	118.94
24	G	608	CHL	CHD-C4C-C3C	-3.33	119.95	124.84
24	9	608	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	0	1621	LUT	C15-C14-C13	-3.33	122.56	127.31
25	1	610	CLA	C4A-NA-C1A	3.33	108.20	106.71
34	d	404	BCR	C33-C5-C6	-3.33	120.79	124.53
24	n	606	CHL	CHC-C4B-NB	-3.33	120.73	124.26
34	C	516	BCR	C20-C21-C22	-3.33	122.56	127.31
25	r	603	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
24	1	606	CHL	CHB-C1B-NB	-3.32	120.74	124.26
25	7	610	CLA	C4A-NA-C1A	3.32	108.20	106.71
25	R	601	CLA	CHB-C4A-NA	3.32	129.10	124.51
25	R	603	CLA	CAA-C2A-C3A	-3.32	103.68	112.78
34	c	514	BCR	C20-C21-C22	-3.32	122.57	127.31
24	3	605	CHL	CAC-C3C-C4C	3.32	129.12	124.81
24	6	605	CHL	C3B-C4B-NB	3.32	113.59	110.52
24	y	609	CHL	CHB-C4A-NA	3.32	129.10	124.51
24	s	601	CHL	C4A-NA-C1A	-3.32	105.22	106.71
27	r	622	XAT	C24-C23-C22	-3.32	104.37	110.77
24	N	608	CHL	CMB-C2B-C1B	3.32	130.42	125.37
24	2	609	CHL	CAC-C3C-C4C	3.31	129.11	124.81
27	q	1622	XAT	C35-C34-C33	-3.31	122.58	127.31
24	g	608	CHL	CAC-C3C-C4C	3.31	129.11	124.81
33	A	408	PHO	C2D-C1D-ND	-3.31	107.24	109.53
24	8	605	CHL	CAC-C3C-C4C	3.31	129.11	124.81
27	p	1622	XAT	C11-C10-C9	-3.31	122.58	127.31
34	b	620	BCR	C20-C21-C22	-3.31	122.58	127.31
25	B	617	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
24	s	608	CHL	CHD-C4C-C3C	-3.31	119.98	124.84
27	5	1622	XAT	C11-C10-C9	-3.31	122.59	127.31
24	p	607	CHL	CHB-C1B-NB	-3.31	120.76	124.26
25	c	513	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
25	0	614	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
24	y	605	CHL	CHB-C1B-NB	-3.30	120.76	124.26
27	4	1622	XAT	C4-C3-C2	-3.30	104.41	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	614	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	s	612	CLA	CHB-C1B-NB	3.29	127.74	124.26
25	c	512	CLA	CHB-C4A-NA	3.29	129.07	124.51
27	1	1622	XAT	C26-C27-C28	-3.29	119.03	125.99
24	g	601	CHL	CHC-C4B-NB	-3.29	120.77	124.26
24	p	601	CHL	CHB-C4A-NA	3.29	129.06	124.51
28	g	1623	NEX	C39-C29-C30	-3.29	118.31	122.92
25	7	614	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
28	y	1623	NEX	C28-C29-C30	3.29	123.99	118.94
24	6	609	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
24	G	608	CHL	CAC-C3C-C4C	3.29	129.08	124.81
25	B	614	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
28	Y	1623	NEX	C26-C27-C28	-3.29	119.05	125.99
34	B	620	BCR	C16-C17-C18	-3.28	122.62	127.31
24	6	608	CHL	CAC-C3C-C4C	3.28	129.07	124.81
24	g	605	CHL	CHD-C4C-C3C	-3.28	120.01	124.84
28	3	1623	NEX	C11-C10-C9	-3.28	122.63	127.31
29	8	2630	LHG	O7-C7-C8	3.28	118.57	111.50
25	s	612	CLA	CHB-C4A-NA	3.28	129.05	124.51
24	G	601	CHL	CHC-C4B-NB	-3.28	120.78	124.26
24	6	605	CHL	CHC-C4B-NB	-3.28	120.78	124.26
24	s	601	CHL	CMD-C2D-C3D	-3.28	120.07	127.61
24	N	608	CHL	C3B-C4B-NB	3.28	113.56	110.52
25	b	614	CLA	CMB-C2B-C1B	-3.28	120.38	125.37
25	1	604	CLA	CHC-C4B-NB	3.28	127.73	124.26
24	y	601	CHL	CHD-C4C-C3C	-3.28	120.02	124.84
25	4	610	CLA	C1-C2-C3	-3.28	120.38	126.04
24	0	607	CHL	CHB-C1B-NB	-3.28	120.79	124.26
28	7	1623	NEX	C2-C1-C6	3.27	112.39	109.21
26	s	1621	LUT	C11-C10-C9	-3.27	122.64	127.31
39	d	405	PL9	C7-C8-C9	-3.27	121.34	126.79
28	2	1623	NEX	C39-C29-C30	-3.27	118.34	122.92
25	d	402	CLA	CAC-C3C-C4C	3.27	129.05	124.81
28	2	1623	NEX	C27-C28-C29	-3.27	120.46	125.53
24	Y	608	CHL	CHB-C1B-NB	-3.27	120.80	124.26
26	8	1620	LUT	C15-C14-C13	-3.27	122.65	127.31
25	3	603	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
24	n	607	CHL	CAC-C3C-C4C	3.27	129.05	124.81
26	9	1621	LUT	C22-C23-C24	-3.27	108.02	111.74
25	S	612	CLA	CHB-C4A-NA	3.27	129.03	124.51
24	8	605	CHL	CHC-C4B-NB	-3.27	120.80	124.26
25	y	604	CLA	CHC-C4B-NB	3.27	127.71	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	519	DGD	C3G-O3G-C1D	-3.27	107.36	113.74
27	G	1622	XAT	C15-C14-C13	-3.26	122.65	127.31
24	y	601	CHL	CHC-C4B-NB	-3.26	120.80	124.26
27	9	1622	XAT	C35-C34-C33	-3.26	122.66	127.31
25	n	610	CLA	C4A-NA-C1A	3.26	108.17	106.71
24	g	609	CHL	CHB-C1B-NB	-3.26	120.81	124.26
25	8	603	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
26	S	1621	LUT	C11-C10-C9	-3.26	122.66	127.31
24	G	601	CHL	CHB-C4A-NA	3.26	129.02	124.51
34	b	620	BCR	C16-C17-C18	-3.26	122.66	127.31
24	R	608	CHL	C2A-C3A-C4A	-3.26	96.61	101.87
25	4	612	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
26	4	1621	LUT	C10-C11-C12	-3.25	113.06	123.22
24	N	609	CHL	C3B-C4B-NB	3.25	113.53	110.52
25	c	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	n	602	CLA	C4A-NA-C1A	3.25	108.17	106.71
24	S	606	CHL	C3B-C4B-NB	3.25	113.53	110.52
24	7	609	CHL	C3B-C4B-NB	3.25	113.53	110.52
24	9	607	CHL	CHD-C4C-C3C	-3.25	120.06	124.84
25	C	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	q	603	CLA	CHB-C4A-NA	3.25	129.00	124.51
24	s	606	CHL	C3B-C4B-NB	3.25	113.53	110.52
24	0	606	CHL	CMD-C2D-C3D	-3.25	120.14	127.61
24	Y	601	CHL	CHC-C4B-NB	-3.25	120.82	124.26
24	2	607	CHL	CHD-C4C-C3C	-3.25	120.07	124.84
28	y	1623	NEX	C26-C27-C28	-3.24	119.13	125.99
29	3	2630	LHG	O7-C7-C8	3.24	118.49	111.50
26	2	1621	LUT	C22-C23-C24	-3.24	108.05	111.74
24	Y	605	CHL	CMB-C2B-C1B	3.24	130.31	125.37
28	p	1623	NEX	O24-C25-C38	3.24	118.94	115.06
24	9	606	CHL	CAC-C3C-C4C	3.24	129.01	124.81
24	n	605	CHL	CGD-CBD-CAD	-3.24	100.25	110.73
25	D	402	CLA	CAC-C3C-C4C	3.24	129.01	124.81
25	p	612	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
24	5	605	CHL	CHD-C4C-C3C	-3.24	120.08	124.84
27	n	1622	XAT	C26-C27-C28	-3.24	119.15	125.99
24	3	605	CHL	CHC-C4B-NB	-3.24	120.83	124.26
24	p	601	CHL	CAC-C3C-C4C	3.23	129.01	124.81
28	7	1623	NEX	C24-C23-C22	-3.23	104.53	110.77
24	g	601	CHL	CHB-C4A-NA	3.23	128.98	124.51
27	2	1622	XAT	C35-C34-C33	-3.23	122.70	127.31
28	p	1623	NEX	C31-C30-C29	-3.23	122.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	619	BCR	C16-C17-C18	-3.23	122.70	127.31
24	r	608	CHL	C2A-C3A-C4A	-3.23	96.65	101.87
24	1	608	CHL	C3B-C4B-NB	3.23	113.51	110.52
25	b	604	CLA	CHB-C1B-NB	3.23	127.67	124.26
24	y	605	CHL	CMB-C2B-C1B	3.23	130.29	125.37
34	d	404	BCR	C28-C27-C26	-3.23	108.31	114.08
24	3	609	CHL	CAC-C3C-C4C	3.23	129.00	124.81
27	7	1622	XAT	C36-C21-C26	3.23	118.76	110.05
24	5	608	CHL	C3B-C4B-NB	3.23	113.51	110.52
25	S	612	CLA	CHB-C1B-NB	3.23	127.67	124.26
28	r	623	NEX	O24-C25-C38	3.22	118.92	115.06
24	2	608	CHL	CAC-C3C-C4C	3.22	128.99	124.81
26	p	1620	LUT	C7-C8-C9	-3.22	121.36	126.23
25	g	610	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
24	3	607	CHL	C3B-C4B-NB	3.22	113.50	110.52
24	6	605	CHL	CHD-C4C-C3C	-3.22	120.11	124.84
34	D	404	BCR	C28-C27-C26	-3.22	108.33	114.08
28	s	1623	NEX	C17-C1-C6	-3.22	107.59	110.47
26	2	1620	LUT	C11-C10-C9	-3.22	122.72	127.31
33	A	409	PHO	O2D-CGD-O1D	-3.22	117.55	123.84
29	L	101	LHG	O8-C23-C24	3.21	122.00	111.91
25	G	610	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
24	3	606	CHL	CHC-C4B-NB	-3.21	120.86	124.26
25	1	614	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	3	613	CLA	CHB-C4A-NA	3.21	128.95	124.51
27	G	1622	XAT	C27-C28-C29	-3.21	120.55	125.53
25	2	613	CLA	CHB-C4A-NA	3.21	128.95	124.51
25	C	512	CLA	CHB-C4A-NA	3.21	128.95	124.51
27	2	1622	XAT	C26-C27-C28	-3.21	119.20	125.99
24	8	606	CHL	CHC-C4B-NB	-3.21	120.86	124.26
24	3	606	CHL	CMD-C2D-C3D	-3.21	120.23	127.61
25	B	609	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
29	l	101	LHG	O8-C23-C24	3.21	121.97	111.91
24	Y	609	CHL	CHB-C4A-NA	3.20	128.94	124.51
24	G	609	CHL	O2A-CGA-CBA	3.20	121.96	111.91
25	C	507	CLA	CHB-C4A-NA	3.20	128.94	124.51
28	R	623	NEX	O24-C25-C38	3.20	118.89	115.06
28	3	1623	NEX	C35-C34-C33	-3.20	122.74	127.31
33	a	409	PHO	O2D-CGD-O1D	-3.20	117.58	123.84
25	b	609	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
28	q	1623	NEX	C26-C27-C28	-3.20	119.23	125.99
27	5	1622	XAT	C35-C34-C33	-3.20	122.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	1622	XAT	C31-C30-C29	-3.20	122.75	127.31
24	9	609	CHL	CAC-C3C-C4C	3.20	128.96	124.81
24	G	605	CHL	CHD-C4C-C3C	-3.20	120.14	124.84
34	C	514	BCR	C7-C8-C9	-3.20	121.41	126.23
24	6	605	CHL	CAC-C3C-C4C	3.20	128.96	124.81
27	g	1622	XAT	C27-C28-C29	-3.20	120.57	125.53
27	p	1622	XAT	C35-C34-C33	-3.20	122.75	127.31
24	0	606	CHL	CHB-C1B-NB	-3.19	120.88	124.26
25	Y	604	CLA	CHC-C4B-NB	3.19	127.64	124.26
24	1	607	CHL	OMC-CMC-C2C	-3.19	118.47	125.69
24	p	608	CHL	CHB-C1B-NB	-3.19	120.88	124.26
24	9	601	CHL	CMD-C2D-C3D	-3.19	120.27	127.61
24	8	601	CHL	CAC-C3C-C4C	3.19	128.95	124.81
27	5	1622	XAT	C4-C3-C2	-3.19	104.61	110.77
34	B	618	BCR	C29-C30-C25	3.19	115.39	110.48
34	c	514	BCR	C7-C8-C9	-3.19	121.42	126.23
36	c	521	LMG	C7-O1-C1	-3.19	107.51	113.74
27	3	1622	XAT	C35-C34-C33	-3.19	122.76	127.31
34	B	619	BCR	C16-C17-C18	-3.19	122.76	127.31
25	g	614	CLA	C4A-NA-C1A	3.19	108.14	106.71
34	b	618	BCR	C29-C30-C25	3.18	115.38	110.48
24	2	601	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
24	p	601	CHL	CMB-C2B-C1B	3.18	130.22	125.37
24	p	605	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
24	4	607	CHL	CHC-C4B-NB	-3.18	120.89	124.26
28	7	1623	NEX	C26-C27-C28	-3.18	119.27	125.99
25	Y	612	CLA	CHB-C1B-NB	3.18	127.62	124.26
25	S	612	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
28	1	1623	NEX	C11-C12-C13	-3.18	117.49	126.42
24	g	609	CHL	O2A-CGA-CBA	3.18	121.88	111.91
29	C	2630	LHG	O7-C7-C8	3.18	118.34	111.50
24	s	608	CHL	O2A-CGA-CBA	3.17	121.87	111.91
24	8	606	CHL	CMD-C2D-C3D	-3.17	120.31	127.61
27	8	1622	XAT	C35-C34-C33	-3.17	122.78	127.31
26	0	1621	LUT	C7-C8-C9	-3.17	121.44	126.23
25	y	604	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
36	C	521	LMG	C7-O1-C1	-3.17	107.55	113.74
24	n	605	CHL	CMD-C2D-C3D	-3.17	120.33	127.61
24	G	601	CHL	CMB-C2B-C1B	3.17	130.19	125.37
25	0	612	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
34	c	517	BCR	C15-C16-C17	-3.17	116.99	123.47
25	q	602	CLA	O2D-CGD-O1D	-3.17	117.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	509	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
25	Y	604	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	N	612	CLA	CHB-C4A-NA	3.17	128.89	124.51
24	s	607	CHL	CAC-C3C-C4C	3.16	128.92	124.81
25	8	613	CLA	CHB-C4A-NA	3.16	128.89	124.51
26	4	1620	LUT	C15-C14-C13	-3.16	122.80	127.31
25	y	612	CLA	CHB-C1B-NB	3.16	127.61	124.26
24	8	607	CHL	C3B-C4B-NB	3.16	113.45	110.52
25	9	613	CLA	CHB-C4A-NA	3.16	128.88	124.51
25	s	612	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
34	C	515	BCR	C15-C16-C17	-3.16	117.00	123.47
24	q	606	CHL	O2A-CGA-CBA	3.16	121.82	111.91
24	1	606	CHL	CAC-C3C-C4C	3.16	128.91	124.81
27	7	1622	XAT	C31-C30-C29	-3.16	122.80	127.31
25	B	617	CLA	CHB-C4A-NA	3.16	128.88	124.51
27	n	1622	XAT	C15-C35-C34	-3.16	117.01	123.47
25	y	612	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
25	G	614	CLA	C4A-NA-C1A	3.16	108.12	106.71
24	9	607	CHL	CAC-C3C-C4C	3.15	128.90	124.81
25	s	605	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
27	6	1622	XAT	C15-C35-C34	-3.15	117.01	123.47
34	c	515	BCR	C15-C16-C17	-3.15	117.02	123.47
24	S	601	CHL	C4A-NA-C1A	-3.15	105.29	106.71
24	N	605	CHL	CMB-C2B-C1B	3.15	130.17	125.37
24	6	607	CHL	CMB-C2B-C1B	3.15	130.17	125.37
25	S	614	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	s	614	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
24	3	601	CHL	CAC-C3C-C4C	3.15	128.90	124.81
25	g	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
25	Y	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
25	a	405	CLA	CMB-C2B-C1B	-3.15	120.58	125.37
25	G	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
27	1	1622	XAT	C36-C21-C26	3.15	118.54	110.05
25	b	617	CLA	CHB-C4A-NA	3.15	128.86	124.51
24	1	606	CHL	OMC-CMC-C2C	-3.14	118.58	125.69
27	0	1622	XAT	C6-C7-C8	-3.14	119.35	125.99
28	y	1623	NEX	C11-C10-C9	-3.14	122.83	127.31
24	g	601	CHL	CMB-C2B-C1B	3.14	130.16	125.37
27	p	1622	XAT	C6-C7-C8	-3.14	119.35	125.99
25	c	507	CLA	CHB-C4A-NA	3.14	128.86	124.51
25	c	502	CLA	CHB-C4A-NA	3.14	128.85	124.51
24	S	608	CHL	O2A-CGA-CBA	3.14	121.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	612	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	G	611	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
36	h	102	LMG	O8-C28-C29	3.14	121.75	111.91
34	b	619	BCR	C33-C5-C4	3.14	119.64	113.62
24	8	601	CHL	CHB-C4A-NA	3.13	128.85	124.51
25	3	611	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
26	s	1621	LUT	C18-C5-C6	-3.13	121.01	124.53
24	5	601	CHL	CAC-C3C-C4C	3.13	128.88	124.81
24	S	607	CHL	CAC-C3C-C4C	3.13	128.88	124.81
24	5	606	CHL	CHD-C4C-C3C	-3.13	120.24	124.84
25	C	509	CLA	CAA-C2A-C3A	-3.13	104.21	112.78
24	5	608	CHL	CAC-C3C-C4C	3.13	128.87	124.81
28	G	1623	NEX	C19-C9-C10	-3.13	118.54	122.92
34	C	517	BCR	C15-C16-C17	-3.13	117.07	123.47
24	R	606	CHL	O2A-CGA-CBA	3.13	121.72	111.91
26	Y	1621	LUT	C7-C8-C9	-3.13	121.51	126.23
24	n	605	CHL	O2A-CGA-CBA	3.13	121.72	111.91
28	7	1623	NEX	C11-C12-C13	-3.13	117.64	126.42
24	R	608	CHL	C3B-C4B-NB	3.12	113.41	110.52
25	6	604	CLA	CHC-C4B-NB	3.12	127.56	124.26
24	N	601	CHL	CHB-C4A-NA	3.12	128.83	124.51
27	N	1622	XAT	O24-C25-C38	3.12	118.80	115.06
24	r	606	CHL	O2A-CGA-CBA	3.12	121.71	111.91
24	1	606	CHL	CHC-C4B-NB	-3.12	120.95	124.26
25	8	613	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
34	B	619	BCR	C33-C5-C4	3.12	119.61	113.62
24	g	609	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
24	N	605	CHL	CGD-CBD-CAD	-3.12	100.63	110.73
24	G	609	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
25	g	611	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
25	B	604	CLA	CHB-C1B-NB	3.12	127.56	124.26
24	p	607	CHL	C4A-NA-C1A	-3.12	105.30	106.71
24	S	608	CHL	C3B-C4B-NB	3.12	113.41	110.52
25	A	405	CLA	CHB-C1B-NB	3.12	127.56	124.26
36	H	102	LMG	O8-C28-C29	3.12	121.69	111.91
24	3	609	CHL	C3B-C4B-NB	3.12	113.41	110.52
24	S	601	CHL	OMC-CMC-C2C	-3.12	118.64	125.69
26	S	1621	LUT	C18-C5-C6	-3.12	121.03	124.53
24	4	606	CHL	O2A-CGA-CBA	3.11	121.68	111.91
25	B	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	b	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	9	612	CLA	CHB-C4A-NA	3.11	128.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	519	DGD	C2G-O2G-C1B	-3.11	110.13	117.79
24	n	601	CHL	CAC-C3C-C4C	3.11	128.85	124.81
24	0	608	CHL	CAC-C3C-C4C	3.11	128.85	124.81
25	n	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
27	3	1622	XAT	C27-C28-C29	-3.11	120.71	125.53
25	y	603	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
24	p	607	CHL	C3B-C4B-NB	3.11	113.40	110.52
24	9	601	CHL	CMB-C2B-C1B	3.11	130.10	125.37
25	A	405	CLA	CMB-C2B-C1B	-3.11	120.64	125.37
24	2	601	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
24	S	601	CHL	CHD-C4C-C3C	-3.11	120.28	124.84
25	3	613	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
34	h	101	BCR	C20-C21-C22	-3.10	122.88	127.31
25	C	502	CLA	CHB-C4A-NA	3.10	128.81	124.51
27	N	1622	XAT	C18-C5-C4	3.10	117.77	114.28
26	y	1621	LUT	C7-C8-C9	-3.10	121.55	126.23
24	N	607	CHL	CMD-C2D-C3D	-3.10	120.48	127.61
24	s	608	CHL	C3B-C4B-NB	3.10	113.39	110.52
26	3	1621	LUT	C15-C14-C13	-3.10	122.88	127.31
25	C	507	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
24	7	607	CHL	OMC-CMC-C2C	-3.10	118.67	125.69
24	R	608	CHL	C4A-NA-C1A	-3.10	105.31	106.71
24	5	607	CHL	CHB-C1B-NB	-3.10	120.98	124.26
25	p	610	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	G	609	CHL	C3B-C4B-NB	3.10	113.39	110.52
24	g	608	CHL	C3B-C4B-NB	3.10	113.39	110.52
24	6	608	CHL	O2A-CGA-CBA	3.10	121.63	111.91
26	6	1621	LUT	C31-C30-C29	-3.10	122.89	127.31
35	A	412	SQD	O8-S-O7	3.10	118.84	111.27
25	r	610	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	8	605	CHL	O2A-CGA-CBA	3.09	121.61	111.91
25	9	614	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	y	608	CHL	CHB-C1B-NB	-3.09	120.98	124.26
24	r	608	CHL	C3B-C4B-NB	3.09	113.38	110.52
24	q	601	CHL	CHB-C1B-NB	-3.09	120.99	124.26
24	8	601	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
34	H	101	BCR	C20-C21-C22	-3.09	122.90	127.31
25	S	610	CLA	CHB-C1B-NB	3.09	127.53	124.26
26	1	1620	LUT	C21-C26-C27	-3.09	108.80	112.70
24	8	601	CHL	CMB-C2B-C1B	3.09	130.07	125.37
25	B	616	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
25	Y	610	CLA	O2D-CGD-O1D	-3.08	117.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	408	PHO	CMB-C2B-C3B	3.08	130.45	124.68
25	p	603	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
26	7	1620	LUT	C21-C26-C27	-3.08	108.80	112.70
24	y	601	CHL	C4-C3-C5	3.08	120.46	115.27
27	3	1622	XAT	C31-C30-C29	-3.08	122.91	127.31
25	Y	603	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
33	a	408	PHO	CMB-C2B-C3B	3.08	130.44	124.68
24	8	609	CHL	C3B-C4B-NB	3.08	113.37	110.52
26	y	1621	LUT	C22-C23-C24	-3.08	108.23	111.74
37	C	519	DGD	C2G-O2G-C1B	-3.08	110.21	117.79
25	c	509	CLA	CHB-C4A-NA	3.08	128.77	124.51
29	c	2630	LHG	O7-C7-C8	3.08	118.14	111.50
24	g	609	CHL	C3B-C4B-NB	3.08	113.37	110.52
26	1	1621	LUT	C22-C23-C24	-3.08	108.24	111.74
24	Y	608	CHL	CHC-C4B-NB	-3.08	121.00	124.26
24	S	601	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
27	0	1622	XAT	C15-C14-C13	-3.08	122.92	127.31
25	c	513	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
34	B	618	BCR	C27-C26-C25	-3.08	118.27	122.73
26	s	1620	LUT	C35-C34-C33	-3.08	122.92	127.31
25	S	605	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
34	c	514	BCR	C11-C10-C9	-3.07	122.92	127.31
25	b	616	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	5	609	CHL	CMD-C2D-C3D	-3.07	120.54	127.61
25	R	610	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	a	405	CLA	CHB-C1B-NB	3.07	127.51	124.26
25	8	612	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
25	A	406	CLA	C4A-NA-C1A	3.07	108.09	106.71
25	a	406	CLA	C4A-NA-C1A	3.07	108.09	106.71
28	0	1623	NEX	C11-C10-C9	-3.07	122.93	127.31
25	p	612	CLA	CHB-C4A-NA	3.07	128.76	124.51
25	6	610	CLA	C4A-NA-C1A	3.07	108.09	106.71
25	8	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
27	5	1622	XAT	C15-C35-C34	-3.07	117.19	123.47
25	0	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
25	R	601	CLA	CHC-C4B-NB	3.07	127.50	124.26
25	R	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
24	9	609	CHL	CMD-C2D-C3D	-3.07	120.56	127.61
24	7	605	CHL	C3B-C4B-NB	3.07	113.36	110.52
24	Y	601	CHL	C4-C3-C5	3.07	120.43	115.27
27	N	1622	XAT	C26-C27-C28	-3.07	119.51	125.99
25	0	602	CLA	C4A-NA-C1A	3.07	108.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	404	BCR	C20-C21-C22	-3.06	122.94	127.31
25	C	509	CLA	CHB-C4A-NA	3.06	128.75	124.51
25	3	612	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
35	D	413	SQD	O9-S-C6	3.06	110.58	106.94
24	s	601	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
24	9	607	CHL	C3B-C4B-NB	3.06	113.36	110.52
25	r	611	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
34	B	620	BCR	C33-C5-C4	3.06	119.50	113.62
24	y	608	CHL	CHC-C4B-NB	-3.06	121.02	124.26
27	n	1622	XAT	O24-C25-C38	3.06	118.72	115.06
25	3	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	b	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	c	501	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
27	9	1622	XAT	C27-C28-C29	-3.06	120.78	125.53
35	d	413	SQD	O9-S-C6	3.06	110.58	106.94
24	Y	606	CHL	OMC-CMC-C2C	-3.06	118.77	125.69
25	2	603	CLA	CHB-C4A-NA	3.06	128.74	124.51
34	b	619	BCR	C20-C21-C22	-3.06	122.94	127.31
25	q	613	CLA	CMB-C2B-C1B	-3.06	120.71	125.37
27	0	1622	XAT	C36-C21-C26	3.06	118.30	110.05
24	p	607	CHL	CAC-C3C-C4C	3.06	128.78	124.81
25	5	603	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	5	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	A	410	CLA	CMB-C2B-C1B	-3.06	120.71	125.37
28	9	1623	NEX	C27-C28-C29	-3.06	120.79	125.53
24	N	605	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
25	r	603	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	0	603	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
35	a	412	SQD	O8-S-O7	3.06	118.74	111.27
25	B	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	y	606	CHL	OMC-CMC-C2C	-3.06	118.78	125.69
34	d	404	BCR	C20-C21-C22	-3.05	122.95	127.31
24	5	601	CHL	CMB-C2B-C1B	3.05	130.02	125.37
34	b	618	BCR	C27-C26-C25	-3.05	118.30	122.73
25	n	612	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
24	0	605	CHL	CHC-C4B-NB	-3.05	121.03	124.26
25	6	603	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
24	6	607	CHL	C3B-C4B-NB	3.05	113.35	110.52
25	2	614	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
28	8	1623	NEX	C35-C34-C33	-3.05	122.95	127.31
24	4	608	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
24	4	606	CHL	CHD-C4C-C3C	-3.05	120.36	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	619	BCR	C20-C21-C22	-3.05	122.96	127.31
25	s	610	CLA	CHB-C1B-NB	3.05	127.48	124.26
27	y	1622	XAT	C35-C34-C33	-3.05	122.96	127.31
26	N	1621	LUT	C18-C5-C6	-3.05	121.11	124.53
24	s	601	CHL	OMC-CMC-C2C	-3.05	118.80	125.69
25	C	513	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	N	611	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	C	510	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
34	b	620	BCR	C33-C5-C4	3.04	119.46	113.62
24	6	609	CHL	C3B-C4B-NB	3.04	113.34	110.52
25	c	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	R	612	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
25	r	612	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
24	0	608	CHL	C3B-C4B-NB	3.04	113.34	110.52
27	Y	1622	XAT	C35-C34-C33	-3.04	122.97	127.31
24	n	607	CHL	CMD-C2D-C3D	-3.04	120.62	127.61
24	R	606	CHL	CHB-C4A-NA	3.04	128.72	124.51
25	r	601	CLA	CHC-C4B-NB	3.04	127.47	124.26
27	n	1622	XAT	C18-C5-C4	3.04	117.70	114.28
25	b	612	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	9	610	CLA	C4A-NA-C1A	3.04	108.07	106.71
26	2	1621	LUT	C11-C10-C9	-3.04	122.97	127.31
26	Y	1621	LUT	C10-C11-C12	-3.04	113.74	123.22
26	p	1621	LUT	C35-C15-C14	-3.04	117.26	123.47
24	n	601	CHL	CHB-C4A-NA	3.03	128.71	124.51
25	4	613	CLA	CHB-C4A-NA	3.03	128.71	124.51
25	a	410	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
26	y	1621	LUT	C10-C11-C12	-3.03	113.75	123.22
26	n	1621	LUT	C18-C5-C6	-3.03	121.12	124.53
24	r	606	CHL	CHB-C4A-NA	3.03	128.71	124.51
25	1	603	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
25	B	605	CLA	CAA-CBA-CGA	-3.03	104.39	113.25
25	5	613	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	G	601	CHL	C1-C2-C3	-3.03	120.80	126.04
24	3	609	CHL	CHB-C4A-NA	3.03	128.70	124.51
28	r	623	NEX	C31-C30-C29	-3.03	122.99	127.31
24	r	606	CHL	OMC-CMC-C2C	-3.03	118.84	125.69
34	C	514	BCR	C11-C10-C9	-3.03	122.99	127.31
24	g	605	CHL	C1C-C2C-C3C	-3.03	104.71	107.11
24	5	608	CHL	CHB-C1B-NB	-3.03	121.05	124.26
25	Y	604	CLA	CMB-C2B-C1B	-3.03	120.76	125.37
25	2	612	CLA	CHB-C4A-NA	3.02	128.69	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r	623	NEX	C39-C29-C30	-3.02	118.69	122.92
24	N	605	CHL	O2A-CGA-CBA	3.02	121.39	111.91
25	B	605	CLA	C1-C2-C3	-3.02	120.81	126.04
24	5	607	CHL	C3B-C4B-NB	3.02	113.32	110.52
24	9	607	CHL	CMB-C2B-C1B	3.02	129.97	125.37
25	c	510	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
25	q	610	CLA	C1-C2-C3	-3.02	120.82	126.04
25	5	610	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	8	611	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	c	511	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
28	q	1623	NEX	C15-C35-C34	-3.02	117.29	123.47
26	0	1621	LUT	C31-C30-C29	-3.02	123.00	127.31
24	r	608	CHL	C4A-NA-C1A	-3.02	105.35	106.71
24	p	606	CHL	CMD-C2D-C3D	-3.02	120.67	127.61
24	7	605	CHL	CAC-C3C-C4C	3.02	128.73	124.81
25	C	501	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	506	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	n	608	CHL	CHB-C4A-NA	3.02	128.68	124.51
25	y	604	CLA	CMB-C2B-C1B	-3.02	120.78	125.37
27	1	1622	XAT	C4-C3-C2	-3.02	104.95	110.77
24	2	601	CHL	CMB-C2B-C1B	3.01	129.96	125.37
24	R	606	CHL	OMC-CMC-C2C	-3.01	118.87	125.69
24	q	601	CHL	C3B-C4B-NB	3.01	113.31	110.52
25	R	611	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	N	612	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
25	3	603	CLA	CHB-C4A-NA	3.01	128.67	124.51
25	4	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	8	1621	LUT	C15-C14-C13	-3.01	123.02	127.31
25	r	612	CLA	CHB-C4A-NA	3.01	128.67	124.51
27	7	1622	XAT	C4-C3-C2	-3.01	104.96	110.77
26	n	1620	LUT	C21-C26-C27	-3.01	108.90	112.70
24	3	605	CHL	C4A-NA-C1A	3.01	108.06	106.71
24	G	605	CHL	CHC-C4B-NB	-3.01	121.07	124.26
27	Y	1622	XAT	C26-C27-C28	-3.01	119.64	125.99
25	0	613	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
24	0	608	CHL	CHB-C1B-NB	-3.01	121.08	124.26
26	S	1620	LUT	C35-C34-C33	-3.00	123.02	127.31
24	Y	607	CHL	CAA-C2A-C3A	-3.00	104.55	112.78
24	p	609	CHL	CMD-C2D-C3D	-3.00	120.70	127.61
24	0	608	CHL	O2A-CGA-CBA	3.00	121.33	111.91
34	c	516	BCR	C10-C11-C12	-3.00	113.85	123.22
25	B	612	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	516	BCR	C10-C11-C12	-3.00	113.85	123.22
27	y	1622	XAT	C26-C27-C28	-3.00	119.65	125.99
25	r	609	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	g	601	CHL	C1-C2-C3	-3.00	120.86	126.04
28	3	1623	NEX	C28-C29-C30	3.00	123.54	118.94
25	6	612	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
25	8	612	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	6	606	CHL	C3B-C4B-NB	3.00	113.30	110.52
24	G	607	CHL	C3B-C4B-NB	3.00	113.30	110.52
25	c	511	CLA	CMB-C2B-C1B	-3.00	120.81	125.37
24	0	609	CHL	CMB-C2B-C1B	3.00	129.93	125.37
25	R	613	CLA	CHC-C4B-NB	3.00	127.43	124.26
25	0	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
29	R	2630	LHG	C5-O7-C7	-2.99	110.42	117.79
24	8	607	CHL	C1-O2A-CGA	2.99	124.30	116.44
25	R	609	CLA	CHB-C4A-NA	2.99	128.65	124.51
24	n	606	CHL	CMB-C2B-C1B	2.99	129.93	125.37
25	6	604	CLA	CHB-C1B-NB	2.99	127.42	124.26
28	4	1623	NEX	C15-C35-C34	-2.99	117.34	123.47
25	b	605	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
24	Y	601	CHL	C3B-C4B-NB	2.99	113.29	110.52
25	7	603	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
24	G	609	CHL	CAC-C3C-C4C	2.99	128.69	124.81
24	g	609	CHL	CAC-C3C-C4C	2.99	128.69	124.81
37	C	518	DGD	O1G-C1A-C2A	2.99	121.29	111.91
24	0	607	CHL	CHC-C4B-NB	-2.99	121.09	124.26
29	r	2630	LHG	C5-O7-C7	-2.99	110.43	117.79
24	N	601	CHL	C4-C3-C5	2.99	120.30	115.27
35	D	413	SQD	C44-O6-C1	-2.99	107.90	113.74
26	G	1621	LUT	C31-C30-C29	-2.99	123.05	127.31
24	g	601	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
24	Y	608	CHL	C3B-C4B-NB	2.99	113.28	110.52
25	s	605	CLA	C4A-NA-C1A	2.99	108.05	106.71
25	Y	610	CLA	CMB-C2B-C1B	-2.98	120.82	125.37
34	C	514	BCR	C24-C23-C22	-2.98	121.72	126.23
28	R	623	NEX	C31-C30-C29	-2.98	123.05	127.31
24	3	609	CHL	CMB-C2B-C1B	2.98	129.91	125.37
25	r	613	CLA	CHC-C4B-NB	2.98	127.42	124.26
24	G	608	CHL	C3B-C4B-NB	2.98	113.28	110.52
25	s	612	CLA	CHC-C4B-NB	2.98	127.42	124.26
28	S	1623	NEX	C39-C29-C30	-2.98	118.75	122.92
34	b	620	BCR	C15-C14-C13	-2.98	123.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	r	622	XAT	C10-C11-C12	-2.98	113.91	123.22
24	r	607	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
24	g	607	CHL	C3B-C4B-NB	2.98	113.28	110.52
25	s	609	CLA	CMA-C3A-C2A	-2.98	109.14	116.10
24	2	606	CHL	CMB-C2B-C1B	2.98	129.91	125.37
24	5	601	CHL	CMD-C2D-C3D	-2.98	120.76	127.61
25	C	511	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	9	604	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	7	606	CHL	OMC-CMC-C2C	-2.98	118.95	125.69
25	G	604	CLA	CHB-C1B-NB	2.98	127.41	124.26
24	y	607	CHL	CAA-C2A-C3A	-2.98	104.63	112.78
25	D	403	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
25	b	605	CLA	C1-C2-C3	-2.97	120.90	126.04
24	n	609	CHL	OMC-CMC-C2C	-2.97	118.96	125.69
24	3	608	CHL	CHC-C4B-NB	-2.97	121.11	124.26
27	9	1622	XAT	C24-C23-C22	-2.97	105.03	110.77
25	N	614	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
27	g	1622	XAT	C35-C34-C33	-2.97	123.07	127.31
34	c	516	BCR	C33-C5-C6	-2.97	121.19	124.53
25	4	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	n	1620	LUT	C15-C14-C13	-2.97	123.07	127.31
24	G	601	CHL	C4-C3-C5	2.97	120.27	115.27
24	8	609	CHL	CAC-C3C-C4C	2.97	128.67	124.81
24	Y	606	CHL	C4-C3-C5	2.97	120.27	115.27
24	y	606	CHL	C4-C3-C5	2.97	120.27	115.27
35	d	413	SQD	C44-O6-C1	-2.97	107.94	113.74
24	s	607	CHL	CHD-C4C-C3C	-2.97	120.47	124.84
27	R	622	XAT	C10-C11-C12	-2.97	113.95	123.22
24	G	601	CHL	C4D-CHA-C1A	-2.97	117.64	121.25
27	2	1622	XAT	C24-C23-C22	-2.97	105.04	110.77
24	G	601	CHL	CHB-C1B-NB	-2.97	121.11	124.26
28	2	1623	NEX	C15-C14-C13	-2.97	123.07	127.31
25	b	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
27	8	1622	XAT	C27-C28-C29	-2.97	120.93	125.53
25	C	502	CLA	CMC-C2C-C3C	2.97	134.17	126.12
24	g	605	CHL	CHC-C4B-NB	-2.97	121.12	124.26
24	g	606	CHL	CHB-C1B-NB	-2.97	121.12	124.26
25	s	602	CLA	CHB-C1B-NB	2.97	127.40	124.26
25	R	612	CLA	CHB-C4A-NA	2.96	128.61	124.51
29	7	2630	LHG	O8-C23-C24	2.96	121.21	111.91
26	5	1620	LUT	C7-C8-C9	-2.96	121.76	126.23
25	y	603	CLA	O2D-CGD-O1D	-2.96	118.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	q	1622	XAT	C4-C3-C2	-2.96	105.05	110.77
37	c	518	DGD	O1G-C1A-C2A	2.96	121.20	111.91
28	R	623	NEX	C39-C29-C30	-2.96	118.78	122.92
34	C	516	BCR	C15-C14-C13	-2.96	123.08	127.31
27	p	1622	XAT	C4-C3-C2	-2.96	105.06	110.77
24	s	608	CHL	CMB-C2B-C1B	2.96	129.88	125.37
27	6	1622	XAT	C36-C21-C26	2.96	118.03	110.05
26	s	1621	LUT	C21-C26-C27	-2.96	108.96	112.70
25	y	610	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
26	p	1620	LUT	C11-C10-C9	-2.96	123.09	127.31
24	G	606	CHL	CHB-C1B-NB	-2.96	121.13	124.26
26	7	1621	LUT	C22-C23-C24	-2.95	108.38	111.74
28	s	1623	NEX	C26-C27-C28	-2.95	119.75	125.99
24	R	607	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
25	c	502	CLA	CMC-C2C-C3C	2.95	134.14	126.12
25	Y	603	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	8	609	CHL	CHB-C1B-NB	-2.95	121.13	124.26
35	d	413	SQD	O48-C23-C24	2.95	121.17	111.91
25	d	403	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
24	S	608	CHL	CMB-C2B-C1B	2.95	129.87	125.37
34	B	620	BCR	C11-C10-C9	-2.95	123.10	127.31
25	S	609	CLA	CMA-C3A-C2A	-2.95	109.21	116.10
35	D	413	SQD	O48-C23-C24	2.95	121.17	111.91
34	B	620	BCR	C15-C14-C13	-2.95	123.10	127.31
24	y	607	CHL	C1-C2-C3	-2.95	120.94	126.04
24	R	608	CHL	CAA-C2A-C3A	-2.95	104.70	112.78
24	7	601	CHL	CHB-C1B-NB	-2.95	121.14	124.26
34	C	515	BCR	C33-C5-C6	-2.95	121.22	124.53
24	r	608	CHL	CAA-C2A-C3A	-2.95	104.70	112.78
28	S	1623	NEX	C26-C27-C28	-2.95	119.76	125.99
24	7	601	CHL	CHB-C4A-NA	2.95	128.59	124.51
25	7	613	CLA	CHB-C4A-NA	2.95	128.59	124.51
24	G	607	CHL	O2A-CGA-O1A	-2.95	116.15	123.59
26	1	1621	LUT	C7-C8-C9	-2.95	121.78	126.23
25	R	611	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	9	603	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	n	614	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	9	611	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
34	d	404	BCR	C38-C26-C25	-2.94	121.22	124.53
24	0	601	CHL	C3B-C4B-NB	2.94	113.25	110.52
25	q	612	CLA	CAA-C2A-C3A	-2.94	104.71	112.78
39	d	405	PL9	C22-C23-C24	-2.94	120.57	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	605	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	g	601	CHL	CHB-C1B-NB	-2.94	121.14	124.26
25	6	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	y	610	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	2	608	CHL	CMB-C2B-C1B	2.94	129.85	125.37
28	9	1623	NEX	C39-C29-C30	-2.94	118.80	122.92
24	R	606	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
24	3	601	CHL	CHB-C4A-NA	2.94	128.58	124.51
24	r	606	CHL	CMD-C2D-C3D	-2.94	120.85	127.61
25	C	505	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
25	r	611	CLA	CHB-C4A-NA	2.94	128.58	124.51
34	c	515	BCR	C33-C5-C6	-2.94	121.23	124.53
24	6	609	CHL	CMB-C2B-C1B	2.94	129.85	125.37
25	C	511	CLA	CMB-C2B-C1B	-2.94	120.89	125.37
25	1	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
24	n	601	CHL	CMB-C2B-C1B	2.94	129.84	125.37
25	8	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
34	b	618	BCR	C11-C10-C9	-2.94	123.12	127.31
24	p	608	CHL	CHB-C4A-NA	2.94	128.57	124.51
24	n	601	CHL	C4-C3-C5	2.94	120.21	115.27
24	8	609	CHL	CMB-C2B-C1B	2.94	129.84	125.37
24	2	606	CHL	O2A-CGA-CBA	2.94	121.12	111.91
25	6	612	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	B	608	CLA	CHB-C4A-NA	2.94	128.57	124.51
39	D	405	PL9	C22-C23-C24	-2.93	120.59	127.66
25	c	505	CLA	CMB-C2B-C1B	-2.93	120.90	125.37
24	p	607	CHL	C2A-C3A-C4A	-2.93	97.13	101.87
25	C	510	CLA	CMB-C2B-C3B	2.93	133.69	126.59
24	7	608	CHL	CHB-C4A-NA	2.93	128.57	124.51
26	3	1620	LUT	C31-C30-C29	-2.93	123.12	127.31
24	S	607	CHL	CHD-C4C-C3C	-2.93	120.53	124.84
25	R	616	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	Y	607	CHL	O2A-CGA-CBA	2.93	121.11	111.91
24	3	605	CHL	O2A-CGA-CBA	2.93	121.11	111.91
29	1	2630	LHG	O8-C23-C24	2.93	121.11	111.91
25	S	602	CLA	CHB-C1B-NB	2.93	127.36	124.26
28	g	1623	NEX	C2-C1-C6	2.93	112.06	109.21
24	G	601	CHL	C1C-C2C-C3C	-2.93	104.79	107.11
25	Y	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	7	1621	LUT	C15-C35-C34	-2.93	117.48	123.47
27	p	1622	XAT	C27-C28-C29	-2.93	120.99	125.53
25	S	605	CLA	C4A-NA-C1A	2.93	108.02	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	516	BCR	C33-C5-C6	-2.93	121.24	124.53
28	1	1623	NEX	C24-C23-C22	-2.93	105.12	110.77
29	Y	2630	LHG	C5-O7-C7	-2.93	110.59	117.79
24	2	609	CHL	CMD-C2D-C3D	-2.93	120.88	127.61
24	4	605	CHL	CMB-C2B-C1B	2.92	129.82	125.37
26	9	1620	LUT	C35-C15-C14	-2.92	117.48	123.47
24	y	608	CHL	CAC-C3C-C4C	2.92	128.60	124.81
24	5	601	CHL	C1C-C2C-C3C	-2.92	104.79	107.11
24	5	607	CHL	C1C-C2C-C3C	-2.92	104.79	107.11
24	5	607	CHL	C4-C3-C5	2.92	120.19	115.27
24	g	601	CHL	CBC-CAC-C3C	-2.92	104.37	112.43
27	2	1622	XAT	C15-C35-C34	-2.92	117.49	123.47
24	7	606	CHL	CMD-C2D-C3D	-2.92	120.89	127.61
29	n	2630	LHG	O8-C23-C24	2.92	121.08	111.91
24	G	605	CHL	CAA-C2A-C3A	-2.92	104.78	112.78
24	g	605	CHL	CAA-C2A-C3A	-2.92	104.78	112.78
25	y	614	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	R	609	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	r	620	LUT	C31-C30-C29	-2.92	123.14	127.31
25	g	604	CLA	CHB-C1B-NB	2.92	127.35	124.26
24	3	607	CHL	O2A-CGA-CBA	2.92	121.07	111.91
24	Y	608	CHL	O2A-CGA-CBA	2.92	121.06	111.91
24	y	601	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
25	c	513	CLA	CHB-C4A-NA	2.92	128.55	124.51
24	G	601	CHL	C4A-NA-C1A	-2.92	105.39	106.71
25	C	502	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
36	d	412	LMG	O8-C28-C29	2.92	121.06	111.91
24	1	607	CHL	CMB-C2B-C1B	2.92	129.81	125.37
26	R	620	LUT	C31-C30-C29	-2.91	123.15	127.31
25	6	613	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	Y	608	CHL	CAC-C3C-C4C	2.91	128.59	124.81
25	r	616	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	0	609	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
24	5	608	CHL	CHB-C4A-NA	2.91	128.54	124.51
34	b	620	BCR	C11-C10-C9	-2.91	123.15	127.31
24	1	608	CHL	O2A-CGA-CBA	2.91	121.05	111.91
24	4	609	CHL	O2A-CGA-CBA	2.91	121.05	111.91
25	p	611	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
34	c	516	BCR	C15-C14-C13	-2.91	123.16	127.31
25	C	505	CLA	CHB-C1B-NB	2.91	127.34	124.26
34	D	404	BCR	C38-C26-C25	-2.91	121.26	124.53
25	S	612	CLA	CHC-C4B-NB	2.91	127.34	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	609	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
24	2	607	CHL	CMB-C2B-C1B	2.91	129.80	125.37
25	1	611	CLA	CHB-C4A-NA	2.91	128.53	124.51
25	B	605	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	s	609	CLA	CAA-C2A-C3A	-2.91	109.31	116.10
24	3	601	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
25	3	612	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	s	601	CHL	CAC-C3C-C4C	2.91	128.58	124.81
24	q	609	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
25	C	505	CLA	C1-C2-C3	-2.90	121.02	126.04
24	g	607	CHL	O2A-CGA-O1A	-2.90	116.26	123.59
24	G	606	CHL	O2A-CGA-CBA	2.90	121.02	111.91
27	3	1622	XAT	C4-C3-C2	-2.90	105.17	110.77
25	4	612	CLA	CHB-C4A-NA	2.90	128.52	124.51
24	g	607	CHL	OMC-CMC-C2C	-2.90	119.13	125.69
24	p	606	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
25	6	602	CLA	C4A-NA-C1A	2.90	108.01	106.71
24	N	601	CHL	CMB-C2B-C1B	2.90	129.78	125.37
25	r	613	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	B	605	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
26	6	1621	LUT	C7-C8-C9	-2.90	121.86	126.23
26	9	1620	LUT	C15-C14-C13	-2.90	123.18	127.31
24	1	605	CHL	C3B-C4B-NB	2.90	113.20	110.52
25	1	613	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	a	405	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
24	1	601	CHL	CHB-C4A-NA	2.90	128.52	124.51
28	5	1623	NEX	C39-C29-C30	-2.90	118.87	122.92
24	n	608	CHL	O2A-CGA-CBA	2.89	120.99	111.91
27	p	1622	XAT	C15-C35-C34	-2.89	117.55	123.47
24	1	606	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
25	q	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	c	502	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	4	607	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
25	3	604	CLA	CMB-C2B-C3B	2.89	133.60	126.59
25	c	510	CLA	CMB-C2B-C3B	2.89	133.60	126.59
25	7	612	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
24	p	606	CHL	CMB-C2B-C1B	2.89	129.78	125.37
26	y	1620	LUT	C19-C9-C8	2.89	122.64	118.08
24	p	601	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
24	q	605	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
24	g	601	CHL	C4-C3-C5	2.89	120.14	115.27
25	B	607	CLA	CHD-C1D-ND	-2.89	121.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	618	BCR	C11-C10-C9	-2.89	123.18	127.31
28	4	1623	NEX	O24-C25-C38	2.89	118.52	115.06
26	y	1621	LUT	C16-C1-C6	-2.89	105.61	110.30
26	1	1621	LUT	C15-C35-C34	-2.89	117.55	123.47
25	B	612	CLA	CHB-C1B-NB	2.89	127.32	124.26
25	b	612	CLA	CHB-C1B-NB	2.89	127.32	124.26
24	8	605	CHL	CMB-C2B-C1B	2.89	129.77	125.37
24	6	606	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
25	b	605	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
24	y	601	CHL	C3B-C4B-NB	2.89	113.19	110.52
24	9	609	CHL	CHC-C4B-NB	-2.89	121.20	124.26
26	N	1620	LUT	C10-C11-C12	-2.89	114.21	123.22
28	1	1623	NEX	C28-C29-C30	2.89	123.37	118.94
24	g	609	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
25	4	610	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	y	601	CHL	C1-C2-C3	-2.89	121.05	126.04
25	b	616	CLA	CHB-C4A-NA	2.88	128.50	124.51
24	6	606	CHL	C1C-C2C-C3C	-2.88	104.83	107.11
24	y	608	CHL	O2A-CGA-CBA	2.88	120.96	111.91
25	A	407	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	y	609	CHL	CED-O2D-CGD	2.88	122.46	115.94
39	d	405	PL9	C7-C3-C2	-2.88	119.51	123.30
27	p	1622	XAT	C7-C8-C9	-2.88	121.06	125.53
24	y	605	CHL	CAC-C3C-C4C	2.88	128.55	124.81
25	A	405	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	g	606	CHL	O2A-CGA-CBA	2.88	120.95	111.91
39	D	405	PL9	C7-C3-C2	-2.88	119.51	123.30
25	b	612	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
28	0	1623	NEX	C28-C29-C30	2.88	123.36	118.94
24	N	607	CHL	C1-C2-C3	-2.88	121.07	126.04
24	0	601	CHL	CMB-C2B-C1B	2.88	129.75	125.37
25	S	602	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	Y	1620	LUT	C19-C9-C8	2.88	122.61	118.08
24	y	608	CHL	C3B-C4B-NB	2.88	113.18	110.52
29	y	2630	LHG	O8-C23-C24	2.88	120.93	111.91
25	7	611	CLA	CHB-C4A-NA	2.88	128.49	124.51
25	S	609	CLA	CAA-C2A-C3A	-2.88	109.39	116.10
25	4	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	g	1623	NEX	C35-C34-C33	-2.87	123.21	127.31
28	r	623	NEX	C24-C23-C22	-2.87	105.22	110.77
25	S	602	CLA	CHB-C4A-NA	2.87	128.49	124.51
24	3	607	CHL	CHB-C1B-NB	-2.87	121.22	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	609	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	7	1622	XAT	C27-C28-C29	-2.87	121.07	125.53
24	G	607	CHL	OMC-CMC-C2C	-2.87	119.19	125.69
25	c	505	CLA	C1-C2-C3	-2.87	121.08	126.04
28	R	623	NEX	C24-C23-C22	-2.87	105.23	110.77
24	8	605	CHL	OMC-CMC-C2C	-2.87	119.19	125.69
25	D	402	CLA	CHB-C1B-NB	2.87	127.30	124.26
24	2	608	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
25	2	604	CLA	CHB-C4A-NA	2.87	128.48	124.51
34	c	514	BCR	C24-C23-C22	-2.87	121.90	126.23
24	2	607	CHL	C3B-C4B-NB	2.87	113.18	110.52
27	0	1622	XAT	C4-C3-C2	-2.87	105.23	110.77
26	N	1620	LUT	C21-C26-C27	-2.87	109.07	112.70
24	G	605	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
24	9	601	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
25	R	613	CLA	CHB-C4A-NA	2.87	128.48	124.51
24	n	607	CHL	CHB-C1B-NB	-2.87	121.22	124.26
24	6	606	CHL	CHB-C1B-NB	-2.87	121.22	124.26
28	p	1623	NEX	C39-C29-C30	-2.87	118.91	122.92
28	r	623	NEX	C4-C3-C2	-2.87	105.24	110.77
25	Y	602	CLA	CMB-C2B-C1B	-2.87	121.00	125.37
24	y	601	CHL	CHB-C4A-NA	2.87	128.47	124.51
26	q	1620	LUT	C15-C14-C13	-2.87	123.22	127.31
24	G	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
26	g	1621	LUT	C38-C25-C24	-2.86	117.43	123.56
33	a	408	PHO	O1D-CGD-CBD	2.86	129.51	124.74
29	N	2630	LHG	O8-C23-C24	2.86	120.89	111.91
36	D	412	LMG	O8-C28-C29	2.86	120.89	111.91
24	3	605	CHL	CMB-C2B-C1B	2.86	129.73	125.37
25	9	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
33	A	408	PHO	O1D-CGD-CBD	2.86	129.51	124.74
26	Y	1621	LUT	C16-C1-C6	-2.86	105.66	110.30
27	n	1622	XAT	C35-C34-C33	-2.86	123.22	127.31
25	c	505	CLA	CHB-C1B-NB	2.86	127.29	124.26
24	3	608	CHL	C3B-C4B-NB	2.86	113.17	110.52
24	Y	605	CHL	CAC-C3C-C4C	2.86	128.52	124.81
24	N	601	CHL	CAC-C3C-C4C	2.86	128.52	124.81
35	D	413	SQD	O47-C7-C8	2.86	117.66	111.50
24	G	609	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
25	a	407	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	4	605	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
25	N	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	604	CLA	CHC-C4B-NB	2.86	127.28	124.26
34	c	515	BCR	C16-C17-C18	-2.86	123.23	127.31
26	G	1621	LUT	C38-C25-C24	-2.86	117.45	123.56
35	d	413	SQD	O47-C7-C8	2.86	117.66	111.50
26	6	1621	LUT	C10-C11-C12	-2.86	114.30	123.22
24	5	607	CHL	O2A-CGA-CBA	2.86	120.87	111.91
24	3	609	CHL	CHB-C1B-NB	-2.86	121.23	124.26
25	0	613	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	0	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	b	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	4	612	CLA	CHC-C4B-NB	2.86	127.28	124.26
28	n	1623	NEX	C11-C10-C9	-2.85	123.24	127.31
24	6	608	CHL	C3B-C4B-NB	2.85	113.16	110.52
24	g	608	CHL	C1C-C2C-C3C	-2.85	104.85	107.11
34	C	516	BCR	C16-C15-C14	-2.85	117.63	123.47
36	s	2631	LMG	O8-C28-C29	2.85	120.86	111.91
26	S	1621	LUT	C21-C26-C27	-2.85	109.09	112.70
24	9	606	CHL	O2A-CGA-CBA	2.85	120.86	111.91
25	b	607	CLA	CHD-C1D-ND	-2.85	121.83	124.45
36	B	622	LMG	C8-O7-C10	-2.85	110.77	117.79
25	n	604	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
24	r	607	CHL	CMB-C2B-C1B	2.85	129.71	125.37
29	q	2630	LHG	O8-C23-C24	2.85	120.86	111.91
24	Y	609	CHL	O2A-CGA-CBA	2.85	120.85	111.91
25	G	612	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	p	611	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	B	612	CLA	CMB-C2B-C1B	-2.85	121.03	125.37
25	s	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
24	R	608	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
24	9	608	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
25	b	607	CLA	CHB-C1B-NB	2.85	127.27	124.26
33	A	408	PHO	O2D-CGD-O1D	-2.85	118.27	123.84
33	a	408	PHO	O2D-CGD-O1D	-2.85	118.27	123.84
28	g	1623	NEX	C15-C35-C34	-2.85	117.64	123.47
34	C	516	BCR	C28-C27-C26	-2.85	108.99	114.08
24	N	607	CHL	CHB-C1B-NB	-2.85	121.24	124.26
24	9	605	CHL	O2A-CGA-CBA	2.85	120.84	111.91
27	8	1622	XAT	C4-C3-C2	-2.85	105.28	110.77
24	4	607	CHL	CMB-C2B-C1B	2.85	129.70	125.37
25	d	402	CLA	CHB-C1B-NB	2.84	127.27	124.26
25	5	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	S	604	CLA	CHB-C4A-NA	2.84	128.44	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	615	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	y	609	CHL	O2A-CGA-CBA	2.84	120.82	111.91
25	R	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
34	c	516	BCR	C28-C27-C26	-2.84	109.00	114.08
25	y	602	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
24	n	605	CHL	CBA-CAA-C2A	-2.84	105.48	113.86
25	g	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	s	1620	LUT	C35-C15-C14	-2.84	117.66	123.47
24	2	607	CHL	CAC-C3C-C4C	2.84	128.49	124.81
24	g	601	CHL	C4D-CHA-C1A	-2.84	117.79	121.25
34	c	516	BCR	C16-C15-C14	-2.84	117.66	123.47
24	N	608	CHL	CHB-C4A-NA	2.84	128.44	124.51
35	B	621	SQD	O48-C23-C24	2.84	120.81	111.91
24	N	608	CHL	O2A-CGA-CBA	2.84	120.81	111.91
24	r	608	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
25	B	611	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	8	608	CHL	C3B-C4B-NB	2.84	113.15	110.52
25	B	616	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	7	612	CLA	CHB-C4A-NA	2.84	128.43	124.51
24	q	607	CHL	O2A-CGA-CBA	2.84	120.81	111.91
24	q	605	CHL	CHC-C4B-NB	-2.84	121.25	124.26
25	b	615	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	Y	1621	LUT	C22-C23-C24	-2.84	108.51	111.74
24	n	605	CHL	CMB-C2B-C1B	2.84	129.69	125.37
25	7	603	CLA	CHB-C4A-NA	2.83	128.43	124.51
24	5	609	CHL	C4-C3-C5	2.83	120.04	115.27
24	p	609	CHL	C1C-C2C-C3C	-2.83	104.86	107.11
24	1	601	CHL	CHB-C1B-NB	-2.83	121.26	124.26
24	8	609	CHL	CHB-C4A-NA	2.83	128.43	124.51
25	1	612	CLA	CHB-C4A-NA	2.83	128.43	124.51
24	n	609	CHL	CHD-C4C-C3C	-2.83	120.68	124.84
25	N	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	Y	607	CHL	C1-C2-C3	-2.83	121.14	126.04
35	b	621	SQD	O48-C23-C24	2.83	120.79	111.91
25	y	610	CLA	C4A-NA-C1A	2.83	107.98	106.71
25	r	604	CLA	CHB-C4A-NA	2.83	128.43	124.51
24	9	608	CHL	CMB-C2B-C1B	2.83	129.68	125.37
25	6	602	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	7	601	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	R	606	CHL	C3B-C4B-NB	2.83	113.14	110.52
24	p	608	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	q	601	CHL	O2A-CGA-CBA	2.83	120.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	605	CHL	CHC-C4B-NB	-2.83	121.26	124.26
25	q	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	1	605	CHL	CAC-C3C-C4C	2.83	128.48	124.81
27	y	1622	XAT	C27-C28-C29	-2.83	121.14	125.53
24	R	606	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	g	606	CHL	CMB-C2B-C1B	2.83	129.68	125.37
24	r	606	CHL	CMB-C2B-C1B	2.83	129.68	125.37
27	9	1622	XAT	C15-C35-C34	-2.83	117.68	123.47
24	8	608	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
25	C	513	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	n	609	CHL	C4-C3-C5	2.83	120.03	115.27
24	5	609	CHL	O2A-CGA-CBA	2.83	120.77	111.91
24	0	606	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
24	R	607	CHL	CMB-C2B-C1B	2.82	129.67	125.37
26	S	1620	LUT	C35-C15-C14	-2.82	117.69	123.47
24	q	605	CHL	CMB-C2B-C1B	2.82	129.67	125.37
25	6	611	CLA	CHB-C4A-NA	2.82	128.41	124.51
34	b	620	BCR	C1-C6-C5	-2.82	118.64	122.61
25	3	614	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	r	623	NEX	C35-C34-C33	-2.82	123.28	127.31
34	c	515	BCR	C20-C21-C22	-2.82	123.28	127.31
24	g	605	CHL	CMB-C2B-C1B	2.82	129.67	125.37
29	9	2630	LHG	O8-C23-C24	2.82	120.76	111.91
26	8	1620	LUT	C31-C30-C29	-2.82	123.29	127.31
24	9	605	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
24	5	609	CHL	C1C-C2C-C3C	-2.82	104.88	107.11
25	y	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	d	411	LMG	O8-C28-C29	2.82	120.75	111.91
25	s	602	CLA	CHB-C4A-NA	2.82	128.41	124.51
28	q	1623	NEX	O24-C25-C38	2.82	118.43	115.06
26	Y	1620	LUT	C10-C11-C12	-2.82	114.43	123.22
24	p	609	CHL	C4-C3-C5	2.82	120.01	115.27
26	r	620	LUT	C10-C11-C12	-2.82	114.43	123.22
24	7	609	CHL	CMB-C2B-C1B	2.82	129.66	125.37
24	N	609	CHL	C4-C3-C5	2.82	120.01	115.27
24	2	605	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
24	5	605	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
24	6	601	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
24	5	608	CHL	CMB-C2B-C1B	2.81	129.66	125.37
24	8	601	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
26	R	620	LUT	C10-C11-C12	-2.81	114.44	123.22
25	B	610	CLA	CHB-C1B-NB	2.81	127.24	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	607	CLA	CHB-C1B-NB	2.81	127.23	124.26
24	2	608	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
36	b	622	LMG	C8-O7-C10	-2.81	110.87	117.79
25	G	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
27	6	1622	XAT	C4-C3-C2	-2.81	105.34	110.77
24	3	605	CHL	OMC-CMC-C2C	-2.81	119.33	125.69
25	G	603	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
26	y	1620	LUT	C10-C11-C12	-2.81	114.45	123.22
24	7	607	CHL	CMB-C2B-C1B	2.81	129.65	125.37
24	y	607	CHL	O2A-CGA-CBA	2.81	120.72	111.91
28	8	1623	NEX	C28-C29-C30	2.81	123.25	118.94
27	R	622	XAT	C35-C34-C33	-2.81	123.30	127.31
24	2	605	CHL	O2A-CGA-CBA	2.81	120.72	111.91
25	a	410	CLA	C1-C2-C3	-2.81	121.19	126.04
24	q	601	CHL	CHB-C4A-NA	2.81	128.40	124.51
25	3	602	CLA	CHB-C1B-NB	2.81	127.23	124.26
25	p	602	CLA	CHB-C1B-NB	2.81	127.23	124.26
25	8	604	CLA	CMB-C2B-C3B	2.81	133.39	126.59
25	B	614	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	0	614	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	G	603	CLA	CHB-C4A-NA	2.81	128.39	124.51
24	p	609	CHL	O2A-CGA-CBA	2.81	120.71	111.91
26	g	1621	LUT	C31-C30-C29	-2.81	123.31	127.31
27	r	622	XAT	C35-C34-C33	-2.81	123.31	127.31
24	y	607	CHL	CHB-C1B-NB	-2.80	121.29	124.26
25	8	602	CLA	CHB-C1B-NB	2.80	127.23	124.26
24	7	605	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
25	B	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	7	609	CHL	C4-C3-C5	2.80	119.98	115.27
24	0	607	CHL	CHB-C4A-NA	2.80	128.39	124.51
25	b	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	2	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	n	609	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	2	605	CHL	C3B-C4B-NB	2.80	113.11	110.52
24	G	607	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	6	609	CHL	C1-C2-C3	-2.80	121.20	126.04
36	S	2631	LMG	O8-C28-C29	2.80	120.69	111.91
24	G	608	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
24	G	606	CHL	CMB-C2B-C1B	2.80	129.63	125.37
24	g	607	CHL	CMB-C2B-C1B	2.80	129.63	125.37
27	G	1622	XAT	C35-C34-C33	-2.80	123.32	127.31
25	C	507	CLA	CAA-C2A-C3A	-2.80	105.12	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	411	LMG	O8-C28-C29	2.80	120.69	111.91
25	N	604	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	b	615	CLA	CHB-C4A-NA	2.80	128.38	124.51
24	0	601	CHL	O2A-CGA-CBA	2.80	120.69	111.91
26	s	1620	LUT	C38-C25-C24	-2.80	117.58	123.56
28	s	1623	NEX	C39-C29-C30	-2.80	119.01	122.92
24	1	609	CHL	CMB-C2B-C1B	2.80	129.63	125.37
28	r	623	NEX	C15-C35-C34	-2.80	117.75	123.47
25	y	611	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	s	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	3	607	CHL	CAA-C2A-C3A	-2.80	105.12	112.78
24	2	606	CHL	C3B-C4B-NB	2.80	113.11	110.52
24	8	605	CHL	C4A-NA-C1A	2.79	107.96	106.71
24	2	608	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
25	b	604	CLA	C3B-C4B-NB	-2.79	107.92	110.52
25	6	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	B	613	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
25	b	613	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
28	n	1623	NEX	C26-C27-C28	-2.79	120.09	125.99
24	2	607	CHL	O2A-CGA-CBA	2.79	120.66	111.91
29	c	2630	LHG	C5-O7-C7	-2.79	110.93	117.79
25	Y	603	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	Y	602	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	g	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
28	q	1623	NEX	C2-C1-C6	2.79	111.92	109.21
34	C	515	BCR	C16-C17-C18	-2.79	123.33	127.31
24	1	609	CHL	C4-C3-C5	2.79	119.96	115.27
25	p	610	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	q	604	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	A	410	CLA	C1-C2-C3	-2.78	121.23	126.04
24	9	607	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
25	B	604	CLA	CHC-C4B-NB	2.78	127.20	124.26
39	d	405	PL9	C12-C13-C14	-2.78	120.96	127.66
25	a	405	CLA	CBA-CAA-C2A	-2.78	105.65	113.86
27	Y	1622	XAT	C27-C28-C29	-2.78	121.22	125.53
36	c	521	LMG	O8-C28-C29	2.78	120.63	111.91
24	Y	601	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
26	S	1620	LUT	C38-C25-C24	-2.78	117.61	123.56
25	3	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	8	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	g	611	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	9	607	CHL	O2A-CGA-CBA	2.78	120.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	502	CLA	CHC-C4B-NB	2.78	127.20	124.26
25	2	613	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	8	614	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
24	8	607	CHL	CHB-C1B-NB	-2.77	121.32	124.26
25	g	603	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	Y	611	CLA	CHB-C1B-NB	2.77	127.19	124.26
25	5	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	b	614	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	r	606	CHL	C3B-C4B-NB	2.77	113.09	110.52
26	s	1620	LUT	C10-C11-C12	-2.77	114.57	123.22
25	4	603	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
25	A	405	CLA	CBA-CAA-C2A	-2.77	105.68	113.86
25	B	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	G	613	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	9	605	CHL	C3B-C4B-NB	2.77	113.08	110.52
25	B	604	CLA	C3B-C4B-NB	-2.77	107.95	110.52
25	5	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	5	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	0	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
34	B	620	BCR	C1-C6-C5	-2.77	118.71	122.61
25	S	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	4	605	CHL	CHC-C4B-NB	-2.77	121.33	124.26
25	q	612	CLA	CHC-C4B-NB	2.77	127.19	124.26
25	B	611	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	2	601	CHL	C4A-NA-C1A	-2.77	105.46	106.71
24	1	606	CHL	O2A-CGA-CBA	2.77	120.59	111.91
24	4	607	CHL	CHD-C4C-C3C	-2.76	120.78	124.84
36	C	521	LMG	O8-C28-C29	2.76	120.58	111.91
29	3	2630	LHG	O8-C23-C24	2.76	120.58	111.91
28	G	1623	NEX	C15-C35-C34	-2.76	117.81	123.47
28	N	1623	NEX	C26-C27-C28	-2.76	120.15	125.99
25	0	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	g	614	CLA	CHB-C1B-NB	2.76	127.18	124.26
24	n	607	CHL	CMB-C2B-C1B	2.76	129.57	125.37
25	4	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	q	607	CHL	CMB-C2B-C1B	2.76	129.57	125.37
24	y	609	CHL	CHB-C1B-NB	-2.76	121.33	124.26
25	p	603	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	Y	601	CHL	CHB-C1B-NB	-2.76	121.34	124.26
25	g	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	S	601	CHL	CAC-C3C-C4C	2.76	128.39	124.81
25	9	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	607	CHL	CHC-C4B-NB	-2.76	121.34	124.26
25	Y	611	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	p	612	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	c	503	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
25	S	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
24	5	605	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
25	2	602	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
27	5	1622	XAT	C31-C30-C29	-2.75	123.38	127.31
24	3	607	CHL	CHC-C4B-NB	-2.75	121.34	124.26
24	q	605	CHL	C3B-C4B-NB	2.75	113.07	110.52
25	C	503	CLA	CAA-CBA-CGA	-2.75	105.21	113.25
25	5	602	CLA	CHB-C1B-NB	2.75	127.17	124.26
24	G	608	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
26	7	1620	LUT	C10-C11-C12	-2.75	114.63	123.22
26	4	1621	LUT	C18-C5-C6	-2.75	121.44	124.53
26	S	1620	LUT	C10-C11-C12	-2.75	114.63	123.22
25	3	611	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	Y	607	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
25	s	602	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	N	609	CHL	CMB-C2B-C1B	2.75	129.56	125.37
25	B	617	CLA	CHC-C4B-NB	2.75	127.17	124.26
26	n	1621	LUT	C38-C25-C24	-2.75	117.68	123.56
25	b	614	CLA	CMB-C2B-C3B	2.75	133.25	126.59
25	b	611	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	y	607	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
29	c	2630	LHG	O8-C23-C24	2.75	120.53	111.91
27	Y	1622	XAT	C15-C35-C34	-2.75	117.84	123.47
25	b	610	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	g	601	CHL	C4A-NA-C1A	-2.75	105.47	106.71
24	Y	607	CHL	CHB-C1B-NB	-2.75	121.35	124.26
25	b	610	CLA	CHB-C1B-NB	2.75	127.17	124.26
25	B	607	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	4	1621	LUT	C38-C25-C24	-2.75	117.68	123.56
34	C	515	BCR	C20-C21-C22	-2.75	123.39	127.31
24	1	601	CHL	CMB-C2B-C1B	2.74	129.55	125.37
24	1	609	CHL	O2A-CGA-CBA	2.74	120.52	111.91
25	S	602	CLA	C3B-C4B-NB	-2.74	107.97	110.52
34	H	101	BCR	C29-C30-C25	2.74	114.70	110.48
24	Y	609	CHL	CHB-C1B-NB	-2.74	121.35	124.26
25	B	614	CLA	CMB-C2B-C3B	2.74	133.23	126.59
24	p	605	CHL	CHD-C4C-C3C	-2.74	120.81	124.84
25	n	610	CLA	O2D-CGD-O1D	-2.74	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	609	CHL	CMB-C2B-C1B	2.74	129.55	125.37
24	9	609	CHL	C4-C3-C5	2.74	119.88	115.27
25	q	602	CLA	CHB-C1B-NB	2.74	127.16	124.26
24	9	608	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
28	9	1623	NEX	C31-C30-C29	-2.74	123.40	127.31
24	q	607	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
24	3	608	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
34	b	620	BCR	C28-C27-C26	-2.74	109.19	114.08
25	n	604	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	5	1621	LUT	C7-C8-C9	-2.74	122.10	126.23
26	0	1621	LUT	C18-C5-C6	-2.74	121.45	124.53
25	8	604	CLA	CHB-C1B-NB	2.74	127.16	124.26
25	b	614	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	0	609	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
28	6	1623	NEX	C28-C29-C30	2.74	123.14	118.94
24	9	601	CHL	O2A-CGA-CBA	2.74	120.50	111.91
24	n	607	CHL	O2A-CGA-CBA	2.74	120.50	111.91
25	7	614	CLA	CHB-C4A-NA	2.74	128.29	124.51
25	q	611	CLA	CHB-C4A-NA	2.74	128.29	124.51
24	N	605	CHL	CBA-CAA-C2A	-2.73	105.79	113.86
24	7	609	CHL	CHC-C4B-NB	-2.73	121.36	124.26
24	p	605	CHL	CHC-C4B-NB	-2.73	121.36	124.26
24	y	609	CHL	C1C-C2C-C3C	-2.73	104.94	107.11
26	8	1620	LUT	C35-C15-C14	-2.73	117.87	123.47
24	2	609	CHL	CHD-C4C-C3C	-2.73	120.82	124.84
28	7	1623	NEX	C4-C3-C2	-2.73	105.49	110.77
24	0	601	CHL	CAC-C3C-C4C	2.73	128.36	124.81
28	0	1623	NEX	C30-C31-C32	-2.73	114.69	123.22
29	C	2630	LHG	O8-C23-C24	2.73	120.48	111.91
24	7	608	CHL	CMB-C2B-C1B	2.73	129.53	125.37
26	6	1621	LUT	C38-C25-C24	-2.73	117.72	123.56
25	9	613	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	y	601	CHL	CHB-C1B-NB	-2.73	121.37	124.26
29	D	410	LHG	O8-C23-C24	2.73	120.47	111.91
24	N	601	CHL	CGD-CBD-CAD	-2.73	101.89	110.73
24	7	609	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	6	614	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	8	611	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	8	607	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	7	604	CLA	CHB-C1B-NB	2.73	127.15	124.26
24	7	608	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	4	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	1621	LUT	C18-C5-C6	-2.73	121.46	124.53
25	y	612	CLA	C1-C2-C3	-2.73	121.32	126.04
25	C	501	CLA	CHB-C4A-NA	2.73	128.28	124.51
27	y	1622	XAT	C15-C35-C34	-2.73	117.89	123.47
39	D	405	PL9	C12-C13-C14	-2.73	121.09	127.66
25	p	613	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	y	603	CLA	CHB-C4A-NA	2.73	128.28	124.51
24	5	606	CHL	CMB-C2B-C1B	2.73	129.52	125.37
24	7	606	CHL	O2A-CGA-CBA	2.73	120.47	111.91
26	3	1621	LUT	C30-C31-C32	-2.73	114.71	123.22
25	B	615	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	2	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
25	y	611	CLA	CHB-C1B-NB	2.73	127.14	124.26
27	8	1622	XAT	C15-C35-C34	-2.73	117.89	123.47
25	a	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	r	620	LUT	C2-C3-C4	2.73	114.03	110.30
24	2	609	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
25	c	508	CLA	C3B-C4B-NB	-2.72	107.99	110.52
25	C	512	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
24	s	606	CHL	C4A-NA-C1A	-2.72	105.48	106.71
24	4	608	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
24	6	609	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
25	5	602	CLA	CMB-C2B-C1B	-2.72	121.22	125.37
25	c	502	CLA	CHC-C4B-NB	2.72	127.14	124.26
24	q	609	CHL	CHD-C1D-C2D	2.72	131.19	125.48
26	6	1621	LUT	C2-C3-C4	-2.72	106.58	110.30
24	2	609	CHL	C4-C3-C5	2.72	119.85	115.27
25	b	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
24	N	606	CHL	CMB-C2B-C1B	2.72	129.51	125.37
28	g	1623	NEX	C4-C3-C2	-2.72	105.52	110.77
34	h	101	BCR	C29-C30-C25	2.72	114.67	110.48
24	Y	607	CHL	CHC-C4B-NB	-2.72	121.38	124.26
24	q	605	CHL	O2A-CGA-CBA	2.72	120.44	111.91
26	9	1620	LUT	C11-C10-C9	-2.72	123.43	127.31
24	3	606	CHL	CMB-C2B-C1B	2.72	129.51	125.37
26	1	1620	LUT	C10-C11-C12	-2.72	114.73	123.22
26	R	620	LUT	C2-C3-C4	2.72	114.03	110.30
24	Y	608	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
29	d	410	LHG	O8-C23-C24	2.72	120.44	111.91
27	y	1622	XAT	C36-C21-C26	2.72	117.38	110.05
24	Y	601	CHL	CHB-C4A-NA	2.72	128.27	124.51
34	c	515	BCR	C11-C10-C9	-2.72	123.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	603	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	7	1620	LUT	C7-C8-C9	-2.72	122.13	126.23
24	6	601	CHL	CAC-C3C-C4C	2.72	128.33	124.81
24	8	605	CHL	CHD-C4C-C3C	-2.72	120.85	124.84
28	6	1623	NEX	C30-C31-C32	-2.71	114.75	123.22
25	g	604	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	p	605	CHL	O2D-CGD-O1D	-2.71	118.53	123.84
25	5	611	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	C	508	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	5	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
37	C	520	DGD	O1G-C1A-C2A	2.71	120.42	111.91
37	c	520	DGD	O1G-C1A-C2A	2.71	120.42	111.91
25	r	604	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
24	9	607	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
28	R	623	NEX	C35-C34-C33	-2.71	123.44	127.31
25	A	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	b	611	CLA	CHB-C1B-NB	2.71	127.13	124.26
26	2	1621	LUT	C31-C30-C29	-2.71	123.44	127.31
27	Y	1622	XAT	C36-C21-C26	2.71	117.36	110.05
25	c	508	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
26	N	1620	LUT	C15-C14-C13	-2.71	123.44	127.31
25	R	604	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
24	4	605	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
26	s	1621	LUT	C16-C1-C6	-2.71	105.91	110.30
25	n	603	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	5	1620	LUT	C36-C21-C26	2.71	113.65	109.55
25	d	403	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	y	2630	LHG	C5-O7-C7	-2.71	111.12	117.79
25	s	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	5	607	CHL	C2A-C3A-C4A	-2.71	97.50	101.87
34	B	620	BCR	C28-C27-C26	-2.71	109.24	114.08
24	4	608	CHL	C3B-C4B-NB	2.71	113.03	110.52
26	G	1620	LUT	C10-C11-C12	-2.71	114.77	123.22
25	G	614	CLA	CHB-C1B-NB	2.71	127.12	124.26
25	B	613	CLA	C2A-C1A-CHA	2.71	128.59	123.86
25	c	501	CLA	CHB-C4A-NA	2.71	128.25	124.51
24	0	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
24	p	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
25	g	602	CLA	CHB-C4A-NA	2.71	128.25	124.51
26	1	1620	LUT	C7-C8-C9	-2.70	122.15	126.23
25	s	602	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	q	610	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	1620	LUT	C10-C11-C12	-2.70	114.78	123.22
24	5	605	CHL	C4-C3-C5	2.70	119.82	115.27
24	Y	606	CHL	CMD-C2D-C3D	-2.70	121.39	127.61
25	b	613	CLA	C2A-C1A-CHA	2.70	128.59	123.86
25	D	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	B	614	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
28	R	623	NEX	C15-C35-C34	-2.70	117.94	123.47
29	Y	2630	LHG	O8-C23-C24	2.70	120.39	111.91
24	4	605	CHL	O2A-CGA-CBA	2.70	120.39	111.91
25	4	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	B	604	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	N	610	CLA	CHB-C1B-NB	2.70	127.12	124.26
25	N	603	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	6	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	2	609	CHL	CHB-C4A-NA	2.70	128.24	124.51
25	G	604	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	n	1621	LUT	C19-C9-C8	2.70	122.33	118.08
24	8	608	CHL	CHC-C4B-NB	-2.70	121.40	124.26
25	N	603	CLA	CHC-C4B-NB	2.70	127.11	124.26
24	y	608	CHL	CHB-C4A-NA	2.70	128.24	124.51
25	7	603	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
24	p	607	CHL	CHC-C4B-NB	-2.70	121.40	124.26
24	y	606	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
26	6	1620	LUT	C3-C4-C5	-2.70	106.48	111.85
25	G	602	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	R	602	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	9	601	CHL	C11-C10-C8	-2.69	107.21	115.92
25	n	612	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
26	S	1621	LUT	C16-C1-C6	-2.69	105.93	110.30
24	1	607	CHL	C4-C3-C5	2.69	119.80	115.27
25	b	604	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
36	A	413	LMG	O8-C28-C29	2.69	120.35	111.91
25	7	612	CLA	CHB-C1B-NB	2.69	127.11	124.26
26	4	1620	LUT	C31-C30-C29	-2.69	123.47	127.31
24	G	607	CHL	CAA-C2A-C3A	-2.69	105.41	112.78
26	6	1620	LUT	C1-C2-C3	2.69	119.72	113.64
25	r	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	q	1621	LUT	C19-C9-C8	2.69	122.31	118.08
25	1	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	2	605	CHL	CMB-C2B-C1B	2.69	129.47	125.37
25	n	602	CLA	CHB-C1B-NB	2.69	127.10	124.26
36	a	413	LMG	O8-C28-C29	2.69	120.35	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	601	CHL	O2A-CGA-CBA	2.69	120.35	111.91
25	c	512	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
26	N	1621	LUT	C38-C25-C24	-2.69	117.81	123.56
26	8	1621	LUT	C30-C31-C32	-2.69	114.83	123.22
24	9	609	CHL	CMB-C2B-C1B	2.69	129.46	125.37
26	0	1621	LUT	C38-C25-C24	-2.69	117.81	123.56
24	0	608	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	7	601	CHL	C2A-C1A-CHA	-2.69	119.16	123.86
25	4	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	9	606	CHL	C3B-C4B-NB	2.69	113.01	110.52
25	B	610	CLA	CHC-C4B-NB	2.69	127.10	124.26
24	2	607	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
24	Y	609	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
35	a	412	SQD	O48-C23-C24	2.69	120.33	111.91
24	G	607	CHL	CHB-C4A-NA	2.69	128.22	124.51
26	q	1620	LUT	C38-C25-C24	-2.69	117.81	123.56
24	N	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
25	9	610	CLA	CHB-C1B-NB	2.68	127.10	124.26
24	4	605	CHL	C3B-C4B-NB	2.68	113.00	110.52
29	8	2630	LHG	O8-C23-C24	2.68	120.33	111.91
26	2	1621	LUT	C18-C5-C6	-2.68	121.52	124.53
25	0	604	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	2	607	CHL	CHC-C4B-NB	-2.68	121.42	124.26
25	G	614	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	7	607	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
25	1	612	CLA	CHB-C1B-NB	2.68	127.10	124.26
25	s	604	CLA	CHB-C1B-NB	2.68	127.10	124.26
25	Y	612	CLA	C1-C2-C3	-2.68	121.41	126.04
29	C	2630	LHG	C5-O7-C7	-2.68	111.19	117.79
24	9	609	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
25	r	602	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	p	605	CHL	CMB-C2B-C1B	2.68	129.45	125.37
25	1	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
27	6	1622	XAT	C31-C32-C33	-2.68	118.89	126.42
35	A	412	SQD	O48-C23-C24	2.68	120.32	111.91
25	b	617	CLA	CHC-C4B-NB	2.68	127.09	124.26
24	p	608	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
28	8	1623	NEX	C17-C1-C6	-2.68	108.08	110.47
24	9	606	CHL	CMB-C2B-C1B	2.68	129.45	125.37
25	C	508	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
25	Y	610	CLA	C4A-NA-C1A	2.68	107.91	106.71
24	n	609	CHL	CMD-C2D-C3D	-2.68	121.45	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	1621	LUT	C38-C25-C24	-2.68	117.83	123.56
25	B	611	CLA	CHB-C1B-NB	2.68	127.09	124.26
24	y	606	CHL	CAC-C3C-C4C	2.68	128.28	124.81
24	1	607	CHL	C4D-CHA-C1A	-2.68	117.99	121.25
24	9	605	CHL	CAA-C2A-C3A	-2.68	105.45	112.78
26	S	1621	LUT	C38-C25-C24	-2.68	117.83	123.56
26	y	1621	LUT	C3-C4-C5	-2.67	106.53	111.85
26	y	1620	LUT	C15-C14-C13	-2.67	123.50	127.31
25	4	611	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
24	0	607	CHL	O2A-CGA-CBA	2.67	120.30	111.91
24	n	605	CHL	CHC-C4B-NB	-2.67	121.43	124.26
25	0	603	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	9	612	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	C	504	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	1	1621	LUT	C18-C5-C4	2.67	119.30	114.36
28	S	1623	NEX	O24-C25-C38	2.67	118.26	115.06
24	4	607	CHL	O2A-CGA-CBA	2.67	120.29	111.91
25	R	603	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	g	610	CLA	CHB-C4A-NA	2.67	128.20	124.51
28	s	1623	NEX	O24-C25-C38	2.67	118.25	115.06
24	8	605	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
24	N	607	CHL	CMB-C2B-C1B	2.67	129.43	125.37
25	4	603	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
25	R	613	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
24	q	606	CHL	CHD-C4C-C3C	-2.66	120.92	124.84
25	6	613	CLA	CHB-C4A-NA	2.66	128.20	124.51
24	8	606	CHL	CMB-C2B-C1B	2.66	129.43	125.37
25	q	612	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	q	1621	LUT	C10-C11-C12	-2.66	114.90	123.22
24	8	609	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
25	S	604	CLA	CHB-C1B-NB	2.66	127.08	124.26
34	b	619	BCR	C29-C30-C25	2.66	114.58	110.48
24	S	606	CHL	C4A-NA-C1A	-2.66	105.51	106.71
25	S	611	CLA	C3B-C4B-NB	-2.66	108.05	110.52
26	R	620	LUT	C7-C8-C9	-2.66	122.21	126.23
25	1	604	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	5	606	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
25	2	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	0	1622	XAT	C7-C8-C9	-2.66	121.40	125.53
24	g	607	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
24	7	601	CHL	C4-C3-C5	2.66	119.75	115.27
34	C	515	BCR	C11-C10-C9	-2.66	123.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	606	CHL	CAC-C3C-C4C	2.66	128.26	124.81
24	2	605	CHL	CAA-C2A-C3A	-2.66	105.50	112.78
26	S	1620	LUT	C30-C31-C32	-2.66	114.92	123.22
24	0	607	CHL	O2D-CGD-O1D	-2.66	118.64	123.84
27	p	1622	XAT	C26-C27-C28	-2.66	120.37	125.99
24	1	607	CHL	O2A-CGA-CBA	2.66	120.25	111.91
28	y	1623	NEX	C17-C1-C6	-2.66	108.09	110.47
25	N	602	CLA	CHB-C1B-NB	2.66	127.07	124.26
24	N	608	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
26	Y	1621	LUT	C3-C4-C5	-2.66	106.56	111.85
35	D	413	SQD	O6-C1-C2	2.66	112.45	108.30
24	p	607	CHL	C4D-CHA-C1A	-2.65	118.02	121.25
25	g	602	CLA	C1-C2-C3	-2.65	121.45	126.04
24	y	608	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
24	6	601	CHL	O2A-CGA-CBA	2.65	120.23	111.91
24	2	606	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
25	q	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	r	606	CHL	CHB-C1B-NB	-2.65	121.45	124.26
28	R	623	NEX	C4-C3-C2	-2.65	105.65	110.77
25	C	508	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	2	601	CHL	CHD-C4C-C3C	-2.65	120.94	124.84
25	q	604	CLA	O2D-CGD-CBD	2.65	115.98	111.27
25	A	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	a	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	p	601	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
25	A	406	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
25	B	608	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	g	614	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	n	601	CHL	O2A-CGA-CBA	2.65	120.22	111.91
26	3	1620	LUT	C35-C15-C14	-2.65	118.05	123.47
24	7	607	CHL	O2A-CGA-CBA	2.65	120.22	111.91
25	G	610	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	b	610	CLA	CHC-C4B-NB	2.65	127.06	124.26
24	4	601	CHL	C3B-C4B-NB	2.65	112.97	110.52
24	n	609	CHL	O1D-CGD-CBD	-2.65	119.06	124.48
25	a	406	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
25	y	613	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	9	1621	LUT	C18-C5-C6	-2.65	121.55	124.53
29	Y	2630	LHG	C9-C8-C7	-2.65	103.99	113.62
24	4	609	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
24	5	608	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
25	C	507	CLA	C7-C6-C5	-2.65	106.17	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	0	1620	LUT	C38-C25-C24	-2.65	117.89	123.56
26	R	620	LUT	C16-C1-C6	-2.65	106.00	110.30
28	5	1623	NEX	C31-C30-C29	-2.65	123.53	127.31
26	s	1621	LUT	C35-C15-C14	-2.65	118.05	123.47
25	5	603	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
24	Y	601	CHL	O1D-CGD-CBD	-2.65	119.07	124.48
25	6	603	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	q	610	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	n	606	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
28	Y	1623	NEX	C11-C10-C9	-2.65	123.53	127.31
26	0	1621	LUT	C16-C1-C6	-2.65	106.01	110.30
26	q	1621	LUT	C3-C4-C5	-2.65	106.58	111.85
29	p	2630	LHG	O8-C23-C24	2.65	120.21	111.91
24	4	606	CHL	CMB-C2B-C1B	2.65	129.40	125.37
24	g	609	CHL	C4-C3-C5	2.65	119.72	115.27
24	g	607	CHL	CHB-C4A-NA	2.65	128.17	124.51
25	Y	612	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	c	504	CLA	CHB-C4A-NA	2.65	128.17	124.51
24	G	601	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
26	p	1620	LUT	C38-C25-C24	-2.64	117.90	123.56
25	s	610	CLA	C4A-NA-C1A	2.64	107.89	106.71
25	Y	611	CLA	C3B-C4B-NB	-2.64	108.06	110.52
24	1	605	CHL	CMB-C2B-C1B	2.64	129.40	125.37
24	q	601	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
24	G	609	CHL	C4-C3-C5	2.64	119.72	115.27
34	B	619	BCR	C29-C30-C25	2.64	114.55	110.48
24	3	605	CHL	CHD-C4C-C3C	-2.64	120.95	124.84
25	n	610	CLA	CHB-C1B-NB	2.64	127.06	124.26
26	q	1620	LUT	C1-C2-C3	2.64	119.61	113.64
29	S	2630	LHG	O8-C23-C24	2.64	120.20	111.91
25	b	603	CLA	CMB-C2B-C1B	-2.64	121.34	125.37
28	4	1623	NEX	C11-C12-C13	-2.64	118.99	126.42
25	b	607	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	0	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	7	609	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	R	616	CLA	CHB-C4A-NA	2.64	128.16	124.51
35	d	413	SQD	O6-C1-C2	2.64	112.43	108.30
25	C	508	CLA	CHB-C1B-NB	2.64	127.05	124.26
26	4	1620	LUT	C38-C25-C24	-2.64	117.91	123.56
24	s	606	CHL	CBA-CAA-C2A	-2.64	108.45	114.02
29	2	2630	LHG	O8-C23-C24	2.64	120.19	111.91
25	4	602	CLA	CHB-C1B-NB	2.64	127.05	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1620	LUT	C15-C14-C13	-2.64	123.55	127.31
24	g	601	CHL	C2A-C1A-CHA	-2.64	119.25	123.86
24	7	606	CHL	CMB-C2B-C1B	2.64	129.38	125.37
25	a	407	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	n	603	CLA	CHC-C4B-NB	2.64	127.05	124.26
24	n	609	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	S	612	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
34	b	619	BCR	C15-C16-C17	-2.64	118.08	123.47
25	B	603	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
26	s	1620	LUT	C30-C31-C32	-2.63	115.00	123.22
24	G	606	CHL	CMD-C2D-C3D	-2.63	121.55	127.61
25	G	604	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
24	3	609	CHL	C1C-C2C-C3C	-2.63	105.02	107.11
25	b	608	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	R	606	CHL	CHB-C1B-NB	-2.63	121.47	124.26
28	g	1623	NEX	C31-C30-C29	-2.63	123.55	127.31
24	3	609	CHL	O2A-CGA-CBA	2.63	120.17	111.91
26	3	1621	LUT	C10-C11-C12	-2.63	115.00	123.22
26	5	1620	LUT	C10-C11-C12	-2.63	115.00	123.22
25	r	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	y	1620	LUT	C30-C31-C32	-2.63	115.00	123.22
24	1	605	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
25	n	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	y	601	CHL	O1D-CGD-CBD	-2.63	119.10	124.48
24	Y	601	CHL	C11-C10-C8	-2.63	107.42	115.92
24	q	601	CHL	C4A-NA-C1A	-2.63	105.52	106.71
27	3	1622	XAT	C15-C35-C34	-2.63	118.09	123.47
25	g	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
28	G	1623	NEX	C35-C34-C33	-2.63	123.56	127.31
28	Y	1623	NEX	C30-C31-C32	-2.63	115.02	123.22
25	c	509	CLA	CHC-C4B-NB	2.63	127.04	124.26
26	r	620	LUT	C15-C35-C34	-2.63	118.09	123.47
24	0	605	CHL	CMB-C2B-C1B	2.63	129.37	125.37
24	p	608	CHL	C1C-C2C-C3C	-2.63	105.03	107.11
24	N	607	CHL	O2A-CGA-CBA	2.63	120.15	111.91
26	r	620	LUT	C16-C1-C6	-2.63	106.04	110.30
26	Y	1620	LUT	C30-C31-C32	-2.63	115.02	123.22
25	N	612	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	n	606	CHL	CHB-C4A-NA	2.63	128.14	124.51
25	q	614	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	g	608	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
26	G	1621	LUT	C22-C23-C24	-2.63	108.75	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	601	CHL	C6-C5-C3	-2.63	106.57	113.45
24	N	609	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
24	n	608	CHL	CMD-C2D-C3D	-2.63	121.58	127.61
25	S	613	CLA	CHC-C4B-NB	2.63	127.04	124.26
24	9	606	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
26	1	1621	LUT	C10-C11-C12	-2.62	115.03	123.22
24	2	605	CHL	CMD-C2D-C3D	-2.62	121.58	127.61
26	R	620	LUT	C15-C35-C34	-2.62	118.10	123.47
34	B	618	BCR	C3-C4-C5	-2.62	109.39	114.08
28	4	1623	NEX	C2-C1-C6	2.62	111.76	109.21
25	y	611	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	A	407	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	3	605	CHL	CMD-C2D-C3D	-2.62	121.58	127.61
25	B	616	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
24	q	606	CHL	CMB-C2B-C1B	2.62	129.36	125.37
25	c	506	CLA	CHB-C1B-NB	2.62	127.03	124.26
25	y	612	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	n	609	CHL	O2A-CGA-CBA	2.62	120.14	111.91
26	7	1621	LUT	C10-C11-C12	-2.62	115.03	123.22
28	y	1623	NEX	C30-C31-C32	-2.62	115.03	123.22
24	7	605	CHL	CMB-C2B-C1B	2.62	129.36	125.37
24	4	607	CHL	C3B-C4B-NB	2.62	112.95	110.52
24	N	606	CHL	CHB-C4A-NA	2.62	128.14	124.51
25	c	503	CLA	CHB-C4A-NA	2.62	128.14	124.51
37	C	523	DGD	O1G-C1A-C2A	2.62	120.13	111.91
37	c	523	DGD	O1G-C1A-C2A	2.62	120.13	111.91
25	b	610	CLA	CMB-C2B-C3B	2.62	132.94	126.59
24	g	607	CHL	CAA-C2A-C3A	-2.62	105.60	112.78
25	G	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	9	610	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	9	605	CHL	CMB-C2B-C1B	2.62	129.36	125.37
25	S	613	CLA	CHB-C1B-NB	2.62	127.03	124.26
25	s	613	CLA	CHB-C1B-NB	2.62	127.03	124.26
25	B	610	CLA	CMB-C2B-C3B	2.62	132.93	126.59
24	6	608	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
25	2	614	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	S	604	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	C	503	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	3	1620	LUT	C21-C26-C27	-2.62	109.39	112.70
25	C	506	CLA	CHB-C1B-NB	2.62	127.03	124.26
25	r	616	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	4	1621	LUT	C35-C34-C33	-2.62	123.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	608	CHL	CHB-C4A-NA	2.62	128.13	124.51
25	Y	613	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	N	609	CHL	O2A-CGA-CBA	2.61	120.11	111.91
25	s	604	CLA	CHD-C1D-ND	-2.61	122.05	124.45
25	S	611	CLA	CHB-C1B-NB	2.61	127.02	124.26
25	7	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	7	607	CHL	C4-C3-C5	2.61	119.67	115.27
25	b	617	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	0	611	CLA	C1-C2-C3	-2.61	121.52	126.04
26	r	620	LUT	C7-C8-C9	-2.61	122.29	126.23
25	B	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	c	508	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	3	608	CHL	CMB-C2B-C1B	2.61	129.35	125.37
25	p	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	9	605	CHL	CMD-C2D-C3D	-2.61	121.60	127.61
34	B	619	BCR	C15-C16-C17	-2.61	118.12	123.47
25	p	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	y	609	CHL	C4-C3-C5	2.61	119.66	115.27
25	N	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	0	1621	LUT	C10-C11-C12	-2.61	115.07	123.22
25	b	608	CLA	C7-C6-C5	-2.61	106.27	113.36
25	b	616	CLA	CHB-C1B-NB	2.61	127.02	124.26
25	c	504	CLA	C4-C3-C5	2.61	119.66	115.27
25	b	603	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	5	607	CHL	C4D-CHA-C1A	-2.61	118.08	121.25
28	4	1623	NEX	C17-C1-C6	-2.61	108.14	110.47
29	4	2630	LHG	O8-C23-C24	2.61	120.09	111.91
24	1	601	CHL	C2A-C1A-CHA	-2.61	119.30	123.86
25	9	614	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	c	507	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	g	606	CHL	CMD-C2D-C3D	-2.61	121.62	127.61
25	C	504	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	g	602	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	9	614	CLA	CHC-C4B-NB	2.61	127.02	124.26
25	B	605	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
24	S	607	CHL	CMB-C2B-C1B	2.61	129.34	125.37
25	c	512	CLA	C3B-C4B-NB	-2.61	108.10	110.52
25	G	602	CLA	C1-C2-C3	-2.60	121.54	126.04
25	c	507	CLA	C7-C6-C5	-2.60	106.28	113.36
24	9	605	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
25	s	613	CLA	CHC-C4B-NB	2.60	127.01	124.26
24	S	606	CHL	CBA-CAA-C2A	-2.60	108.52	114.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	1623	NEX	C24-C23-C22	-2.60	105.75	110.77
26	2	1621	LUT	C7-C8-C9	-2.60	122.30	126.23
25	G	602	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
24	5	605	CHL	CHC-C4B-NB	-2.60	121.50	124.26
24	5	607	CHL	C4A-NA-C1A	-2.60	105.54	106.71
24	1	609	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
25	c	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	N	606	CHL	C3B-C4B-NB	2.60	112.93	110.52
25	p	614	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	0	601	CHL	C1-C2-C3	-2.60	121.55	126.04
28	N	1623	NEX	C24-C23-C22	-2.60	105.75	110.77
34	b	618	BCR	C3-C4-C5	-2.60	109.44	114.08
28	Y	1623	NEX	C5-C4-C3	-2.60	108.67	111.75
25	Y	614	CLA	CHB-C1B-NB	2.60	127.01	124.26
28	s	1623	NEX	C15-C35-C34	-2.60	118.15	123.47
25	n	613	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	0	610	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	b	616	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
24	3	607	CHL	C1-O2A-CGA	2.60	123.26	116.44
25	B	617	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
24	s	607	CHL	CMB-C2B-C1B	2.60	129.32	125.37
25	4	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
34	b	619	BCR	C8-C7-C6	-2.60	119.91	127.20
26	5	1621	LUT	C3-C4-C5	-2.60	106.68	111.85
25	B	613	CLA	CMB-C2B-C3B	2.60	132.88	126.59
25	b	613	CLA	CMB-C2B-C3B	2.60	132.88	126.59
25	8	602	CLA	CMB-C2B-C1B	-2.60	121.42	125.37
25	r	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	b	605	CLA	O2A-CGA-O1A	-2.59	117.04	123.59
25	2	610	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	n	601	CHL	CGD-CBD-CAD	-2.59	102.33	110.73
27	5	1622	XAT	C7-C8-C9	-2.59	121.51	125.53
29	s	2630	LHG	O8-C23-C24	2.59	120.05	111.91
24	7	607	CHL	C1-C2-C3	-2.59	121.56	126.04
24	0	606	CHL	O2A-CGA-CBA	2.59	120.04	111.91
24	3	606	CHL	O2D-CGD-O1D	-2.59	118.77	123.84
26	S	1621	LUT	C35-C15-C14	-2.59	118.17	123.47
28	N	1623	NEX	C16-C1-C6	2.59	112.79	110.47
24	6	601	CHL	CMB-C2B-C1B	2.59	129.31	125.37
25	7	613	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
25	1	612	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
25	A	406	CLA	CHC-C4B-NB	2.59	127.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	1620	LUT	C10-C11-C12	-2.59	115.14	123.22
34	A	411	BCR	C11-C10-C9	-2.59	123.62	127.31
34	a	411	BCR	C11-C10-C9	-2.59	123.62	127.31
28	1	1623	NEX	C5-C4-C3	-2.59	108.68	111.75
24	S	601	CHL	C3B-C4B-NB	2.59	112.92	110.52
24	N	601	CHL	O2A-CGA-CBA	2.59	120.03	111.91
24	1	606	CHL	CMB-C2B-C1B	2.59	129.31	125.37
34	B	619	BCR	C8-C7-C6	-2.59	119.94	127.20
24	n	601	CHL	CBC-CAC-C3C	-2.59	105.30	112.43
24	q	601	CHL	CMD-C2D-C3D	-2.59	121.67	127.61
37	c	519	DGD	O3G-C1D-C2D	2.59	112.34	108.30
25	8	604	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
25	C	504	CLA	C4-C3-C5	2.58	119.62	115.27
25	R	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
24	0	609	CHL	C1-C2-C3	-2.58	121.57	126.04
34	c	516	BCR	C7-C8-C9	-2.58	122.33	126.23
24	G	601	CHL	CBC-CAC-C3C	-2.58	105.31	112.43
25	4	603	CLA	C2A-C1A-CHA	2.58	128.38	123.86
24	p	609	CHL	CMB-C2B-C1B	2.58	129.30	125.37
25	c	504	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	n	1620	LUT	C20-C13-C12	2.58	122.15	118.08
24	5	601	CHL	C4-C3-C5	2.58	119.61	115.27
25	G	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	1	1623	NEX	C26-C27-C28	-2.58	120.53	125.99
25	r	602	CLA	C3B-C4B-NB	-2.58	108.12	110.52
25	C	509	CLA	CHC-C4B-NB	2.58	126.99	124.26
24	6	607	CHL	O2A-CGA-CBA	2.58	120.01	111.91
24	q	609	CHL	C3A-C2A-C1A	-2.58	97.47	101.34
25	8	603	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
25	B	609	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	b	609	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	N	1621	LUT	C19-C9-C8	2.58	122.14	118.08
25	R	602	CLA	C3B-C4B-NB	-2.58	108.12	110.52
26	4	1620	LUT	C18-C5-C6	-2.58	121.63	124.53
25	2	611	CLA	CHB-C1B-NB	2.58	126.98	124.26
25	S	604	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
34	D	404	BCR	C38-C26-C27	2.58	118.56	113.62
24	1	609	CHL	CMD-C2D-C3D	-2.58	121.69	127.61
24	y	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
25	C	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
34	d	404	BCR	C38-C26-C27	2.57	118.56	113.62
25	C	512	CLA	C3B-C4B-NB	-2.57	108.13	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	601	CHL	C7-C6-C5	-2.57	106.37	113.36
26	n	1620	LUT	C38-C25-C24	-2.57	118.05	123.56
25	1	612	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
25	9	611	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	3	607	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
25	b	615	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	q	603	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
25	B	603	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
26	q	1621	LUT	C38-C25-C24	-2.57	118.06	123.56
25	6	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	C	510	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
24	8	608	CHL	CMB-C2B-C1B	2.57	129.28	125.37
26	6	1620	LUT	C38-C25-C24	-2.57	118.06	123.56
25	r	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	n	1620	LUT	C10-C11-C12	-2.57	115.21	123.22
34	C	515	BCR	C21-C20-C19	-2.57	115.21	123.22
25	g	610	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
25	7	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	p	603	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
26	s	1621	LUT	C18-C5-C4	2.57	119.11	114.36
24	p	607	CHL	CMB-C2B-C1B	2.57	129.28	125.37
25	a	405	CLA	CMB-C2B-C3B	2.57	132.80	126.59
25	1	610	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	B	612	CLA	CAC-C3C-C4C	2.56	128.14	124.81
25	a	405	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	6	1620	LUT	C10-C11-C12	-2.56	115.22	123.22
25	d	402	CLA	CHC-C4B-NB	2.56	126.97	124.26
25	3	602	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
34	b	618	BCR	C15-C16-C17	-2.56	118.22	123.47
25	3	604	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	q	613	CLA	CMB-C2B-C3B	2.56	132.79	126.59
28	3	1623	NEX	C17-C1-C6	-2.56	108.18	110.47
24	9	607	CHL	CHC-C4B-NB	-2.56	121.55	124.26
24	2	605	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
24	6	606	CHL	O2A-CGA-CBA	2.56	119.94	111.91
24	G	605	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
25	y	614	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	n	602	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
24	4	609	CHL	CHD-C1D-C2D	2.56	130.85	125.48
24	q	605	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
25	B	608	CLA	C7-C6-C5	-2.56	106.41	113.36
25	2	610	CLA	CHB-C1B-NB	2.56	126.97	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	402	CLA	CHC-C4B-NB	2.56	126.97	124.26
26	Y	1620	LUT	C11-C10-C9	-2.56	123.66	127.31
24	Y	605	CHL	CHB-C4A-NA	2.56	128.05	124.51
25	s	612	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	C	507	CLA	C2A-C1A-CHA	2.56	128.33	123.86
25	b	612	CLA	CAC-C3C-C4C	2.56	128.13	124.81
25	N	612	CLA	CHC-C4B-NB	2.56	126.97	124.26
29	l	101	LHG	C5-O7-C7	-2.56	111.49	117.79
25	N	602	CLA	C1-C2-C3	-2.56	121.62	126.04
24	q	606	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
25	3	603	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
26	4	1621	LUT	C15-C14-C13	-2.56	123.66	127.31
26	p	1621	LUT	C15-C14-C13	-2.56	123.66	127.31
25	1	613	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
25	c	511	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	Y	609	CHL	C4-C3-C5	2.56	119.57	115.27
26	5	1620	LUT	C15-C35-C34	-2.56	118.24	123.47
28	5	1623	NEX	C17-C1-C6	-2.56	108.19	110.47
28	G	1623	NEX	C4-C3-C2	-2.55	105.84	110.77
29	4	2630	LHG	C5-O7-C7	-2.55	111.50	117.79
25	A	405	CLA	CMB-C2B-C3B	2.55	132.78	126.59
25	R	612	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
25	a	406	CLA	CHC-C4B-NB	2.55	126.96	124.26
28	6	1623	NEX	C15-C35-C34	-2.55	118.24	123.47
25	c	510	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
34	B	618	BCR	C15-C16-C17	-2.55	118.24	123.47
25	s	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	R	604	CLA	CHB-C1B-NB	2.55	126.96	124.26
24	8	609	CHL	O1D-CGD-CBD	-2.55	119.26	124.48
37	C	519	DGD	O1G-C1A-C2A	2.55	119.92	111.91
26	s	1621	LUT	C15-C14-C13	-2.55	123.67	127.31
24	5	606	CHL	C3B-C4B-NB	2.55	112.88	110.52
25	B	616	CLA	CHB-C1B-NB	2.55	126.96	124.26
25	6	612	CLA	CHB-C1B-NB	2.55	126.96	124.26
34	a	411	BCR	C38-C26-C25	-2.55	121.66	124.53
25	5	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	G	610	CLA	CAA-CBA-CGA	-2.55	105.80	113.25
24	9	609	CHL	O2A-CGA-CBA	2.55	119.91	111.91
24	2	605	CHL	C4D-CHA-C1A	-2.55	118.15	121.25
29	s	2630	LHG	C5-O7-C7	-2.55	111.51	117.79
28	S	1623	NEX	C24-C23-C22	-2.55	105.85	110.77
24	8	607	CHL	C1C-C2C-C3C	-2.55	105.09	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	1621	LUT	C3-C4-C5	-2.55	106.78	111.85
25	A	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	6	605	CHL	CMB-C2B-C1B	2.55	129.25	125.37
25	c	502	CLA	CHC-C1C-NC	2.55	128.07	124.20
24	N	606	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
25	C	511	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	s	613	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
25	A	405	CLA	C3B-C4B-NB	-2.55	108.15	110.52
26	N	1620	LUT	C38-C25-C24	-2.55	118.11	123.56
25	2	614	CLA	CHC-C4B-NB	2.55	126.95	124.26
25	6	602	CLA	CHB-C1B-NB	2.55	126.95	124.26
24	Y	607	CHL	O1D-CGD-CBD	-2.55	119.28	124.48
26	1	1620	LUT	C18-C5-C6	-2.55	121.67	124.53
24	s	601	CHL	C3B-C4B-NB	2.54	112.88	110.52
37	C	518	DGD	C2G-O2G-C1B	-2.54	111.53	117.79
24	g	606	CHL	C4A-NA-C1A	-2.54	105.56	106.71
26	S	1621	LUT	C18-C5-C4	2.54	119.07	114.36
27	0	1622	XAT	C15-C35-C34	-2.54	118.26	123.47
24	0	606	CHL	C6-C7-C8	-2.54	107.69	115.92
24	8	607	CHL	CMD-C2D-C3D	-2.54	121.76	127.61
24	N	601	CHL	O2D-CGD-O1D	-2.54	118.86	123.84
26	4	1621	LUT	C20-C13-C12	2.54	122.08	118.08
24	0	609	CHL	C4-C3-C5	2.54	119.55	115.27
24	3	609	CHL	O1D-CGD-CBD	-2.54	119.28	124.48
25	p	602	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
25	7	612	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
24	1	607	CHL	CHC-C4B-NB	-2.54	121.57	124.26
25	s	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
25	B	612	CLA	C1-C2-C3	-2.54	121.65	126.04
24	p	607	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
25	n	612	CLA	CHC-C4B-NB	2.54	126.95	124.26
25	5	611	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	n	601	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
25	2	603	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
24	0	606	CHL	C3B-C4B-NB	2.54	112.87	110.52
25	g	604	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
24	2	607	CHL	CMD-C2D-C3D	-2.54	121.78	127.61
27	n	1622	XAT	C10-C11-C12	-2.54	115.30	123.22
25	S	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
37	c	519	DGD	O1G-C1A-C2A	2.54	119.87	111.91
34	A	411	BCR	C28-C27-C26	-2.54	109.55	114.08
25	r	613	CLA	CHD-C1D-ND	-2.53	122.12	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	613	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
34	c	514	BCR	C16-C15-C14	-2.53	118.28	123.47
25	S	610	CLA	C4A-NA-C1A	2.53	107.84	106.71
25	5	611	CLA	CHB-C1B-NB	2.53	126.94	124.26
25	0	604	CLA	CHB-C1B-NB	2.53	126.94	124.26
24	p	607	CHL	O2A-CGA-CBA	2.53	119.86	111.91
25	2	611	CLA	CHC-C4B-NB	2.53	126.94	124.26
37	C	519	DGD	O3G-C1D-C2D	2.53	112.26	108.30
24	y	601	CHL	C1-O2A-CGA	2.53	123.09	116.44
29	0	2630	LHG	O8-C23-C24	2.53	119.85	111.91
25	C	509	CLA	C2A-C1A-CHA	2.53	128.28	123.86
25	R	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
26	5	1621	LUT	C38-C25-C24	-2.53	118.15	123.56
25	r	604	CLA	CHB-C1B-NB	2.53	126.93	124.26
24	5	608	CHL	O2A-CGA-CBA	2.53	119.84	111.91
24	g	605	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
24	Y	608	CHL	CMB-C2B-C1B	2.53	129.22	125.37
25	p	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	q	601	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
26	g	1621	LUT	C3-C4-C5	-2.53	106.82	111.85
25	g	614	CLA	C3B-C4B-NB	-2.53	108.17	110.52
34	A	411	BCR	C38-C26-C25	-2.53	121.69	124.53
26	6	1620	LUT	C8-C7-C6	-2.53	120.11	127.20
25	3	614	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	g	605	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
25	3	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
25	r	613	CLA	C4-C3-C5	2.52	119.52	115.27
24	S	601	CHL	CMB-C2B-C1B	2.52	129.21	125.37
25	C	502	CLA	CHC-C1C-NC	2.52	128.03	124.20
25	a	405	CLA	C3B-C4B-NB	-2.52	108.17	110.52
26	S	1621	LUT	C15-C14-C13	-2.52	123.71	127.31
27	N	1622	XAT	C24-C23-C22	-2.52	105.90	110.77
25	4	614	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	5	1623	NEX	C30-C31-C32	-2.52	115.35	123.22
24	0	609	CHL	C3B-C4B-NB	2.52	112.85	110.52
25	B	615	CLA	CHB-C1B-NB	2.52	126.93	124.26
37	c	524	DGD	O1G-C1A-C2A	2.52	119.82	111.91
24	9	605	CHL	C4D-CHA-C1A	-2.52	118.18	121.25
25	D	402	CLA	CBA-CAA-C2A	-2.52	106.42	113.86
25	s	602	CLA	O2D-CGD-CBD	2.52	115.75	111.27
25	s	604	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
24	n	605	CHL	C4-C3-C5	2.52	119.51	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	601	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
27	2	1622	XAT	C31-C32-C33	-2.52	119.34	126.42
37	c	518	DGD	C2G-O2G-C1B	-2.52	111.59	117.79
26	y	1620	LUT	C11-C10-C9	-2.52	123.72	127.31
25	N	602	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
25	7	610	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	3	607	CHL	C1C-C2C-C3C	-2.52	105.12	107.11
34	a	411	BCR	C28-C27-C26	-2.52	109.58	114.08
24	0	601	CHL	CHC-C4B-NB	-2.52	121.59	124.26
25	9	602	CLA	C4-C3-C5	2.52	119.50	115.27
25	s	611	CLA	CHB-C1B-NB	2.52	126.92	124.26
25	S	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	6	606	CHL	C6-C7-C8	-2.52	107.79	115.92
25	R	602	CLA	O2D-CGD-CBD	2.51	115.74	111.27
28	s	1623	NEX	C31-C32-C33	-2.51	119.35	126.42
25	c	505	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
24	G	605	CHL	O2D-CGD-O1D	-2.51	118.92	123.84
25	n	612	CLA	CHB-C1B-NB	2.51	126.92	124.26
27	8	1622	XAT	C10-C11-C12	-2.51	115.38	123.22
27	n	1622	XAT	C24-C23-C22	-2.51	105.92	110.77
25	Y	610	CLA	CMB-C2B-C3B	2.51	132.67	126.59
28	n	1623	NEX	C16-C1-C6	2.51	112.72	110.47
25	C	503	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	8	607	CHL	CHC-C4B-NB	-2.51	121.60	124.26
25	1	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	Y	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	y	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	c	515	BCR	C21-C20-C19	-2.51	115.38	123.22
24	p	608	CHL	O2A-CGA-CBA	2.51	119.79	111.91
25	b	612	CLA	C1-C2-C3	-2.51	121.70	126.04
29	D	408	LHG	O8-C23-C24	2.51	119.78	111.91
24	N	609	CHL	O1D-CGD-CBD	-2.51	119.35	124.48
24	6	605	CHL	CMD-C2D-C3D	-2.51	121.84	127.61
24	s	608	CHL	O2A-CGA-O1A	-2.51	117.26	123.59
24	y	607	CHL	O1D-CGD-CBD	-2.51	119.35	124.48
29	d	408	LHG	O8-C23-C24	2.51	119.78	111.91
25	9	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	6	1620	LUT	C18-C5-C6	-2.51	121.71	124.53
24	0	608	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
29	S	2630	LHG	C5-O7-C7	-2.51	111.62	117.79
25	2	604	CLA	CHB-C1B-NB	2.51	126.91	124.26
25	c	508	CLA	CHB-C1B-NB	2.51	126.91	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	1623	NEX	C4-C3-C2	-2.51	105.93	110.77
24	G	601	CHL	CGD-CBD-CAD	-2.51	102.62	110.73
26	8	1621	LUT	C10-C11-C12	-2.51	115.40	123.22
25	B	609	CLA	CMB-C2B-C3B	2.51	132.66	126.59
25	y	610	CLA	CMB-C2B-C3B	2.51	132.66	126.59
25	Y	612	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	q	1623	NEX	C11-C12-C13	-2.50	119.38	126.42
24	y	608	CHL	CMB-C2B-C1B	2.50	129.18	125.37
25	7	613	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
26	7	1620	LUT	C38-C25-C24	-2.50	118.20	123.56
34	C	514	BCR	C16-C15-C14	-2.50	118.34	123.47
24	9	609	CHL	CHD-C4C-C3C	-2.50	121.16	124.84
25	d	402	CLA	CBA-CAA-C2A	-2.50	106.47	113.86
24	n	605	CHL	C1-C2-C3	-2.50	121.71	126.04
24	G	606	CHL	CHC-C4B-NB	-2.50	121.61	124.26
24	n	601	CHL	C2A-C1A-CHA	-2.50	119.48	123.86
25	n	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	1	607	CHL	C3B-C4B-NB	2.50	112.84	110.52
25	5	604	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
27	n	1622	XAT	C40-C33-C32	2.50	122.02	118.08
25	0	612	CLA	CHB-C1B-NB	2.50	126.91	124.26
37	C	524	DGD	O1G-C1A-C2A	2.50	119.76	111.91
28	G	1623	NEX	C31-C30-C29	-2.50	123.74	127.31
25	A	410	CLA	C3B-C4B-NB	-2.50	108.19	110.52
25	b	609	CLA	CMB-C2B-C3B	2.50	132.65	126.59
25	c	509	CLA	C2A-C1A-CHA	2.50	128.23	123.86
25	1	612	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
25	G	603	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
26	8	1620	LUT	C11-C10-C9	-2.50	123.74	127.31
24	1	607	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
24	5	608	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
24	y	607	CHL	C11-C10-C8	-2.50	107.84	115.92
25	B	615	CLA	CHC-C4B-NB	2.50	126.90	124.26
25	0	613	CLA	CHD-C1D-ND	-2.50	122.16	124.45
24	r	607	CHL	C4D-CHA-C1A	-2.50	118.21	121.25
25	R	603	CLA	CHC-C4B-NB	2.50	126.90	124.26
24	g	601	CHL	CGD-CBD-CAD	-2.50	102.65	110.73
28	2	1623	NEX	C28-C29-C30	2.50	122.77	118.94
25	5	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
25	3	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	C	505	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	q	611	CLA	O2D-CGD-O1D	-2.50	118.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	605	CHL	O1D-CGD-CBD	-2.49	119.38	124.48
25	1	602	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
34	A	411	BCR	C10-C11-C12	-2.49	115.43	123.22
34	a	411	BCR	C10-C11-C12	-2.49	115.43	123.22
26	s	1620	LUT	C3-C4-C5	-2.49	106.88	111.85
25	S	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	g	606	CHL	CHC-C4B-NB	-2.49	121.62	124.26
25	0	602	CLA	CHB-C1B-NB	2.49	126.90	124.26
25	g	614	CLA	CHC-C4B-NB	2.49	126.90	124.26
25	a	410	CLA	C3B-C4B-NB	-2.49	108.20	110.52
25	N	610	CLA	C1-C2-C3	-2.49	121.73	126.04
25	c	511	CLA	O2D-CGD-CBD	2.49	115.70	111.27
24	6	606	CHL	CMB-C2B-C1B	2.49	129.17	125.37
25	r	602	CLA	O2D-CGD-CBD	2.49	115.70	111.27
25	0	604	CLA	CHD-C1D-ND	-2.49	122.16	124.45
25	9	614	CLA	CHB-C1B-NB	2.49	126.90	124.26
28	s	1623	NEX	C24-C23-C22	-2.49	105.96	110.77
25	2	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	9	1621	LUT	C11-C10-C9	-2.49	123.75	127.31
25	y	612	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	1	1621	LUT	C2-C3-C4	2.49	113.71	110.30
26	3	1620	LUT	C18-C5-C6	-2.49	121.73	124.53
26	2	1621	LUT	C1-C2-C3	2.49	119.27	113.64
24	S	608	CHL	O2A-CGA-O1A	-2.49	117.31	123.59
24	9	601	CHL	CAA-CBA-CGA	-2.49	105.98	113.25
24	G	601	CHL	O2A-CGA-CBA	2.49	119.72	111.91
24	R	607	CHL	C4D-CHA-C1A	-2.49	118.22	121.25
24	p	607	CHL	C1-C2-C3	-2.49	121.74	126.04
34	a	411	BCR	C21-C20-C19	-2.49	115.45	123.22
24	2	609	CHL	O2A-CGA-CBA	2.49	119.72	111.91
34	H	101	BCR	C38-C26-C27	2.49	118.40	113.62
26	1	1620	LUT	C38-C25-C24	-2.49	118.23	123.56
24	2	606	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
24	q	606	CHL	CED-O2D-CGD	2.49	121.56	115.94
26	y	1621	LUT	C38-C25-C24	-2.49	118.24	123.56
25	7	602	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
27	g	1622	XAT	C15-C35-C34	-2.49	118.38	123.47
25	8	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	2	1620	LUT	C38-C25-C24	-2.49	118.24	123.56
25	A	406	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
25	a	406	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
25	a	410	CLA	O2D-CGD-O1D	-2.49	118.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	q	1623	NEX	C27-C28-C29	-2.49	121.67	125.53
25	A	410	CLA	CMB-C2B-C3B	2.49	132.61	126.59
25	g	603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	r	608	CHL	O2A-CGA-CBA	2.49	119.71	111.91
25	a	410	CLA	CMB-C2B-C3B	2.49	132.61	126.59
25	1	613	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	6	609	CHL	O2A-CGA-CBA	2.49	119.71	111.91
26	Y	1621	LUT	C38-C25-C24	-2.49	118.24	123.56
25	D	403	CLA	CHD-C1D-ND	-2.49	122.17	124.45
26	5	1620	LUT	C22-C23-C24	-2.48	108.91	111.74
25	9	611	CLA	CHC-C4B-NB	2.48	126.89	124.26
26	9	1620	LUT	C38-C25-C24	-2.48	118.25	123.56
25	9	603	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
26	0	1620	LUT	C35-C15-C14	-2.48	118.39	123.47
25	C	503	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
24	p	601	CHL	O2A-CGA-CBA	2.48	119.70	111.91
27	N	1622	XAT	C10-C11-C12	-2.48	115.47	123.22
24	R	608	CHL	O2A-CGA-CBA	2.48	119.70	111.91
26	1	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
25	2	614	CLA	CHB-C1B-NB	2.48	126.88	124.26
25	b	615	CLA	CHC-C4B-NB	2.48	126.88	124.26
26	y	1621	LUT	C15-C35-C34	-2.48	118.39	123.47
34	C	516	BCR	C7-C8-C9	-2.48	122.49	126.23
25	n	610	CLA	C1-C2-C3	-2.48	121.75	126.04
26	7	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
25	9	611	CLA	CHB-C1B-NB	2.48	126.88	124.26
24	1	601	CHL	CHC-C4B-NB	-2.48	121.63	124.26
24	2	601	CHL	C4-C3-C5	2.48	119.44	115.27
24	8	609	CHL	C4A-NA-C1A	-2.48	105.59	106.71
25	C	507	CLA	CHC-C4B-NB	2.48	126.88	124.26
24	S	606	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
25	S	602	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
25	B	603	CLA	CHB-C1B-NB	2.48	126.88	124.26
25	c	507	CLA	C2A-C1A-CHA	2.48	128.19	123.86
26	3	1621	LUT	C38-C25-C24	-2.47	118.27	123.56
25	r	603	CLA	CHC-C4B-NB	2.47	126.88	124.26
28	S	1623	NEX	C2-C1-C6	2.47	111.61	109.21
25	s	614	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
24	g	605	CHL	O2A-CGA-CBA	2.47	119.67	111.91
24	0	601	CHL	C6-C7-C8	-2.47	107.93	115.92
24	n	607	CHL	C1-O2A-CGA	2.47	122.93	116.44
25	C	504	CLA	C3B-C4B-NB	-2.47	108.22	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	410	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	1	1621	LUT	C1-C2-C3	2.47	119.22	113.64
24	s	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
25	s	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	5	605	CHL	CAC-C3C-C4C	2.47	128.01	124.81
24	N	601	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
26	S	1620	LUT	C3-C4-C5	-2.47	106.94	111.85
36	a	413	LMG	C7-O1-C1	-2.47	108.92	113.74
24	4	606	CHL	CMD-C2D-C3D	-2.47	121.94	127.61
25	s	611	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
25	g	613	CLA	CHC-C4B-NB	2.47	126.87	124.26
28	S	1623	NEX	C31-C32-C33	-2.47	119.49	126.42
24	y	601	CHL	C11-C10-C8	-2.47	107.95	115.92
24	7	601	CHL	O1D-CGD-CBD	-2.47	119.44	124.48
25	R	610	CLA	C1-C2-C3	-2.47	121.78	126.04
26	4	1620	LUT	C1-C2-C3	2.47	119.21	113.64
28	7	1623	NEX	C19-C9-C10	-2.47	119.47	122.92
34	h	101	BCR	C38-C26-C27	2.46	118.35	113.62
25	S	603	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
25	8	602	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
24	5	607	CHL	CHC-C4B-NB	-2.46	121.65	124.26
24	5	601	CHL	O1D-CGD-CBD	-2.46	119.44	124.48
34	A	411	BCR	C21-C20-C19	-2.46	115.53	123.22
25	s	612	CLA	CHB-C1B-C2B	-2.46	120.28	127.24
25	y	610	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
29	G	2630	LHG	C6-C5-C4	-2.46	105.96	111.79
25	C	506	CLA	C3B-C4B-NB	-2.46	108.23	110.52
26	Y	1621	LUT	C15-C35-C34	-2.46	118.43	123.47
26	n	1620	LUT	C31-C30-C29	-2.46	123.80	127.31
24	8	606	CHL	CHD-C4C-C3C	-2.46	121.22	124.84
28	r	623	NEX	C30-C31-C32	-2.46	115.54	123.22
26	N	1620	LUT	C35-C15-C14	-2.46	118.44	123.47
25	R	613	CLA	C4-C3-C5	2.46	119.41	115.27
25	n	602	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	n	1623	NEX	O4-C5-C18	-2.46	105.02	109.39
26	8	1621	LUT	C38-C25-C24	-2.46	118.30	123.56
24	Y	601	CHL	C1-C2-C3	-2.46	121.79	126.04
25	n	611	CLA	CHC-C4B-NB	2.46	126.86	124.26
24	9	606	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
24	4	601	CHL	C4-C3-C5	2.46	119.41	115.27
26	6	1620	LUT	C19-C9-C8	2.46	121.95	118.08
24	7	609	CHL	CMD-C2D-C3D	-2.46	121.96	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	605	CHL	O2A-CGA-CBA	2.46	119.62	111.91
24	6	608	CHL	CMB-C2B-C1B	2.46	129.11	125.37
24	7	607	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
24	8	606	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
25	B	607	CLA	CMB-C2B-C1B	-2.46	121.63	125.37
24	4	601	CHL	C1C-C2C-C3C	-2.46	105.17	107.11
25	N	602	CLA	C3B-C4B-NB	-2.46	108.24	110.52
25	C	505	CLA	CMB-C2B-C3B	2.45	132.53	126.59
25	C	511	CLA	O2D-CGD-CBD	2.45	115.63	111.27
26	9	1621	LUT	C38-C25-C24	-2.45	118.31	123.56
25	s	602	CLA	CMB-C2B-C1B	-2.45	121.63	125.37
25	r	610	CLA	C1-C2-C3	-2.45	121.80	126.04
26	p	1621	LUT	C31-C30-C29	-2.45	123.81	127.31
25	Y	602	CLA	CMB-C2B-C3B	2.45	132.53	126.59
25	4	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
25	S	614	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
24	5	601	CHL	C11-C10-C8	-2.45	107.99	115.92
25	8	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	Y	612	CLA	C3B-C4B-NB	-2.45	108.24	110.52
24	n	601	CHL	C11-C10-C8	-2.45	108.00	115.92
26	p	1621	LUT	C38-C25-C24	-2.45	118.32	123.56
25	r	601	CLA	CHA-C1A-NA	-2.45	120.79	126.40
26	9	1621	LUT	C31-C30-C29	-2.45	123.81	127.31
24	4	601	CHL	O1D-CGD-CBD	-2.45	119.47	124.48
25	s	610	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
25	N	611	CLA	CHC-C4B-NB	2.45	126.85	124.26
25	0	604	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
24	q	605	CHL	CHD-C4C-C3C	-2.45	121.24	124.84
24	7	601	CHL	CGD-CBD-CAD	-2.45	102.81	110.73
25	b	603	CLA	CHB-C1B-NB	2.45	126.85	124.26
25	y	614	CLA	CHC-C4B-NB	2.45	126.85	124.26
24	N	605	CHL	C1-C2-C3	-2.45	121.81	126.04
24	R	607	CHL	C4-C3-C5	2.45	119.39	115.27
24	0	605	CHL	CMD-C2D-C3D	-2.44	121.99	127.61
29	g	2630	LHG	C6-C5-C4	-2.44	106.01	111.79
24	y	608	CHL	CMD-C2D-C3D	-2.44	121.99	127.61
25	c	503	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	c	506	CLA	C3B-C4B-NB	-2.44	108.25	110.52
25	Y	610	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
25	D	402	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
24	n	606	CHL	C3B-C4B-NB	2.44	112.78	110.52
25	Y	614	CLA	C3B-C4B-NB	-2.44	108.25	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	613	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	6	609	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
24	0	608	CHL	CHC-C4B-NB	-2.44	121.67	124.26
25	S	612	CLA	CHB-C1B-C2B	-2.44	120.34	127.24
25	d	403	CLA	CHD-C1D-ND	-2.44	122.21	124.45
34	C	517	BCR	C1-C6-C5	-2.44	119.18	122.61
25	9	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	y	602	CLA	CMB-C2B-C3B	2.44	132.50	126.59
24	2	609	CHL	CHC-C4B-NB	-2.44	121.67	124.26
25	c	505	CLA	CMB-C2B-C3B	2.44	132.50	126.59
24	5	601	CHL	CHB-C4A-NA	2.44	127.88	124.51
24	8	607	CHL	C4-C3-C5	2.44	119.37	115.27
25	C	507	CLA	O2D-CGD-CBD	2.44	115.60	111.27
25	S	611	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	c	507	CLA	CHC-C4B-NB	2.44	126.84	124.26
26	y	1620	LUT	C38-C25-C24	-2.44	118.34	123.56
26	1	1621	LUT	C11-C10-C9	-2.44	123.83	127.31
24	0	606	CHL	CMB-C2B-C1B	2.44	129.08	125.37
26	4	1620	LUT	C3-C4-C5	-2.44	107.00	111.85
34	d	404	BCR	C35-C13-C12	2.44	121.92	118.08
24	5	606	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
24	7	605	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
25	p	602	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
24	0	609	CHL	O2A-CGA-CBA	2.44	119.55	111.91
24	0	609	CHL	O1D-CGD-CBD	-2.44	119.50	124.48
34	D	404	BCR	C35-C13-C12	2.44	121.91	118.08
25	d	402	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
25	y	614	CLA	C3B-C4B-NB	-2.44	108.26	110.52
25	R	601	CLA	CHA-C1A-NA	-2.43	120.82	126.40
26	9	1621	LUT	C7-C8-C9	-2.43	122.56	126.23
24	0	607	CHL	CMB-C2B-C1B	2.43	129.08	125.37
26	6	1621	LUT	C16-C1-C6	-2.43	106.35	110.30
25	s	612	CLA	C2B-C1B-NB	2.43	111.86	110.23
24	7	607	CHL	CMD-C2D-C3D	-2.43	122.01	127.61
25	S	610	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	s	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
26	4	1620	LUT	C16-C1-C6	-2.43	106.35	110.30
24	5	605	CHL	CMB-C2B-C1B	2.43	129.07	125.37
26	9	1621	LUT	C18-C5-C4	2.43	118.86	114.36
25	1	604	CLA	CHB-C1B-NB	2.43	126.83	124.26
24	Y	608	CHL	CMD-C2D-C3D	-2.43	122.02	127.61
28	R	623	NEX	C30-C31-C32	-2.43	115.63	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	612	CLA	C2B-C1B-NB	2.43	111.86	110.23
25	y	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	c	504	CLA	C3B-C4B-NB	-2.43	108.26	110.52
26	3	1620	LUT	C11-C10-C9	-2.43	123.84	127.31
39	d	405	PL9	O1-C4-C3	-2.43	118.04	120.72
25	N	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	p	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	q	607	CHL	CHD-C4C-C3C	-2.43	121.27	124.84
26	1	1621	LUT	C18-C5-C6	-2.43	121.80	124.53
24	1	607	CHL	CMD-C2D-C3D	-2.43	122.03	127.61
24	1	601	CHL	O1D-CGD-CBD	-2.43	119.52	124.48
24	N	601	CHL	C1-C2-C3	-2.43	121.84	126.04
26	5	1620	LUT	C11-C10-C9	-2.43	123.85	127.31
25	G	613	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
24	p	601	CHL	C4-C3-C5	2.43	119.35	115.27
34	H	101	BCR	C2-C3-C4	-2.43	105.96	111.38
27	3	1622	XAT	C10-C11-C12	-2.43	115.65	123.22
34	c	514	BCR	C21-C20-C19	-2.43	115.65	123.22
25	c	507	CLA	O2D-CGD-CBD	2.42	115.58	111.27
24	7	601	CHL	CHC-C4B-NB	-2.42	121.69	124.26
24	6	607	CHL	OMC-CMC-C2C	-2.42	120.20	125.69
28	G	1623	NEX	C5-C4-C3	-2.42	108.88	111.75
24	G	601	CHL	C4D-C3D-CAD	2.42	110.95	108.10
25	B	609	CLA	CHC-C4B-NB	2.42	126.82	124.26
26	8	1620	LUT	C21-C26-C27	-2.42	109.64	112.70
25	0	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
25	Y	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
28	3	1623	NEX	C2-C1-C6	2.42	111.57	109.21
24	n	607	CHL	C4-C3-C5	2.42	119.35	115.27
24	4	601	CHL	CMB-C2B-C1B	2.42	129.06	125.37
25	b	607	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
29	g	2630	LHG	C5-O7-C7	-2.42	111.83	117.79
24	1	607	CHL	C1-C2-C3	-2.42	121.85	126.04
25	q	613	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
25	p	614	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	3	1622	XAT	C11-C10-C9	-2.42	123.86	127.31
24	6	609	CHL	C4-C3-C5	2.42	119.34	115.27
28	0	1623	NEX	C15-C35-C34	-2.42	118.52	123.47
25	d	402	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	y	612	CLA	C3B-C4B-NB	-2.42	108.27	110.52
24	g	601	CHL	O1D-CGD-CBD	-2.42	119.54	124.48
24	8	609	CHL	O2A-CGA-CBA	2.42	119.49	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	1621	LUT	C3-C4-C5	-2.42	107.04	111.85
34	H	101	BCR	C30-C25-C26	-2.42	119.21	122.61
24	s	606	CHL	CMD-C2D-C3D	-2.42	122.06	127.61
25	1	610	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
36	A	413	LMG	C7-O1-C1	-2.42	109.02	113.74
25	n	602	CLA	C1-C2-C3	-2.41	121.87	126.04
24	s	608	CHL	CMD-C2D-C3D	-2.41	122.06	127.61
25	b	611	CLA	CAA-CBA-CGA	-2.41	106.20	113.25
29	6	2630	LHG	O8-C23-C24	2.41	119.48	111.91
25	3	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	G	611	CLA	O2D-CGD-CBD	2.41	115.56	111.27
24	s	601	CHL	CMB-C2B-C1B	2.41	129.04	125.37
25	4	612	CLA	CHB-C1B-NB	2.41	126.81	124.26
25	q	602	CLA	CHD-C1D-ND	-2.41	122.24	124.45
34	b	618	BCR	C33-C5-C6	-2.41	121.82	124.53
24	0	608	CHL	CMB-C2B-C1B	2.41	129.04	125.37
28	4	1623	NEX	C39-C29-C30	-2.41	119.54	122.92
25	1	604	CLA	C3B-C4B-NB	-2.41	108.28	110.52
28	1	1623	NEX	C30-C31-C32	-2.41	115.69	123.22
24	1	608	CHL	CMB-C2B-C1B	2.41	129.04	125.37
25	3	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	q	601	CHL	CMB-C2B-C1B	2.41	129.04	125.37
25	6	610	CLA	CHB-C1B-NB	2.41	126.81	124.26
25	b	606	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	Y	614	CLA	CHC-C4B-NB	2.41	126.81	124.26
24	S	608	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
24	7	608	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
25	9	603	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
26	8	1620	LUT	C10-C11-C12	-2.41	115.71	123.22
34	C	514	BCR	C21-C20-C19	-2.41	115.71	123.22
28	8	1623	NEX	C4-C3-C2	-2.41	106.13	110.77
36	a	413	LMG	C8-O7-C10	-2.41	111.87	117.79
28	9	1623	NEX	O24-C25-C38	2.41	117.94	115.06
25	B	611	CLA	CAA-CBA-CGA	-2.40	106.23	113.25
25	b	609	CLA	CHC-C4B-NB	2.40	126.80	124.26
34	h	101	BCR	C2-C3-C4	-2.40	106.01	111.38
25	c	501	CLA	CHC-C4B-NB	2.40	126.80	124.26
29	5	2630	LHG	O8-C23-C24	2.40	119.45	111.91
34	c	517	BCR	C1-C6-C5	-2.40	119.23	122.61
24	2	609	CHL	CMB-C2B-C1B	2.40	129.03	125.37
24	1	601	CHL	CGD-CBD-CAD	-2.40	102.96	110.73
24	6	605	CHL	C1C-C2C-C3C	-2.40	105.21	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	B	618	BCR	C38-C26-C27	2.40	118.23	113.62
29	G	2630	LHG	C5-O7-C7	-2.40	111.88	117.79
24	3	608	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
24	0	605	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
24	8	608	CHL	O2A-CGA-CBA	2.40	119.44	111.91
27	N	1622	XAT	C5-C4-C3	-2.40	108.00	112.75
24	N	606	CHL	CAA-C2A-C3A	-2.40	106.21	112.78
25	S	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	c	505	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	4	1620	LUT	C11-C10-C9	-2.40	123.89	127.31
24	3	608	CHL	O2A-CGA-CBA	2.40	119.43	111.91
26	7	1620	LUT	C18-C5-C6	-2.40	121.83	124.53
28	g	1623	NEX	C24-C23-C22	-2.40	106.14	110.77
24	n	606	CHL	CAA-C2A-C3A	-2.40	106.21	112.78
25	n	610	CLA	C3B-C4B-NB	-2.40	108.29	110.52
24	3	607	CHL	C4-C3-C5	2.40	119.30	115.27
24	4	605	CHL	CHD-C4C-C3C	-2.40	121.32	124.84
24	p	605	CHL	O1D-CGD-CBD	-2.40	119.58	124.48
24	5	605	CHL	C3B-C4B-NB	2.40	112.74	110.52
29	L	101	LHG	C5-O7-C7	-2.40	111.89	117.79
24	S	606	CHL	CMD-C2D-C3D	-2.40	122.10	127.61
25	g	612	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
24	n	605	CHL	CAA-C2A-C3A	-2.40	106.22	112.78
27	n	1622	XAT	C5-C4-C3	-2.39	108.01	112.75
24	r	606	CHL	C4-C3-C5	2.39	119.30	115.27
24	8	608	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
36	A	413	LMG	C8-O7-C10	-2.39	111.90	117.79
24	y	605	CHL	OMC-CMC-C2C	-2.39	120.28	125.69
25	Y	611	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
25	2	603	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
25	B	606	CLA	C3B-C4B-NB	-2.39	108.30	110.52
34	d	404	BCR	C33-C5-C4	2.39	118.21	113.62
24	p	607	CHL	CMD-C2D-C3D	-2.39	122.11	127.61
28	S	1623	NEX	C15-C35-C34	-2.39	118.58	123.47
25	Y	613	CLA	CHB-C1B-NB	2.39	126.79	124.26
25	b	602	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	Y	1620	LUT	C21-C26-C27	-2.39	109.68	112.70
25	b	616	CLA	C2A-C1A-CHA	2.39	128.03	123.86
25	8	614	CLA	CHD-C1D-ND	-2.39	122.26	124.45
24	n	606	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
24	y	601	CHL	C1C-C2C-C3C	-2.39	105.22	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	602	CLA	C3B-C4B-NB	-2.39	108.30	110.52
26	5	1620	LUT	C38-C25-C24	-2.39	118.45	123.56
24	S	607	CHL	CMD-C2D-C3D	-2.39	122.13	127.61
24	5	605	CHL	O2A-CGA-CBA	2.39	119.39	111.91
24	n	601	CHL	C1-C2-C3	-2.39	121.92	126.04
28	S	1623	NEX	C11-C12-C13	-2.38	119.72	126.42
24	N	605	CHL	C4-C3-C5	2.38	119.28	115.27
24	g	601	CHL	O2A-CGA-CBA	2.38	119.39	111.91
34	b	618	BCR	C38-C26-C27	2.38	118.19	113.62
24	Y	605	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
24	7	606	CHL	C3B-C4B-NB	2.38	112.73	110.52
25	G	614	CLA	C3B-C4B-NB	-2.38	108.30	110.52
24	1	609	CHL	CHC-C4B-NB	-2.38	121.73	124.26
24	p	605	CHL	C3B-C4B-NB	2.38	112.72	110.52
25	B	602	CLA	C3B-C4B-NB	-2.38	108.31	110.52
27	9	1622	XAT	C31-C32-C33	-2.38	119.73	126.42
34	B	619	BCR	C3-C4-C5	-2.38	109.83	114.08
26	4	1621	LUT	C19-C9-C8	2.38	121.83	118.08
25	B	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	y	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	5	607	CHL	CMB-C2B-C1B	2.38	128.99	125.37
24	0	601	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
34	b	619	BCR	C3-C4-C5	-2.38	109.83	114.08
24	G	601	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
28	y	1623	NEX	C2-C1-C6	2.38	111.52	109.21
24	r	607	CHL	CHC-C4B-NB	-2.38	121.74	124.26
24	R	606	CHL	C4-C3-C5	2.38	119.27	115.27
24	6	607	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
28	G	1623	NEX	C24-C23-C22	-2.38	106.18	110.77
24	r	606	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
25	s	610	CLA	O2D-CGD-CBD	2.38	115.49	111.27
28	Y	1623	NEX	C11-C12-C13	-2.38	119.74	126.42
34	B	618	BCR	C33-C5-C6	-2.38	121.86	124.53
25	g	611	CLA	O2D-CGD-CBD	2.37	115.49	111.27
25	y	613	CLA	CHB-C1B-NB	2.37	126.77	124.26
25	c	511	CLA	CMB-C2B-C3B	2.37	132.34	126.59
24	6	601	CHL	C6-C5-C3	-2.37	107.23	113.45
27	G	1622	XAT	C15-C35-C34	-2.37	118.61	123.47
25	4	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	g	602	CLA	CMB-C2B-C1B	-2.37	121.75	125.37
25	Y	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	B	616	CLA	CAC-C3C-C4C	2.37	127.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1620	LUT	C38-C25-C24	-2.37	118.48	123.56
25	4	612	CLA	C2A-C1A-CHA	2.37	128.01	123.86
25	S	612	CLA	C2A-C1A-CHA	2.37	128.01	123.86
28	R	623	NEX	C17-C1-C6	-2.37	108.35	110.47
25	B	617	CLA	CHB-C1B-NB	2.37	126.77	124.26
25	N	612	CLA	CHB-C1B-NB	2.37	126.77	124.26
27	0	1622	XAT	C26-C27-C28	-2.37	120.98	125.99
27	3	1622	XAT	C31-C32-C33	-2.37	119.75	126.42
34	h	101	BCR	C30-C25-C26	-2.37	119.27	122.61
25	C	505	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	p	605	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
25	2	602	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
24	3	605	CHL	CED-O2D-CGD	2.37	121.30	115.94
25	B	616	CLA	C2A-C1A-CHA	2.37	128.00	123.86
25	8	610	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	S	1621	LUT	C1-C2-C3	2.37	118.99	113.64
24	2	601	CHL	C11-C10-C8	-2.37	108.26	115.92
25	5	604	CLA	CHC-C4B-NB	2.37	126.77	124.26
34	D	404	BCR	C33-C5-C4	2.37	118.17	113.62
24	g	608	CHL	CMB-C2B-C1B	2.37	128.98	125.37
39	D	405	PL9	O1-C4-C3	-2.37	118.11	120.72
25	b	605	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
25	b	608	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
25	B	603	CLA	CHC-C4B-NB	2.37	126.76	124.26
24	9	601	CHL	C1-C2-C3	-2.37	121.95	126.04
29	n	2630	LHG	C5-O7-C7	-2.37	111.96	117.79
29	7	2630	LHG	C5-O7-C7	-2.37	111.97	117.79
26	2	1620	LUT	C21-C26-C27	-2.37	109.71	112.70
25	2	610	CLA	CMB-C2B-C1B	-2.37	121.77	125.37
27	8	1622	XAT	C11-C10-C9	-2.36	123.94	127.31
26	S	1620	LUT	C8-C7-C6	-2.36	120.56	127.20
26	s	1621	LUT	C1-C2-C3	2.36	118.98	113.64
24	y	606	CHL	O2A-CGA-CBA	2.36	119.33	111.91
28	9	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
25	1	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	S	607	CHL	C3B-C4B-NB	2.36	112.71	110.52
24	N	601	CHL	C11-C10-C8	-2.36	108.28	115.92
25	4	602	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
25	4	603	CLA	CMB-C2B-C3B	2.36	132.31	126.59
25	3	612	CLA	C2A-C1A-CHA	2.36	127.99	123.86
24	6	607	CHL	C11-C10-C8	-2.36	108.28	115.92
24	p	605	CHL	C4D-CHA-C1A	-2.36	118.38	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	1623	NEX	C19-C9-C10	-2.36	119.61	122.92
25	5	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	Y	606	CHL	O2A-CGA-CBA	2.36	119.32	111.91
29	G	2630	LHG	O8-C23-C24	2.36	119.31	111.91
26	y	1620	LUT	C16-C1-C6	-2.36	106.47	110.30
25	1	612	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
28	r	623	NEX	C40-C33-C32	2.36	121.80	118.08
25	B	606	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	r	606	CHL	O2A-CGA-O1A	-2.36	117.64	123.59
26	6	1620	LUT	C35-C15-C14	-2.36	118.64	123.47
25	s	612	CLA	C2A-C1A-CHA	2.36	127.98	123.86
29	N	2630	LHG	C5-O7-C7	-2.36	111.99	117.79
24	R	606	CHL	O2A-CGA-O1A	-2.36	117.64	123.59
26	9	1621	LUT	C36-C21-C26	2.36	113.12	109.55
25	1	610	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
24	R	606	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
28	4	1623	NEX	C35-C34-C33	-2.36	123.95	127.31
28	7	1623	NEX	C28-C29-C30	2.36	122.56	118.94
24	R	608	CHL	CMD-C2D-C3D	-2.36	122.19	127.61
24	p	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
25	s	609	CLA	C1D-ND-C4D	-2.36	104.66	106.33
24	G	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
29	g	2630	LHG	O8-C23-C24	2.36	119.30	111.91
24	N	605	CHL	CAA-C2A-C3A	-2.36	106.33	112.78
24	2	601	CHL	C11-C12-C13	-2.36	108.31	115.92
24	y	605	CHL	C1C-C2C-C3C	-2.36	105.25	107.11
24	q	605	CHL	CED-O2D-CGD	2.36	121.26	115.94
35	A	412	SQD	C45-O47-C7	-2.35	111.99	117.79
26	R	620	LUT	C11-C10-C9	-2.35	123.95	127.31
28	N	1623	NEX	C30-C31-C32	-2.35	115.87	123.22
26	q	1621	LUT	C15-C35-C34	-2.35	118.66	123.47
25	B	605	CLA	CHC-C4B-NB	2.35	126.75	124.26
25	0	604	CLA	CHC-C4B-NB	2.35	126.75	124.26
35	b	623	SQD	C45-O47-C7	-2.35	112.00	117.79
24	6	609	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
35	a	412	SQD	C45-O47-C7	-2.35	112.00	117.79
24	8	605	CHL	CED-O2D-CGD	2.35	121.25	115.94
26	0	1620	LUT	C18-C5-C6	-2.35	121.89	124.53
24	n	601	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
29	y	2630	LHG	C9-C8-C7	-2.35	105.07	113.62
25	5	602	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	5	612	CLA	C2A-C1A-CHA	2.35	127.97	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	601	CHL	C1-C2-C3	-2.35	121.98	126.04
28	p	1623	NEX	C11-C12-C13	-2.35	119.81	126.42
25	D	402	CLA	C3B-C4B-NB	-2.35	108.33	110.52
28	2	1623	NEX	C11-C12-C13	-2.35	119.81	126.42
25	c	509	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	s	607	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
25	9	612	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	9	601	CHL	C11-C12-C13	-2.35	108.33	115.92
26	9	1621	LUT	C1-C2-C3	2.35	118.95	113.64
26	R	620	LUT	C8-C7-C6	-2.35	120.60	127.20
25	N	604	CLA	CHB-C1B-NB	2.35	126.74	124.26
26	g	1621	LUT	C8-C7-C6	-2.35	120.61	127.20
24	r	608	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
25	Y	603	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
25	b	606	CLA	C3B-C4B-NB	-2.35	108.34	110.52
27	6	1622	XAT	C28-C29-C30	2.35	122.54	118.94
26	s	1620	LUT	C8-C7-C6	-2.35	120.61	127.20
34	B	620	BCR	C29-C28-C27	-2.35	106.13	111.38
24	7	607	CHL	C3B-C4B-NB	2.35	112.69	110.52
28	R	623	NEX	C40-C33-C32	2.35	121.77	118.08
24	6	601	CHL	C1-C2-C3	-2.35	121.99	126.04
25	n	603	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	b	617	CLA	CHB-C1B-NB	2.35	126.74	124.26
25	q	603	CLA	CMB-C2B-C1B	-2.35	121.80	125.37
24	Y	601	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
24	Y	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
35	b	621	SQD	O8-S-C6	2.34	109.48	105.74
25	C	503	CLA	CMB-C2B-C3B	2.34	132.27	126.59
25	q	602	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
24	1	605	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
25	B	616	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	b	616	CLA	CAC-C3C-C4C	2.34	127.85	124.81
25	B	607	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	b	607	CLA	O2D-CGD-CBD	2.34	115.43	111.27
24	9	605	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
24	8	601	CHL	O2A-CGA-CBA	2.34	119.26	111.91
33	A	409	PHO	O1D-CGD-CBD	2.34	128.64	124.74
25	C	511	CLA	CMB-C2B-C3B	2.34	132.26	126.59
25	G	613	CLA	CHC-C4B-NB	2.34	126.74	124.26
28	9	1623	NEX	C24-C23-C22	-2.34	106.25	110.77
25	8	603	CLA	C2A-C1A-CHA	2.34	127.95	123.86
25	3	614	CLA	CHD-C1D-ND	-2.34	122.30	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
24	r	607	CHL	OMC-CMC-C2C	-2.34	120.39	125.69
27	g	1622	XAT	C10-C11-C12	-2.34	115.92	123.22
25	2	604	CLA	CHD-C1D-ND	-2.34	122.30	124.45
25	N	610	CLA	C3B-C4B-NB	-2.34	108.34	110.52
24	3	606	CHL	CHD-C4C-C3C	-2.34	121.40	124.84
25	9	612	CLA	CHC-C4B-NB	2.34	126.73	124.26
25	y	603	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
36	H	102	LMG	C6-C5-C4	-2.34	107.53	113.00
24	7	608	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
24	q	609	CHL	C2A-C3A-C4A	-2.34	98.09	101.87
26	r	620	LUT	C8-C7-C6	-2.34	120.64	127.20
25	s	610	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
24	R	607	CHL	CHC-C4B-NB	-2.34	121.78	124.26
34	h	101	BCR	C16-C15-C14	-2.34	118.69	123.47
25	s	604	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
28	s	1623	NEX	C11-C12-C13	-2.34	119.85	126.42
25	n	604	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	C	509	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
26	N	1620	LUT	C8-C7-C6	-2.34	120.64	127.20
24	2	605	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	Y	609	CHL	C1-C2-C3	-2.34	122.00	126.04
24	N	601	CHL	O1D-CGD-CBD	-2.34	119.71	124.48
25	1	602	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	1	610	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	2	602	CLA	CHC-C4B-NB	2.34	126.73	124.26
25	S	604	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	6	604	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	9	608	CHL	CHC-C4B-NB	-2.33	121.79	124.26
25	S	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	s	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
24	p	606	CHL	C3B-C4B-NB	2.33	112.68	110.52
25	N	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	a	407	CLA	CHC-C4B-NB	2.33	126.73	124.26
25	y	602	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	q	603	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
35	B	621	SQD	O8-S-C6	2.33	109.46	105.74
25	7	604	CLA	CAC-C3C-C2C	-2.33	123.54	127.53
34	H	101	BCR	C16-C15-C14	-2.33	118.70	123.47
24	q	601	CHL	C4-C3-C5	2.33	119.19	115.27
24	G	606	CHL	C1C-C2C-C3C	-2.33	105.26	107.11
24	3	609	CHL	OMC-CMC-C2C	-2.33	120.42	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	1620	LUT	C36-C21-C26	2.33	113.08	109.55
25	Y	603	CLA	O2D-CGD-CBD	2.33	115.41	111.27
26	3	1620	LUT	C30-C31-C32	-2.33	115.94	123.22
24	s	607	CHL	C3B-C4B-NB	2.33	112.68	110.52
24	3	601	CHL	CHC-C4B-NB	-2.33	121.79	124.26
25	Y	613	CLA	CHC-C4B-NB	2.33	126.72	124.26
34	C	517	BCR	C10-C11-C12	-2.33	115.95	123.22
26	2	1621	LUT	C38-C25-C24	-2.33	118.58	123.56
27	4	1622	XAT	C7-C8-C9	-2.33	121.92	125.53
25	C	507	CLA	CHA-C1A-NA	-2.33	121.07	126.40
24	y	601	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
24	R	607	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
25	b	616	CLA	O2D-CGD-CBD	2.33	115.40	111.27
25	6	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	c	513	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
25	n	614	CLA	CHD-C1D-ND	-2.33	122.32	124.45
25	7	613	CLA	CMB-C2B-C3B	2.33	132.22	126.59
28	7	1623	NEX	C15-C35-C34	-2.33	118.71	123.47
25	b	605	CLA	CHC-C4B-NB	2.33	126.72	124.26
26	r	620	LUT	C11-C10-C9	-2.32	123.99	127.31
25	G	614	CLA	CHC-C4B-NB	2.32	126.72	124.26
34	b	620	BCR	C29-C28-C27	-2.32	106.18	111.38
25	9	602	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
25	y	603	CLA	O2D-CGD-CBD	2.32	115.40	111.27
33	a	409	PHO	O1D-CGD-CBD	2.32	128.61	124.74
26	S	1621	LUT	C31-C30-C29	-2.32	124.00	127.31
25	0	610	CLA	CHB-C1B-NB	2.32	126.72	124.26
24	4	601	CHL	C1-O2A-CGA	2.32	122.54	116.44
24	N	606	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
25	4	613	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
26	Y	1620	LUT	C7-C8-C9	-2.32	122.73	126.23
26	4	1620	LUT	C31-C32-C33	-2.32	119.90	126.42
24	2	607	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
25	R	601	CLA	CAA-C2A-C1A	2.32	119.57	111.97
24	2	601	CHL	C1-C2-C3	-2.32	122.03	126.04
24	n	606	CHL	C2A-C1A-CHA	-2.32	119.81	123.86
25	c	510	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	r	607	CHL	C4-C3-C5	2.32	119.17	115.27
34	c	517	BCR	C10-C11-C12	-2.32	115.99	123.22
24	s	606	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
24	5	601	CHL	C1-O2A-CGA	2.32	122.52	116.44
27	N	1622	XAT	C7-C8-C9	-2.32	121.94	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	409	LHG	O8-C23-C24	2.32	119.18	111.91
24	n	607	CHL	O1D-CGD-CBD	-2.32	119.75	124.48
24	q	609	CHL	O2A-CGA-CBA	2.32	119.17	111.91
24	Y	605	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
39	D	405	PL9	C32-C33-C34	-2.31	122.09	127.66
39	d	405	PL9	C32-C33-C34	-2.31	122.09	127.66
28	n	1623	NEX	C30-C31-C32	-2.31	115.99	123.22
25	7	610	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
26	q	1620	LUT	C19-C9-C8	2.31	121.72	118.08
25	R	604	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
25	B	603	CLA	CMB-C2B-C3B	2.31	132.19	126.59
25	8	610	CLA	CHB-C1B-NB	2.31	126.70	124.26
24	6	601	CHL	CHB-C4A-NA	2.31	127.71	124.51
26	G	1621	LUT	C8-C7-C6	-2.31	120.71	127.20
24	1	608	CHL	CMD-C2D-C3D	-2.31	122.30	127.61
26	s	1621	LUT	C31-C30-C29	-2.31	124.01	127.31
26	Y	1620	LUT	C2-C3-C4	-2.31	107.14	110.30
26	7	1620	LUT	C30-C31-C32	-2.31	116.01	123.22
24	G	606	CHL	CHB-C4A-NA	2.31	127.71	124.51
25	c	512	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	r	2630	LHG	O8-C23-C24	2.31	119.15	111.91
25	7	610	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
36	C	521	LMG	C8-O7-C10	-2.31	112.11	117.79
25	9	614	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	r	610	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
25	8	612	CLA	C2A-C1A-CHA	2.31	127.89	123.86
25	p	604	CLA	CHD-C1D-ND	-2.31	122.33	124.45
24	1	608	CHL	CHB-C4A-NA	2.31	127.70	124.51
24	7	605	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
25	R	610	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	1	1620	LUT	C30-C31-C32	-2.31	116.02	123.22
24	7	607	CHL	CHC-C4B-NB	-2.31	121.82	124.26
25	A	406	CLA	CHB-C1B-NB	2.31	126.70	124.26
25	a	406	CLA	CHB-C1B-NB	2.31	126.70	124.26
25	d	403	CLA	O2D-CGD-CBD	2.31	115.36	111.27
29	R	2630	LHG	O8-C23-C24	2.31	119.14	111.91
25	C	510	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	7	609	CHL	O1D-CGD-CBD	-2.31	119.77	124.48
25	c	508	CLA	CMB-C2B-C3B	2.30	132.17	126.59
24	y	609	CHL	C1-C2-C3	-2.30	122.06	126.04
25	C	512	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
24	6	601	CHL	C2A-C1A-CHA	-2.30	119.83	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	610	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	2	611	CLA	C3B-C4B-NB	-2.30	108.38	110.52
24	Y	609	CHL	CMD-C2D-C3D	-2.30	122.31	127.61
36	c	521	LMG	C8-O7-C10	-2.30	112.12	117.79
25	1	613	CLA	CMB-C2B-C3B	2.30	132.17	126.59
24	q	608	CHL	CMB-C2B-C1B	2.30	128.88	125.37
25	2	612	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
24	r	607	CHL	CMD-C2D-C3D	-2.30	122.32	127.61
25	S	609	CLA	C1D-ND-C4D	-2.30	104.70	106.33
24	4	601	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
40	f	101	HEM	CMC-C2C-C1C	-2.30	120.66	124.71
26	Y	1620	LUT	C16-C1-C6	-2.30	106.57	110.30
24	5	605	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
40	f	101	HEM	CBA-CAA-C2A	-2.30	106.23	112.63
24	N	601	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
26	6	1620	LUT	C39-C29-C28	2.30	121.70	118.08
39	d	405	PL9	C36-C37-C38	-2.30	104.32	111.88
24	6	606	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
24	9	601	CHL	C4-C3-C5	2.30	119.14	115.27
26	5	1620	LUT	C8-C9-C10	-2.30	115.41	118.94
39	D	405	PL9	C36-C37-C38	-2.30	104.32	111.88
28	5	1623	NEX	C11-C12-C13	-2.30	119.95	126.42
24	p	609	CHL	CHD-C4C-C3C	-2.30	121.46	124.84
24	R	608	CHL	CMB-C2B-C1B	2.30	128.87	125.37
24	R	606	CHL	C4A-NA-C1A	-2.30	105.67	106.71
28	G	1623	NEX	C11-C12-C13	-2.30	119.96	126.42
24	S	606	CHL	OMC-CMC-C2C	-2.30	120.49	125.69
25	C	503	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	b	603	CLA	CMB-C2B-C3B	2.30	132.16	126.59
24	6	607	CHL	CMD-C2D-C3D	-2.30	122.33	127.61
24	7	606	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
25	R	616	CLA	CHD-C1D-ND	-2.30	122.34	124.45
25	N	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	2	603	CLA	C2A-C1A-CHA	2.30	127.88	123.86
25	2	610	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
26	5	1621	LUT	C20-C13-C12	2.30	121.70	118.08
24	S	601	CHL	O2A-CGA-CBA	2.30	121.41	114.03
24	y	606	CHL	CHB-C4A-NA	2.30	127.69	124.51
25	y	613	CLA	CHC-C4B-NB	2.30	126.69	124.26
26	n	1620	LUT	C35-C15-C14	-2.30	118.77	123.47
28	5	1623	NEX	C35-C15-C14	-2.30	118.77	123.47
24	5	605	CHL	O1D-CGD-CBD	-2.30	119.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	606	CHL	C4A-NA-C1A	-2.30	105.67	106.71
25	r	616	CLA	CHD-C1D-ND	-2.29	122.34	124.45
25	5	612	CLA	CHC-C4B-NB	2.29	126.69	124.26
29	q	2630	LHG	C5-O7-C7	-2.29	112.14	117.79
25	4	614	CLA	CHC-C4B-NB	2.29	126.69	124.26
25	6	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
37	c	520	DGD	C2G-O2G-C1B	-2.29	112.15	117.79
24	R	607	CHL	CMD-C2D-C3D	-2.29	122.34	127.61
24	n	601	CHL	O1D-CGD-CBD	-2.29	119.79	124.48
27	y	1622	XAT	C18-C5-C4	2.29	116.86	114.28
24	n	608	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
25	C	508	CLA	CMB-C2B-C3B	2.29	132.14	126.59
25	2	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	d	402	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
26	p	1621	LUT	C7-C8-C9	-2.29	122.78	126.23
25	7	602	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	1	601	CHL	C4-C3-C5	2.29	119.12	115.27
34	c	514	BCR	C10-C11-C12	-2.29	116.07	123.22
24	p	606	CHL	CED-O2D-CGD	2.29	121.11	115.94
24	5	609	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
24	1	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
25	b	603	CLA	CHC-C4B-NB	2.29	126.68	124.26
24	Y	606	CHL	C3B-C4B-NB	2.29	112.64	110.52
25	3	602	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	4	607	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
25	C	501	CLA	CHC-C4B-NB	2.29	126.68	124.26
25	r	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
24	0	606	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
24	g	606	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
24	3	601	CHL	O1D-CGD-CBD	-2.29	119.81	124.48
24	G	607	CHL	CMD-C2D-C3D	-2.29	122.35	127.61
24	4	608	CHL	O1D-CGD-CBD	-2.29	119.81	124.48
27	7	1622	XAT	O4-C5-C6	-2.29	57.07	58.96
28	6	1623	NEX	C24-C23-C22	-2.29	106.36	110.77
34	C	514	BCR	C33-C5-C6	-2.29	121.96	124.53
25	G	602	CLA	CMB-C2B-C3B	2.29	132.12	126.59
34	B	620	BCR	C21-C20-C19	-2.29	116.08	123.22
24	6	609	CHL	O1D-CGD-CBD	-2.29	119.81	124.48
24	6	606	CHL	CHB-C4A-NA	2.29	127.67	124.51
25	b	610	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
27	n	1622	XAT	C7-C8-C9	-2.28	121.98	125.53
24	N	607	CHL	C6-C5-C3	-2.28	107.47	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	605	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
24	q	609	CHL	C1-O2A-CGA	2.28	122.44	116.44
27	8	1622	XAT	C31-C32-C33	-2.28	120.00	126.42
26	2	1621	LUT	C18-C5-C4	2.28	118.58	114.36
29	d	409	LHG	O8-C23-C24	2.28	119.07	111.91
28	q	1623	NEX	C17-C1-C6	-2.28	108.43	110.47
25	B	610	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
25	r	601	CLA	CAA-C2A-C1A	2.28	119.45	111.97
26	4	1620	LUT	C21-C26-C27	-2.28	109.82	112.70
25	2	602	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	p	606	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
25	q	604	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
25	S	610	CLA	O2D-CGD-CBD	2.28	115.32	111.27
35	B	623	SQD	C45-O47-C7	-2.28	112.18	117.79
25	D	402	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
25	D	403	CLA	O2D-CGD-CBD	2.28	115.32	111.27
25	A	407	CLA	CHC-C4B-NB	2.28	126.67	124.26
25	1	611	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
25	7	611	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
24	5	601	CHL	O2A-CGA-CBA	2.28	119.05	111.91
24	4	605	CHL	C1D-CHD-C4C	-2.28	121.15	126.06
25	c	507	CLA	CHA-C1A-NA	-2.28	121.19	126.40
24	q	605	CHL	C1D-CHD-C4C	-2.28	121.15	126.06
36	B	622	LMG	O8-C28-C29	2.28	119.05	111.91
25	C	502	CLA	C16-C15-C13	-2.28	108.56	115.92
24	0	601	CHL	O2A-CGA-O1A	-2.27	117.85	123.59
35	d	413	SQD	O48-C23-O10	-2.27	117.85	123.59
24	1	605	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
24	q	607	CHL	C3B-C4B-NB	2.27	112.62	110.52
37	C	520	DGD	C2G-O2G-C1B	-2.27	112.19	117.79
27	Y	1622	XAT	C18-C5-C4	2.27	116.84	114.28
25	s	605	CLA	CHB-C4A-NA	2.27	127.66	124.51
25	S	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
28	q	1623	NEX	C39-C29-C30	-2.27	119.74	122.92
25	p	614	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	c	510	CLA	C6-C7-C8	-2.27	108.58	115.92
24	6	608	CHL	CHC-C4B-NB	-2.27	121.85	124.26
25	q	612	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	n	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
27	G	1622	XAT	C10-C11-C12	-2.27	116.13	123.22
36	b	622	LMG	O8-C28-C29	2.27	119.03	111.91
28	g	1623	NEX	C19-C9-C10	-2.27	119.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	607	CHL	CMD-C2D-C3D	-2.27	122.39	127.61
28	q	1623	NEX	C4-C3-C2	-2.27	106.39	110.77
25	r	602	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	B	606	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	s	612	CLA	CHA-C1A-NA	-2.27	121.20	126.40
24	s	601	CHL	O2A-CGA-CBA	2.27	121.32	114.03
25	3	611	CLA	C3B-C4B-NB	-2.27	108.41	110.52
28	N	1623	NEX	C19-C9-C10	-2.27	119.75	122.92
24	3	601	CHL	O2A-CGA-CBA	2.27	119.03	111.91
28	p	1623	NEX	C35-C15-C14	-2.27	118.83	123.47
24	0	605	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
25	b	603	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	0	604	CLA	C3B-C4B-NB	-2.27	108.41	110.52
25	c	503	CLA	C4-C3-C5	2.27	119.08	115.27
24	N	607	CHL	C4D-C3D-CAD	2.27	110.77	108.10
25	B	605	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
28	2	1623	NEX	C24-C23-C22	-2.26	106.40	110.77
25	s	614	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
24	n	607	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
24	S	608	CHL	CHC-C4B-NB	-2.26	121.86	124.26
25	B	609	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	b	609	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	S	605	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	Y	1620	LUT	C3-C4-C5	-2.26	107.34	111.85
28	N	1623	NEX	C28-C29-C30	2.26	122.42	118.94
25	A	406	CLA	CMB-C2B-C3B	2.26	132.07	126.59
24	6	608	CHL	CHB-C4A-NA	2.26	127.64	124.51
25	6	611	CLA	CHD-C1D-ND	-2.26	122.37	124.45
28	g	1623	NEX	C5-C4-C3	-2.26	109.07	111.75
24	5	605	CHL	C1-O2A-CGA	2.26	122.38	116.44
35	D	413	SQD	O48-C23-O10	-2.26	117.88	123.59
24	5	601	CHL	C6-C5-C3	2.26	119.39	113.45
24	4	606	CHL	O2A-CGA-O1A	-2.26	117.88	123.59
25	9	610	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
25	a	406	CLA	CMB-C2B-C3B	2.26	132.07	126.59
25	C	510	CLA	C6-C7-C8	-2.26	108.61	115.92
36	d	412	LMG	C8-O7-C10	-2.26	112.22	117.79
25	8	604	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	3	1621	LUT	C16-C1-C6	-2.26	106.63	110.30
25	0	610	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	G	602	CLA	CHB-C1B-NB	2.26	126.65	124.26
26	0	1621	LUT	C3-C4-C5	-2.26	107.35	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	p	2630	LHG	C5-O7-C7	-2.26	112.23	117.79
25	R	609	CLA	CHB-C1B-NB	2.26	126.65	124.26
24	q	609	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
36	d	411	LMG	C8-O7-C10	-2.26	112.23	117.79
24	9	607	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
25	c	507	CLA	CMB-C2B-C3B	2.26	132.06	126.59
27	1	1622	XAT	O4-C5-C6	-2.26	57.09	58.96
24	8	601	CHL	CHC-C4B-NB	-2.26	121.87	124.26
25	g	604	CLA	C3B-C4B-NB	-2.26	108.42	110.52
24	q	606	CHL	O2A-CGA-O1A	-2.26	117.90	123.59
36	D	412	LMG	C8-O7-C10	-2.26	112.23	117.79
27	5	1622	XAT	C25-C24-C23	2.26	117.21	112.75
25	8	614	CLA	CHB-C1B-NB	2.26	126.64	124.26
35	B	623	SQD	O48-C23-C24	2.26	118.98	111.91
25	N	602	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	8	614	CLA	CHC-C4B-NB	2.25	126.64	124.26
25	S	614	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
25	C	513	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
24	Y	605	CHL	CMD-C2D-C3D	-2.25	122.43	127.61
24	y	605	CHL	CMD-C2D-C3D	-2.25	122.43	127.61
24	2	606	CHL	O2A-CGA-O1A	-2.25	117.91	123.59
25	7	604	CLA	CHC-C4B-NB	2.25	126.64	124.26
25	c	502	CLA	CHC-C1C-C2C	-2.25	120.47	126.73
25	y	612	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
26	9	1620	LUT	C18-C5-C6	-2.25	122.00	124.53
25	R	609	CLA	C3B-C4B-NB	-2.25	108.43	110.52
35	b	623	SQD	O48-C23-C24	2.25	118.97	111.91
34	b	620	BCR	C21-C20-C19	-2.25	116.19	123.22
24	n	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
26	5	1620	LUT	C8-C7-C6	-2.25	120.88	127.20
24	n	601	CHL	C4A-NA-C1A	-2.25	105.69	106.71
25	p	611	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	Y	612	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	3	603	CLA	C2A-C1A-CHA	2.25	127.80	123.86
26	9	1620	LUT	C21-C26-C27	-2.25	109.86	112.70
24	q	608	CHL	CMD-C2D-C3D	-2.25	122.44	127.61
24	3	607	CHL	CMB-C2B-C1B	2.25	128.79	125.37
24	8	609	CHL	C4-C3-C5	2.25	119.06	115.27
26	N	1621	LUT	C1-C2-C3	2.25	118.72	113.64
24	G	606	CHL	C4A-NA-C1A	-2.25	105.69	106.71
24	Y	607	CHL	C1C-C2C-C3C	-2.25	105.33	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	609	CHL	CHC-C4B-NB	-2.25	121.88	124.26
25	c	512	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	C	507	CLA	CMB-C2B-C3B	2.25	132.03	126.59
26	n	1621	LUT	C1-C2-C3	2.25	118.72	113.64
29	5	2630	LHG	C5-O7-C7	-2.25	112.26	117.79
25	B	614	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
25	7	610	CLA	CHB-C1B-NB	2.25	126.64	124.26
24	y	606	CHL	C3B-C4B-NB	2.25	112.60	110.52
25	S	609	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	1	613	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
25	R	602	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	1	2630	LHG	C5-O7-C7	-2.25	112.26	117.79
25	c	503	CLA	CHB-C1B-NB	2.25	126.63	124.26
34	c	517	BCR	C16-C17-C18	-2.25	124.11	127.31
25	r	601	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	Y	604	CLA	CHB-C4A-NA	2.24	127.62	124.51
25	5	602	CLA	CMB-C2B-C3B	2.24	132.02	126.59
25	3	614	CLA	CHC-C4B-NB	2.24	126.63	124.26
25	b	606	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	b	609	CLA	O2D-CGD-CBD	2.24	115.26	111.27
24	8	609	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
24	g	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
28	g	1623	NEX	C5-C6-C1	2.24	121.92	119.70
34	H	101	BCR	C3-C4-C5	-2.24	110.07	114.08
24	G	607	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
25	q	603	CLA	C2A-C1A-CHA	2.24	127.78	123.86
24	R	608	CHL	C11-C10-C8	-2.24	108.68	115.92
25	B	605	CLA	CHB-C1B-NB	2.24	126.63	124.26
24	6	601	CHL	CMD-C2D-C3D	-2.24	122.46	127.61
24	7	607	CHL	C1-O2A-CGA	2.24	122.32	116.44
24	r	608	CHL	CMB-C2B-C1B	2.24	128.78	125.37
25	b	616	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
25	7	610	CLA	C1-C2-C3	-2.24	122.17	126.04
24	Y	605	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	s	608	CHL	CHC-C4B-NB	-2.24	121.89	124.26
27	3	1622	XAT	O4-C5-C6	-2.24	57.11	58.96
25	N	614	CLA	CHD-C1D-ND	-2.24	122.40	124.45
24	N	608	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
24	0	607	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
25	B	609	CLA	O2D-CGD-CBD	2.24	115.25	111.27
25	q	612	CLA	C2A-C1A-CHA	2.24	127.77	123.86
34	c	516	BCR	C34-C9-C8	2.24	121.60	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	h	101	BCR	C3-C4-C5	-2.24	110.08	114.08
24	0	608	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	p	609	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	Y	607	CHL	O2A-C1-C2	2.24	114.52	108.64
25	c	502	CLA	C16-C15-C13	-2.24	108.69	115.92
25	B	608	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
24	7	609	CHL	CHB-C4A-NA	2.24	127.61	124.51
24	y	607	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
36	D	411	LMG	C8-O7-C10	-2.24	112.28	117.79
25	Y	611	CLA	CHC-C4B-NB	2.24	126.62	124.26
25	y	604	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	C	502	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
26	9	1620	LUT	C31-C30-C29	-2.24	124.12	127.31
25	b	614	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
24	Y	609	CHL	CAC-C3C-C4C	2.24	127.71	124.81
25	3	604	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	s	1621	LUT	C39-C29-C28	2.23	121.60	118.08
25	b	612	CLA	CMB-C2B-C3B	2.23	132.00	126.59
24	g	609	CHL	O1D-CGD-CBD	-2.23	119.91	124.48
28	p	1623	NEX	C24-C23-C22	-2.23	106.46	110.77
26	8	1620	LUT	C18-C5-C6	-2.23	122.02	124.53
25	R	604	CLA	CHD-C1D-ND	-2.23	122.40	124.45
24	6	607	CHL	CHC-C4B-NB	-2.23	121.89	124.26
26	S	1621	LUT	C39-C29-C28	2.23	121.60	118.08
27	0	1622	XAT	C35-C34-C33	-2.23	124.12	127.31
26	9	1620	LUT	C20-C13-C14	-2.23	119.80	122.92
24	N	606	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
25	C	511	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
28	4	1623	NEX	C24-C23-C22	-2.23	106.46	110.77
24	r	608	CHL	C11-C10-C8	-2.23	108.70	115.92
25	n	611	CLA	CHB-C1B-NB	2.23	126.62	124.26
24	n	609	CHL	CAA-C2A-C3A	-2.23	106.67	112.78
24	0	609	CHL	CED-O2D-CGD	2.23	120.98	115.94
25	b	605	CLA	CHB-C1B-NB	2.23	126.62	124.26
26	q	1620	LUT	C15-C35-C34	-2.23	118.90	123.47
25	S	602	CLA	O2D-CGD-CBD	2.23	115.23	111.27
24	N	601	CHL	C4D-C3D-CAD	2.23	110.72	108.10
24	G	606	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
25	q	604	CLA	C3B-C4B-NB	-2.23	108.45	110.52
25	y	611	CLA	CHC-C4B-NB	2.23	126.62	124.26
34	d	404	BCR	C23-C24-C25	-2.23	120.94	127.20
24	2	601	CHL	OMC-CMC-C2C	-2.23	120.65	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	607	CLA	C3B-C4B-NB	-2.23	108.45	110.52
26	4	1620	LUT	C7-C8-C9	-2.23	122.87	126.23
25	r	609	CLA	C3B-C4B-NB	-2.23	108.45	110.52
24	r	606	CHL	CAA-CBA-CGA	-2.23	106.75	113.25
25	8	602	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	6	601	CHL	CHC-C4B-NB	-2.23	121.90	124.26
34	C	514	BCR	C10-C11-C12	-2.23	116.27	123.22
24	y	605	CHL	O2D-CGD-O1D	-2.23	119.49	123.84
25	y	602	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
24	r	608	CHL	CHB-C1B-NB	-2.23	121.90	124.26
27	Y	1622	XAT	C10-C11-C12	-2.23	116.27	123.22
25	y	613	CLA	C2D-C1D-ND	-2.23	108.46	110.10
34	b	620	BCR	C39-C30-C25	-2.23	106.69	110.30
36	h	102	LMG	O8-C28-O10	-2.22	117.98	123.59
25	3	614	CLA	CHB-C1B-NB	2.22	126.61	124.26
24	G	606	CHL	CED-O2D-CGD	2.22	120.96	115.94
24	2	601	CHL	O2A-CGA-CBA	2.22	118.88	111.91
34	C	516	BCR	C34-C9-C8	2.22	121.58	118.08
24	6	608	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
26	0	1620	LUT	C39-C29-C28	2.22	121.58	118.08
25	b	603	CLA	C2A-C1A-CHA	2.22	127.74	123.86
25	B	616	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
27	G	1622	XAT	C11-C10-C9	-2.22	124.14	127.31
25	S	614	CLA	CHC-C4B-NB	2.22	126.61	124.26
25	B	612	CLA	CMB-C2B-C3B	2.22	131.96	126.59
24	N	609	CHL	CAA-C2A-C3A	-2.22	106.70	112.78
26	n	1621	LUT	C30-C31-C32	-2.22	116.29	123.22
36	H	102	LMG	O8-C28-O10	-2.22	117.99	123.59
24	s	608	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
25	9	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	g	606	CHL	CED-O2D-CGD	2.22	120.95	115.94
24	r	607	CHL	C7-C6-C5	-2.22	107.33	113.36
24	1	601	CHL	O2A-CGA-CBA	2.22	118.87	111.91
24	8	606	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
25	S	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	D	404	BCR	C23-C24-C25	-2.22	120.97	127.20
26	0	1620	LUT	C19-C9-C8	2.22	121.57	118.08
34	b	619	BCR	C39-C30-C25	-2.22	106.70	110.30
28	4	1623	NEX	C27-C28-C29	-2.22	122.09	125.53
25	q	614	CLA	C3B-C4B-NB	-2.22	108.46	110.52
24	8	607	CHL	CAA-C2A-C3A	-2.22	106.71	112.78
24	9	601	CHL	CHC-C4B-NB	-2.22	121.91	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	608	CHL	CHC-C4B-NB	-2.22	121.91	124.26
25	N	611	CLA	CHB-C1B-NB	2.22	126.60	124.26
24	1	606	CHL	C4-C3-C5	2.22	119.00	115.27
25	G	610	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	N	607	CHL	C1C-C2C-C3C	-2.22	105.36	107.11
24	7	601	CHL	C4D-CHA-C1A	-2.22	118.55	121.25
28	7	1623	NEX	C30-C31-C32	-2.22	116.30	123.22
33	a	409	PHO	O2D-CGD-CBD	2.22	113.80	111.00
25	1	602	CLA	C3B-C4B-NB	-2.22	108.46	110.52
25	G	604	CLA	C3B-C4B-NB	-2.22	108.46	110.52
24	S	601	CHL	O2A-CGA-O1A	-2.22	117.78	123.30
24	5	606	CHL	C4D-CHA-C1A	-2.21	118.55	121.25
27	2	1622	XAT	C7-C8-C9	-2.21	122.09	125.53
33	A	409	PHO	O2D-CGD-CBD	2.21	113.80	111.00
24	R	608	CHL	CHB-C1B-NB	-2.21	121.91	124.26
28	y	1623	NEX	C5-C4-C3	-2.21	109.12	111.75
24	q	601	CHL	C1-O2A-CGA	2.21	122.25	116.44
24	G	608	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
26	q	1620	LUT	C10-C11-C12	-2.21	116.31	123.22
25	Y	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	G	1620	LUT	C8-C7-C6	-2.21	120.99	127.20
24	R	606	CHL	CAA-CBA-CGA	-2.21	106.79	113.25
26	p	1621	LUT	C36-C21-C26	2.21	112.89	109.55
26	Y	1621	LUT	C31-C30-C29	-2.21	124.16	127.31
40	F	101	HEM	CMC-C2C-C1C	-2.21	120.82	124.71
24	5	601	CHL	CHC-C4B-NB	-2.21	121.92	124.26
26	p	1621	LUT	C16-C1-C6	-2.21	106.71	110.30
28	4	1623	NEX	C4-C3-C2	-2.21	106.50	110.77
25	s	609	CLA	CHB-C4A-NA	2.21	127.57	124.51
27	0	1622	XAT	C31-C32-C33	-2.21	120.21	126.42
26	r	620	LUT	C38-C25-C24	-2.21	118.83	123.56
24	5	609	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
37	c	518	DGD	O3G-C3G-C2G	-2.21	105.57	110.90
26	n	1620	LUT	C7-C8-C9	-2.21	122.90	126.23
34	C	517	BCR	C33-C5-C6	-2.21	122.05	124.53
25	3	602	CLA	C3B-C4B-NB	-2.21	108.47	110.52
26	q	1620	LUT	C21-C26-C27	-2.21	109.91	112.70
24	N	607	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
28	g	1623	NEX	C20-C13-C14	-2.21	119.83	122.92
25	n	602	CLA	CAA-CBA-CGA	-2.21	106.81	113.25
24	y	606	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
25	y	604	CLA	CHB-C4A-NA	2.21	127.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	619	BCR	C39-C30-C25	-2.21	106.72	110.30
26	8	1620	LUT	C30-C31-C32	-2.21	116.33	123.22
25	6	611	CLA	C1-C2-C3	-2.21	122.23	126.04
26	y	1620	LUT	C7-C8-C9	-2.20	122.90	126.23
25	n	603	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
25	R	601	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	8	605	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
25	g	602	CLA	CHB-C1B-NB	2.20	126.59	124.26
24	Y	606	CHL	O1D-CGD-CBD	-2.20	119.97	124.48
25	7	612	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
25	Y	604	CLA	CHB-C1B-C2B	-2.20	121.01	127.24
24	q	601	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
26	7	1621	LUT	C31-C30-C29	-2.20	124.17	127.31
28	2	1623	NEX	C31-C30-C29	-2.20	124.17	127.31
25	b	617	CLA	CMB-C2B-C3B	2.20	131.92	126.59
25	g	610	CLA	CHD-C1D-ND	-2.20	122.43	124.45
24	5	601	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
24	3	601	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
24	8	601	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
25	C	512	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	4	604	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
28	2	1623	NEX	O24-C25-C38	2.20	117.69	115.06
25	s	614	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	q	1622	XAT	C24-C23-C22	-2.20	106.52	110.77
25	G	610	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	g	613	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
26	5	1621	LUT	C36-C21-C26	2.20	112.88	109.55
34	b	620	BCR	C34-C9-C10	-2.20	119.84	122.92
37	C	518	DGD	O1G-C1A-O1A	-2.20	118.04	123.59
25	8	602	CLA	CMB-C2B-C3B	2.20	131.91	126.59
34	B	620	BCR	C39-C30-C25	-2.20	106.73	110.30
25	y	604	CLA	CHB-C1B-C2B	-2.20	121.03	127.24
25	7	602	CLA	C3B-C4B-NB	-2.20	108.48	110.52
25	5	604	CLA	CHB-C1B-NB	2.20	126.58	124.26
27	G	1622	XAT	C30-C31-C32	-2.20	116.36	123.22
37	C	518	DGD	O3G-C3G-C2G	-2.20	105.60	110.90
27	9	1622	XAT	C4-C3-C2	-2.20	106.53	110.77
24	0	607	CHL	CMD-C2D-C3D	-2.20	122.56	127.61
26	y	1621	LUT	C31-C30-C29	-2.20	124.18	127.31
24	4	601	CHL	CMD-C2D-C3D	-2.20	122.56	127.61
24	5	605	CHL	C7-C6-C5	-2.20	107.40	113.36
28	q	1623	NEX	C24-C23-C22	-2.20	106.53	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	605	CHL	O1D-CGD-CBD	-2.19	119.99	124.48
39	d	405	PL9	C42-C43-C44	-2.19	122.38	127.66
26	3	1621	LUT	C35-C15-C14	-2.19	118.98	123.47
24	g	605	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
25	r	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	1	1621	LUT	C16-C1-C6	-2.19	106.74	110.30
25	r	609	CLA	CHB-C1B-NB	2.19	126.58	124.26
34	c	514	BCR	C33-C5-C6	-2.19	122.06	124.53
25	y	614	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	B	617	CLA	CMB-C2B-C3B	2.19	131.90	126.59
25	b	617	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
24	s	608	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
25	B	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	s	1621	LUT	C30-C31-C32	-2.19	116.38	123.22
25	3	614	CLA	C3B-C4B-NB	-2.19	108.48	110.52
25	2	610	CLA	CMB-C2B-C3B	2.19	131.90	126.59
24	8	601	CHL	C4-C3-C5	2.19	118.96	115.27
25	R	602	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
37	c	519	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
24	p	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
28	G	1623	NEX	C5-C6-C1	2.19	121.87	119.70
25	B	617	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
24	r	608	CHL	CHB-C4A-NA	2.19	127.54	124.51
34	h	101	BCR	C8-C9-C10	2.19	122.30	118.94
24	6	605	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
26	8	1620	LUT	C38-C25-C24	-2.19	118.87	123.56
25	3	602	CLA	CMB-C2B-C3B	2.19	131.89	126.59
26	5	1621	LUT	C31-C30-C29	-2.19	124.19	127.31
25	Y	614	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	4	607	CHL	C2A-C3A-C4A	-2.19	98.33	101.87
24	n	601	CHL	C4D-C3D-CAD	2.19	110.67	108.10
24	q	608	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
26	3	1620	LUT	C19-C9-C8	2.19	121.52	118.08
34	C	517	BCR	C36-C18-C19	2.19	121.52	118.08
24	r	608	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
27	y	1622	XAT	C10-C11-C12	-2.19	116.39	123.22
24	S	608	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
24	8	606	CHL	O1D-CGD-CBD	-2.19	120.01	124.48
24	q	607	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
25	0	602	CLA	C3B-C4B-NB	-2.19	108.49	110.52
24	2	608	CHL	CHC-C4B-NB	-2.19	121.94	124.26
24	6	609	CHL	CHC-C4B-NB	-2.19	121.94	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	611	CLA	CHC-C4B-NB	2.19	126.57	124.26
26	R	620	LUT	C38-C25-C24	-2.19	118.88	123.56
24	2	607	CHL	C4A-NA-C1A	2.19	107.69	106.71
24	4	605	CHL	C4A-NA-C1A	2.19	107.69	106.71
26	q	1620	LUT	C18-C5-C6	-2.19	122.07	124.53
40	f	101	HEM	CMB-C2B-C1B	-2.19	121.71	125.04
27	R	622	XAT	O24-C25-C26	-2.19	57.15	58.96
34	c	517	BCR	C36-C18-C19	2.18	121.52	118.08
25	C	511	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	r	602	CLA	CAA-CBA-CGA	-2.18	106.87	113.25
24	Y	609	CHL	CHC-C4B-NB	-2.18	121.94	124.26
24	y	609	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
26	Y	1620	LUT	C35-C15-C14	-2.18	119.00	123.47
24	s	601	CHL	O2A-CGA-O1A	-2.18	117.86	123.30
26	y	1620	LUT	C21-C26-C27	-2.18	109.94	112.70
25	Y	602	CLA	CAA-CBA-CGA	-2.18	106.87	113.25
24	1	607	CHL	C1-O2A-CGA	2.18	122.17	116.44
25	6	614	CLA	CMB-C2B-C1B	-2.18	122.04	125.37
26	9	1620	LUT	C16-C1-C6	-2.18	106.76	110.30
25	g	610	CLA	CHB-C1B-NB	2.18	126.57	124.26
24	9	609	CHL	CAA-CBA-CGA	-2.18	106.87	113.25
37	C	519	DGD	O1G-C1A-O1A	-2.18	118.08	123.59
25	5	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	6	601	CHL	C11-C10-C8	-2.18	108.87	115.92
24	1	609	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
24	3	606	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
25	2	612	CLA	CHC-C4B-NB	2.18	126.56	124.26
25	B	606	CLA	CHC-C4B-NB	2.18	126.56	124.26
25	G	612	CLA	CHB-C1B-NB	2.18	126.56	124.26
26	q	1620	LUT	C8-C7-C6	-2.18	121.08	127.20
25	G	610	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	5	604	CLA	CHD-C1D-ND	-2.18	122.45	124.45
39	D	405	PL9	C42-C43-C44	-2.18	122.41	127.66
25	S	604	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	p	614	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	G	603	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
25	B	604	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	N	1620	LUT	C31-C30-C29	-2.18	124.20	127.31
25	7	613	CLA	CHC-C4B-NB	2.18	126.56	124.26
27	8	1622	XAT	O4-C5-C6	-2.18	57.16	58.96
25	b	616	CLA	C11-C12-C13	-2.18	108.88	115.92
25	5	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	1621	LUT	C10-C11-C12	-2.18	116.42	123.22
25	9	604	CLA	CHB-C1B-NB	2.18	126.56	124.26
25	n	614	CLA	CHB-C1B-NB	2.18	126.56	124.26
29	y	2630	LHG	O8-C23-O10	-2.18	118.10	123.59
24	y	609	CHL	CMD-C2D-C3D	-2.18	122.61	127.61
26	g	1620	LUT	C8-C7-C6	-2.18	121.09	127.20
26	3	1620	LUT	C38-C25-C24	-2.18	118.90	123.56
24	y	609	CHL	CAC-C3C-C4C	2.18	127.63	124.81
25	3	610	CLA	CHB-C1B-NB	2.18	126.56	124.26
26	n	1621	LUT	C10-C11-C12	-2.18	116.43	123.22
25	y	614	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	4	605	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
27	7	1622	XAT	O24-C25-C26	-2.17	57.16	58.96
25	8	602	CLA	C3B-C4B-NB	-2.17	108.50	110.52
28	n	1623	NEX	C28-C29-C30	2.17	122.28	118.94
24	q	609	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
25	B	603	CLA	C2A-C1A-CHA	2.17	127.66	123.86
26	N	1621	LUT	C30-C31-C32	-2.17	116.43	123.22
24	S	608	CHL	C4D-CHA-C1A	-2.17	118.60	121.25
26	2	1620	LUT	C16-C1-C6	-2.17	106.77	110.30
27	g	1622	XAT	C30-C31-C32	-2.17	116.44	123.22
24	1	606	CHL	C3B-C4B-NB	2.17	112.53	110.52
24	9	606	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
25	s	604	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	8	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	G	1621	LUT	C3-C4-C5	-2.17	107.53	111.85
26	y	1620	LUT	C35-C15-C14	-2.17	119.03	123.47
25	B	605	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	S	1621	LUT	C30-C31-C32	-2.17	116.44	123.22
25	g	602	CLA	C3B-C4B-NB	-2.17	108.50	110.52
37	C	524	DGD	C6D-C5D-C4D	-2.17	107.56	112.09
24	0	605	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
25	q	610	CLA	CHB-C1B-NB	2.17	126.55	124.26
25	b	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
27	p	1622	XAT	C31-C30-C29	-2.17	124.22	127.31
28	q	1623	NEX	C35-C34-C33	-2.17	124.22	127.31
25	g	610	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	b	612	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	6	602	CLA	C3B-C4B-NB	-2.17	108.50	110.52
24	p	605	CHL	O2A-CGA-CBA	2.17	118.71	111.91
26	2	1620	LUT	C18-C5-C6	-2.17	122.09	124.53
24	Y	609	CHL	O1D-CGD-CBD	-2.17	120.05	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	411	BCR	C20-C21-C22	-2.17	124.22	127.31
26	5	1620	LUT	C35-C15-C14	-2.17	119.03	123.47
25	R	611	CLA	CHC-C4B-NB	2.17	126.55	124.26
25	S	605	CLA	C1-C2-C3	-2.17	123.25	126.75
25	b	606	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	3	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
24	5	609	CHL	CHD-C4C-C3C	-2.17	121.66	124.84
26	7	1621	LUT	C36-C21-C26	2.17	112.83	109.55
25	1	610	CLA	CMB-C2B-C3B	2.17	131.83	126.59
34	c	517	BCR	C33-C5-C6	-2.16	122.10	124.53
37	c	518	DGD	O1G-C1A-O1A	-2.16	118.13	123.59
26	6	1620	LUT	C30-C31-C32	-2.16	116.46	123.22
24	R	608	CHL	CHB-C4A-NA	2.16	127.50	124.51
27	8	1622	XAT	C24-C23-C22	-2.16	106.59	110.77
28	y	1623	NEX	C11-C12-C13	-2.16	120.34	126.42
25	7	613	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
25	g	603	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
24	g	606	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
24	y	607	CHL	C3B-C4B-NB	2.16	112.52	110.52
25	R	612	CLA	CHB-C1B-NB	2.16	126.55	124.26
25	B	606	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
28	9	1623	NEX	C26-C27-C28	-2.16	121.42	125.99
27	6	1622	XAT	C39-C29-C30	-2.16	119.89	122.92
25	r	602	CLA	CHC-C4B-NB	2.16	126.55	124.26
25	B	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	b	605	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	p	1623	NEX	C30-C31-C32	-2.16	116.47	123.22
24	y	605	CHL	CHC-C4B-NB	-2.16	121.97	124.26
25	R	613	CLA	CHB-C1B-NB	2.16	126.55	124.26
24	3	606	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
24	N	609	CHL	C1D-CHD-C4C	-2.16	121.40	126.06
26	0	1620	LUT	C10-C11-C12	-2.16	116.48	123.22
24	6	605	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
24	4	609	CHL	C4-C3-C5	2.16	118.90	115.27
27	9	1622	XAT	C7-C8-C9	-2.16	122.18	125.53
25	g	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	C	517	BCR	C16-C17-C18	-2.16	124.23	127.31
24	p	606	CHL	CHD-C4C-C3C	-2.16	121.67	124.84
34	h	101	BCR	C37-C22-C21	-2.16	119.90	122.92
25	g	614	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	G	1623	NEX	C28-C29-C30	2.16	122.25	118.94
25	r	612	CLA	CHB-C1B-NB	2.16	126.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	608	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
25	2	611	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
25	B	616	CLA	C11-C12-C13	-2.16	108.95	115.92
33	A	408	PHO	OBD-CAD-CBD	-2.16	122.66	125.82
25	9	611	CLA	C3B-C4B-NB	-2.16	108.52	110.52
26	3	1621	LUT	C39-C29-C28	2.16	121.47	118.08
25	9	611	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
28	g	1623	NEX	C26-C27-C28	-2.15	121.44	125.99
25	S	614	CLA	CHB-C1B-NB	2.15	126.54	124.26
24	R	608	CHL	CHC-C4B-NB	-2.15	121.98	124.26
24	Y	605	CHL	CHC-C4B-NB	-2.15	121.98	124.26
25	1	613	CLA	CHC-C4B-NB	2.15	126.54	124.26
25	0	603	CLA	CHD-C1D-ND	-2.15	122.47	124.45
26	8	1621	LUT	C16-C1-C6	-2.15	106.81	110.30
24	n	609	CHL	CBC-CAC-C3C	-2.15	106.50	112.43
24	n	606	CHL	CHB-C1B-NB	-2.15	121.98	124.26
26	4	1620	LUT	C8-C7-C6	-2.15	121.16	127.20
26	G	1621	LUT	C35-C15-C14	-2.15	119.06	123.47
25	C	511	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	y	1621	LUT	C21-C26-C27	-2.15	109.98	112.70
24	n	607	CHL	C3B-C4B-NB	2.15	112.51	110.52
25	4	614	CLA	C3B-C4B-NB	-2.15	108.52	110.52
25	C	505	CLA	C7-C6-C5	-2.15	107.52	113.36
25	s	611	CLA	CHC-C4B-NB	2.15	126.53	124.26
24	g	607	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
25	p	611	CLA	C3B-C4B-NB	-2.15	108.52	110.52
26	4	1621	LUT	C15-C35-C34	-2.15	119.07	123.47
25	c	505	CLA	C7-C6-C5	-2.15	107.52	113.36
25	p	612	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	q	602	CLA	CMB-C2B-C3B	2.15	131.79	126.59
24	y	609	CHL	C2A-C1A-CHA	-2.15	120.10	123.86
24	3	605	CHL	C1-C2-C3	-2.15	122.33	126.04
24	G	609	CHL	CMB-C2B-C1B	2.15	128.64	125.37
24	y	601	CHL	C3A-C2A-C1A	-2.15	98.12	101.34
24	g	609	CHL	CMB-C2B-C1B	2.15	128.64	125.37
25	b	606	CLA	CHC-C4B-NB	2.15	126.53	124.26
24	n	609	CHL	C1D-CHD-C4C	-2.15	121.42	126.06
24	3	601	CHL	C4-C3-C5	2.15	118.88	115.27
34	b	620	BCR	C38-C26-C25	-2.15	122.12	124.53
25	3	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	b	607	CLA	C3B-C4B-NB	-2.15	108.52	110.52
27	y	1622	XAT	C19-C9-C8	2.15	121.46	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	613	CLA	CHB-C1B-NB	2.15	126.53	124.26
24	1	608	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
27	2	1622	XAT	C4-C3-C2	-2.14	106.63	110.77
24	G	605	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
24	n	607	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
25	b	607	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
24	g	608	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
24	G	607	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
25	N	602	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
24	Y	609	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
25	Y	614	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	0	610	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	1	612	CLA	CMB-C2B-C3B	2.14	131.78	126.59
25	5	614	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	4	613	CLA	CHC-C4B-NB	2.14	126.53	124.26
25	2	604	CLA	C3B-C4B-NB	-2.14	108.53	110.52
25	a	410	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
24	7	601	CHL	O2A-CGA-CBA	2.14	118.63	111.91
26	p	1620	LUT	C10-C11-C12	-2.14	116.53	123.22
24	N	608	CHL	CHC-C4B-NB	-2.14	121.99	124.26
25	7	602	CLA	CHB-C1B-NB	2.14	126.52	124.26
24	G	608	CHL	CMB-C2B-C1B	2.14	128.63	125.37
25	Y	612	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
26	N	1621	LUT	C10-C11-C12	-2.14	116.54	123.22
27	1	1622	XAT	C40-C33-C34	-2.14	119.92	122.92
37	c	524	DGD	C6D-C5D-C4D	-2.14	107.62	112.09
24	6	601	CHL	C11-C12-C13	-2.14	109.00	115.92
25	S	611	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
24	Y	607	CHL	C3B-C4B-NB	2.14	112.50	110.52
25	3	611	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	s	614	CLA	CHB-C1B-NB	2.14	126.52	124.26
36	S	2631	LMG	C8-O7-C10	-2.14	112.52	117.79
24	p	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
25	8	611	CLA	CHC-C4B-NB	2.14	126.52	124.26
24	5	607	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
25	9	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
26	G	1621	LUT	C19-C9-C8	2.14	121.44	118.08
26	5	1621	LUT	C18-C5-C6	-2.14	122.13	124.53
34	a	411	BCR	C33-C5-C4	2.14	117.72	113.62
24	G	609	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
24	N	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
40	F	101	HEM	CBD-CAD-C3D	-2.14	106.69	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	408	PHO	OBD-CAD-CBD	-2.13	122.69	125.82
25	3	611	CLA	CHC-C4B-NB	2.13	126.52	124.26
25	g	612	CLA	CHB-C1B-NB	2.13	126.52	124.26
24	1	601	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
40	F	101	HEM	CMB-C2B-C1B	-2.13	121.79	125.04
25	2	602	CLA	C1-C2-C3	-2.13	122.35	126.04
25	b	605	CLA	O2D-CGD-CBD	2.13	115.06	111.27
25	Y	613	CLA	C2D-C1D-ND	-2.13	108.53	110.10
25	7	612	CLA	C3B-C4B-NB	-2.13	108.53	110.52
24	4	605	CHL	CED-O2D-CGD	2.13	120.76	115.94
34	H	101	BCR	C37-C22-C21	-2.13	119.93	122.92
27	r	622	XAT	O24-C25-C26	-2.13	57.19	58.96
24	8	608	CHL	C4D-C3D-CAD	2.13	110.61	108.10
24	8	609	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
25	4	612	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
24	N	607	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
25	B	617	CLA	C2A-C1A-CHA	2.13	127.59	123.86
33	a	408	PHO	C16-C15-C13	-2.13	109.03	115.92
24	1	609	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
24	6	601	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
24	n	609	CHL	CHB-C4A-NA	2.13	127.46	124.51
26	Y	1621	LUT	C21-C26-C27	-2.13	110.01	112.70
25	8	614	CLA	C3B-C4B-NB	-2.13	108.54	110.52
24	8	607	CHL	CAC-C3C-C4C	2.13	127.58	124.81
24	5	609	CHL	CHC-C4B-NB	-2.13	122.00	124.26
28	g	1623	NEX	C17-C1-C6	-2.13	108.56	110.47
26	0	1620	LUT	C8-C7-C6	-2.13	121.22	127.20
25	n	604	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
24	g	601	CHL	C4D-C3D-CAD	2.13	110.61	108.10
25	p	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	9	601	CHL	CHD-C4C-C3C	-2.13	121.71	124.84
27	N	1622	XAT	C40-C33-C32	2.13	121.43	118.08
25	8	611	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	B	605	CLA	O2D-CGD-CBD	2.13	115.05	111.27
25	p	610	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	4	614	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	7	612	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
24	9	609	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
25	9	610	CLA	CMB-C2B-C3B	2.13	131.74	126.59
28	Y	1623	NEX	O24-C25-C26	-2.12	57.20	58.96
25	b	615	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
24	8	607	CHL	CMB-C2B-C1B	2.12	128.60	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	608	CHL	C2A-C1A-CHA	-2.12	120.14	123.86
26	p	1620	LUT	C15-C35-C34	-2.12	119.12	123.47
33	A	408	PHO	C16-C15-C13	-2.12	109.05	115.92
27	1	1622	XAT	O24-C25-C26	-2.12	57.20	58.96
24	6	605	CHL	C4D-CHA-C1A	-2.12	118.66	121.25
25	y	612	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
24	p	601	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
26	0	1621	LUT	C18-C5-C4	2.12	118.29	114.36
24	y	608	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
34	D	404	BCR	C30-C25-C26	-2.12	119.62	122.61
34	C	515	BCR	C36-C18-C19	2.12	121.42	118.08
25	G	611	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
24	1	606	CHL	CAA-C2A-C3A	-2.12	106.97	112.78
25	g	602	CLA	CMB-C2B-C3B	2.12	131.73	126.59
25	q	603	CLA	CMB-C2B-C3B	2.12	131.72	126.59
28	7	1623	NEX	C17-C1-C6	-2.12	108.57	110.47
24	p	605	CHL	C1-O2A-CGA	2.12	122.01	116.44
26	G	1620	LUT	C2-C3-C4	2.12	113.21	110.30
25	C	508	CLA	CHD-C4C-NC	2.12	127.54	124.20
34	C	517	BCR	C33-C5-C4	2.12	117.69	113.62
25	B	607	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
34	A	411	BCR	C33-C5-C4	2.12	117.69	113.62
24	4	606	CHL	CED-O2D-CGD	2.12	120.73	115.94
25	g	611	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
26	Y	1621	LUT	C30-C31-C32	-2.12	116.61	123.22
24	6	606	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
25	g	612	CLA	C3B-C4B-NB	-2.12	108.55	110.52
24	3	608	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
24	8	608	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
25	c	508	CLA	CHD-C4C-NC	2.12	127.54	124.20
25	8	611	CLA	C3B-C4B-NB	-2.12	108.55	110.52
25	7	613	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	y	612	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
25	R	616	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	S	601	CHL	CED-O2D-CGD	2.12	120.72	115.94
26	r	620	LUT	C30-C31-C32	-2.12	116.61	123.22
26	y	1620	LUT	C3-C4-C5	-2.12	107.64	111.85
34	B	620	BCR	C38-C26-C25	-2.12	122.15	124.53
24	1	607	CHL	CAA-CBA-CGA	-2.12	107.07	113.25
25	A	410	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	b	617	CLA	C2A-C1A-CHA	2.12	127.56	123.86
26	9	1620	LUT	C20-C13-C12	2.12	121.41	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	1622	XAT	C40-C33-C32	2.12	121.41	118.08
27	Y	1622	XAT	C19-C9-C8	2.12	121.41	118.08
28	r	623	NEX	C35-C15-C14	-2.12	119.14	123.47
24	s	601	CHL	CED-O2D-CGD	2.12	120.72	115.94
24	5	605	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
25	b	603	CLA	O2D-CGD-CBD	2.11	115.03	111.27
34	B	620	BCR	C16-C15-C14	-2.11	119.14	123.47
25	r	616	CLA	CHB-C1B-NB	2.11	126.50	124.26
24	3	609	CHL	O2D-CGD-O1D	-2.11	119.70	123.84
25	s	614	CLA	C3B-C4B-NB	-2.11	108.55	110.52
34	H	101	BCR	C8-C9-C10	2.11	122.18	118.94
25	8	603	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	7	607	CHL	C2A-C3A-C4A	-2.11	98.46	101.87
28	y	1623	NEX	O24-C25-C26	-2.11	57.21	58.96
25	9	603	CLA	C2A-C1A-CHA	2.11	127.55	123.86
25	S	611	CLA	CHC-C4B-NB	2.11	126.49	124.26
25	A	410	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
25	B	612	CLA	C3B-C4B-NB	-2.11	108.56	110.52
25	a	410	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
36	h	102	LMG	O7-C10-O9	-2.11	118.60	123.70
25	a	407	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
24	Y	601	CHL	CGD-CBD-CAD	-2.11	103.89	110.73
24	6	605	CHL	CAA-C2A-C3A	-2.11	107.00	112.78
25	8	613	CLA	CHD-C1D-ND	-2.11	122.51	124.45
24	8	605	CHL	C1-C2-C3	-2.11	122.39	126.04
25	7	602	CLA	C4-C3-C5	2.11	118.82	115.27
24	S	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
25	b	612	CLA	C3B-C4B-NB	-2.11	108.56	110.52
24	p	605	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
25	6	602	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
24	S	606	CHL	CHB-C4A-NA	2.11	127.43	124.51
27	3	1622	XAT	C24-C23-C22	-2.11	106.70	110.77
25	B	615	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
25	4	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
34	B	620	BCR	C34-C9-C10	-2.11	119.97	122.92
26	8	1620	LUT	C19-C9-C8	2.11	121.40	118.08
24	7	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
34	d	404	BCR	C30-C25-C26	-2.11	119.64	122.61
25	6	614	CLA	O2D-CGD-CBD	2.11	115.01	111.27
24	q	605	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
26	9	1620	LUT	C39-C29-C28	2.11	121.40	118.08
36	d	412	LMG	O8-C28-O10	-2.11	118.27	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
36	s	2631	LMG	C8-O7-C10	-2.11	112.60	117.79
33	a	409	PHO	O2A-CGA-O1A	-2.11	118.28	123.59
25	n	614	CLA	C3B-C4B-NB	-2.11	108.56	110.52
24	6	608	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
24	p	601	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
25	G	612	CLA	CHC-C4B-NB	2.10	126.48	124.26
28	s	1623	NEX	C20-C13-C14	-2.10	119.97	122.92
25	G	612	CLA	C3B-C4B-NB	-2.10	108.56	110.52
25	p	602	CLA	CMB-C2B-C3B	2.10	131.68	126.59
24	6	605	CHL	CAA-C2A-C1A	2.10	118.87	111.97
25	c	501	CLA	O2D-CGD-CBD	2.10	115.00	111.27
25	4	602	CLA	CMB-C2B-C3B	2.10	131.68	126.59
25	N	603	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
25	b	617	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	B	613	CLA	CHA-C1A-NA	-2.10	121.58	126.40
25	9	602	CLA	CMB-C2B-C3B	2.10	131.68	126.59
33	A	409	PHO	O2A-CGA-O1A	-2.10	118.29	123.59
24	n	607	CHL	C1-C2-C3	-2.10	122.41	126.04
24	3	609	CHL	C4-C3-C5	2.10	118.81	115.27
24	8	606	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
25	2	602	CLA	CHB-C1B-NB	2.10	126.48	124.26
24	N	605	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
24	Y	601	CHL	O2A-CGA-CBA	2.10	118.50	111.91
26	R	620	LUT	C30-C31-C32	-2.10	116.66	123.22
26	8	1621	LUT	C35-C15-C14	-2.10	119.17	123.47
25	B	606	CLA	C1-C2-C3	-2.10	122.41	126.04
25	G	604	CLA	CMB-C2B-C3B	2.10	131.67	126.59
25	B	603	CLA	O2D-CGD-CBD	2.10	115.00	111.27
28	5	1623	NEX	C16-C1-C6	2.10	112.35	110.47
24	G	606	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
24	0	609	CHL	C1D-CHD-C4C	-2.10	121.53	126.06
24	n	605	CHL	CBC-CAC-C3C	-2.10	106.64	112.43
36	H	102	LMG	O7-C10-O9	-2.10	118.63	123.70
25	G	602	CLA	C3B-C4B-NB	-2.10	108.57	110.52
27	7	1622	XAT	C35-C15-C14	-2.10	119.17	123.47
34	A	411	BCR	C20-C21-C22	-2.10	124.31	127.31
24	7	606	CHL	C4-C3-C5	2.10	118.80	115.27
26	7	1621	LUT	C3-C4-C5	-2.10	107.67	111.85
35	b	621	SQD	C44-O6-C1	-2.10	109.64	113.74
24	Y	607	CHL	CHB-C1B-C2B	-2.10	121.31	127.24
25	p	612	CLA	CHC-C4B-NB	2.10	126.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	608	CLA	CHB-C1B-NB	2.10	126.48	124.26
24	g	601	CHL	CAA-CBA-CGA	-2.10	107.12	113.25
26	y	1621	LUT	C30-C31-C32	-2.10	116.67	123.22
25	4	604	CLA	C3B-C4B-NB	-2.10	108.57	110.52
25	g	604	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	Y	1620	LUT	C20-C13-C12	2.10	121.38	118.08
24	y	607	CHL	CHB-C1B-C2B	-2.10	121.32	127.24
24	3	607	CHL	C1-C2-C3	-2.10	122.42	126.04
26	n	1620	LUT	C8-C7-C6	-2.10	121.32	127.20
28	7	1623	NEX	C5-C4-C3	-2.10	109.26	111.75
25	q	610	CLA	C3B-C4B-NB	-2.10	108.57	110.52
25	1	610	CLA	C1-C2-C3	-2.10	122.42	126.04
25	5	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	0	1623	NEX	C16-C1-C6	2.10	112.35	110.47
26	p	1621	LUT	C10-C11-C12	-2.10	116.68	123.22
25	5	614	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	0	606	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
25	c	505	CLA	C3B-C4B-NB	-2.09	108.57	110.52
25	g	612	CLA	CHC-C4B-NB	2.09	126.47	124.26
25	N	610	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	c	517	BCR	C33-C5-C4	2.09	117.64	113.62
25	0	613	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
33	a	408	PHO	CMA-C3A-C4A	-2.09	109.79	114.38
25	5	614	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	A	407	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
24	s	606	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
27	4	1622	XAT	C24-C23-C22	-2.09	106.73	110.77
25	y	613	CLA	CAC-C3C-C4C	2.09	127.53	124.81
25	y	610	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	3	601	CHL	C1-O2A-CGA	2.09	121.93	116.44
36	D	412	LMG	O8-C28-O10	-2.09	118.31	123.59
25	3	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
24	8	601	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
40	F	101	HEM	CAA-CBA-CGA	-2.09	109.10	113.60
26	3	1621	LUT	C3-C4-C5	-2.09	107.69	111.85
24	6	601	CHL	CED-O2D-CGD	2.09	120.67	115.94
24	2	606	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
24	1	607	CHL	C1C-C2C-C3C	-2.09	105.45	107.11
24	n	607	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
26	s	1620	LUT	C15-C14-C13	-2.09	124.33	127.31
24	Y	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
24	7	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	612	CLA	C2A-C1A-CHA	2.09	127.51	123.86
24	4	608	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
25	S	605	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	C	511	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	1	1622	XAT	C40-C33-C32	2.09	121.37	118.08
25	7	614	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	0	613	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	5	1621	LUT	C16-C1-C6	-2.09	106.91	110.30
26	8	1621	LUT	C39-C29-C28	2.09	121.36	118.08
25	B	602	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	b	613	CLA	CHA-C1A-NA	-2.09	121.62	126.40
26	6	1620	LUT	C40-C33-C32	2.09	121.36	118.08
34	c	515	BCR	C36-C18-C19	2.09	121.36	118.08
25	b	607	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
35	B	621	SQD	C44-O6-C1	-2.09	109.66	113.74
25	9	614	CLA	C3B-C4B-NB	-2.09	108.58	110.52
29	Y	2630	LHG	O8-C23-O10	-2.09	118.33	123.59
34	b	620	BCR	C16-C15-C14	-2.09	119.20	123.47
24	8	609	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
24	9	601	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
25	6	612	CLA	C2A-C1A-CHA	2.09	127.50	123.86
25	7	610	CLA	CMB-C2B-C3B	2.09	131.64	126.59
25	B	607	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	y	1620	LUT	C2-C3-C4	-2.08	107.45	110.30
25	3	612	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	Y	612	CLA	CMB-C2B-C1B	-2.08	122.19	125.37
26	4	1620	LUT	C18-C5-C4	2.08	118.22	114.36
26	S	1620	LUT	C40-C33-C32	2.08	121.36	118.08
24	1	607	CHL	C2A-C3A-C4A	-2.08	98.50	101.87
25	B	617	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
24	4	607	CHL	CED-O2D-CGD	2.08	120.65	115.94
25	p	602	CLA	CHD-C1D-ND	-2.08	122.54	124.45
33	A	408	PHO	CMA-C3A-C4A	-2.08	109.81	114.38
28	1	1623	NEX	C2-C1-C6	2.08	111.24	109.21
25	g	604	CLA	CMB-C2B-C3B	2.08	131.63	126.59
24	3	608	CHL	C4D-CHA-C1A	-2.08	118.71	121.25
25	1	614	CLA	CHB-C1B-NB	2.08	126.46	124.26
25	9	610	CLA	C1-C2-C3	-2.08	122.44	126.04
25	N	614	CLA	C3B-C4B-NB	-2.08	108.58	110.52
25	p	612	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	S	608	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
27	r	622	XAT	C31-C30-C29	-2.08	124.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	607	CHL	CED-O2D-CGD	2.08	120.64	115.94
24	8	607	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
24	0	605	CHL	CAA-C2A-C1A	2.08	118.80	111.97
25	B	613	CLA	CHC-C4B-NB	2.08	126.46	124.26
25	b	613	CLA	CHC-C4B-NB	2.08	126.46	124.26
25	1	604	CLA	CAC-C3C-C4C	2.08	127.51	124.81
28	3	1623	NEX	C16-C1-C6	2.08	112.33	110.47
24	0	606	CHL	CHB-C4A-NA	2.08	127.39	124.51
24	s	606	CHL	CHB-C4A-NA	2.08	127.39	124.51
25	b	606	CLA	C1-C2-C3	-2.08	122.44	126.04
24	5	606	CHL	CED-O2D-CGD	2.08	120.64	115.94
26	Y	1621	LUT	C36-C21-C26	2.08	112.70	109.55
25	6	610	CLA	C1-C2-C3	-2.08	122.45	126.04
25	n	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	2	1620	LUT	C30-C31-C32	-2.08	116.73	123.22
26	0	1620	LUT	C11-C10-C9	-2.08	124.34	127.31
24	4	606	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
25	y	603	CLA	CBA-CAA-C2A	-2.08	107.73	113.86
25	8	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	1	1621	LUT	C36-C21-C26	2.08	112.69	109.55
25	1	602	CLA	CHB-C1B-NB	2.08	126.46	124.26
26	G	1621	LUT	C16-C1-C6	-2.08	106.93	110.30
24	g	607	CHL	C1C-C2C-C3C	-2.08	105.47	107.11
26	6	1621	LUT	C35-C15-C14	-2.08	119.22	123.47
24	q	607	CHL	CAA-C2A-C3A	-2.08	107.09	112.78
25	C	511	CLA	CHC-C4B-NB	2.08	126.45	124.26
25	7	602	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	6	604	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
25	0	612	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
29	d	408	LHG	C5-O7-C7	-2.08	112.68	117.79
24	9	606	CHL	CED-O2D-CGD	2.08	120.63	115.94
24	s	607	CHL	C1C-C2C-C3C	-2.08	105.47	107.11
24	p	601	CHL	CHC-C4B-NB	-2.08	122.06	124.26
25	4	613	CLA	CMB-C2B-C3B	2.08	131.61	126.59
25	0	612	CLA	C2A-C1A-CHA	2.07	127.49	123.86
26	2	1620	LUT	C39-C29-C28	2.07	121.35	118.08
26	n	1621	LUT	C35-C15-C14	-2.07	119.22	123.47
25	9	613	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
27	2	1622	XAT	O4-C5-C6	-2.07	57.24	58.96
24	4	609	CHL	CAA-CBA-CGA	-2.07	107.19	113.25
24	1	606	CHL	CBC-CAC-C3C	-2.07	106.71	112.43
25	B	608	CLA	CHB-C1B-NB	2.07	126.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	605	CHL	OMC-CMC-C2C	-2.07	121.00	125.69
24	y	607	CHL	C16-C15-C13	-2.07	109.22	115.92
24	7	606	CHL	CAA-C2A-C3A	-2.07	107.10	112.78
25	N	613	CLA	CAC-C3C-C4C	2.07	127.50	124.81
24	g	606	CHL	C4D-CHA-C1A	-2.07	118.73	121.25
26	7	1621	LUT	C18-C5-C6	-2.07	122.20	124.53
25	B	607	CLA	CMB-C2B-C3B	2.07	131.61	126.59
25	s	614	CLA	CHC-C4B-NB	2.07	126.45	124.26
25	R	601	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	q	1621	LUT	C36-C21-C26	2.07	112.68	109.55
24	n	605	CHL	CHB-C4A-NA	2.07	127.37	124.51
25	5	610	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	R	602	CLA	CHC-C4B-NB	2.07	126.45	124.26
25	B	615	CLA	C3B-C4B-NB	-2.07	108.59	110.52
25	c	507	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
39	d	405	PL9	C41-C39-C38	-2.07	116.93	121.12
24	2	609	CHL	O2D-CGD-O1D	-2.07	119.79	123.84
35	b	623	SQD	O6-C44-C45	-2.07	105.91	110.90
29	7	2630	LHG	O8-C23-O10	-2.07	118.37	123.59
24	8	608	CHL	OMC-CMC-C2C	-2.07	121.01	125.69
24	G	608	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
25	C	505	CLA	CHC-C4B-NB	2.07	126.45	124.26
25	3	610	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
33	A	408	PHO	O2A-CGA-O1A	-2.07	118.37	123.59
25	q	612	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
26	y	1620	LUT	C8-C7-C6	-2.07	121.39	127.20
25	3	613	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	n	1623	NEX	O24-C25-C26	-2.07	57.25	58.96
24	y	609	CHL	CHC-C4B-NB	-2.07	122.07	124.26
26	y	1620	LUT	C20-C13-C12	2.07	121.33	118.08
24	p	607	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
25	c	505	CLA	C2D-C1D-ND	-2.07	108.58	110.10
29	4	2630	LHG	O7-C7-O9	-2.07	118.71	123.70
25	q	602	CLA	CHB-C1B-C2B	-2.07	121.40	127.24
24	N	607	CHL	C4-C3-C5	2.07	118.75	115.27
25	0	610	CLA	C1-C2-C3	-2.06	122.47	126.04
27	g	1622	XAT	C40-C33-C32	2.06	121.33	118.08
25	5	604	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
24	8	606	CHL	C3B-C4B-NB	2.06	112.43	110.52
27	q	1622	XAT	O4-C5-C6	-2.06	57.25	58.96
25	p	612	CLA	C2A-C1A-CHA	2.06	127.47	123.86
25	N	614	CLA	CHB-C1B-NB	2.06	126.44	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	9	602	CLA	C6-C7-C8	-2.06	109.25	115.92
39	D	405	PL9	C41-C39-C38	-2.06	116.94	121.12
25	G	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
37	c	524	DGD	O5D-C1E-C2E	2.06	111.52	108.30
25	C	504	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	Y	603	CLA	CBA-CAA-C2A	-2.06	107.77	113.86
28	G	1623	NEX	C26-C27-C28	-2.06	121.63	125.99
34	b	619	BCR	C35-C13-C14	-2.06	120.03	122.92
24	Y	608	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
25	S	614	CLA	C3B-C4B-NB	-2.06	108.60	110.52
33	a	408	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
24	s	607	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
24	1	601	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
25	0	602	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
34	C	515	BCR	C38-C26-C25	-2.06	122.21	124.53
34	B	620	BCR	C3-C4-C5	-2.06	110.40	114.08
28	p	1623	NEX	O24-C25-C26	-2.06	57.25	58.96
25	B	616	CLA	C2C-C1C-NC	2.06	111.90	109.97
25	S	602	CLA	CMB-C2B-C3B	2.06	131.58	126.59
34	B	620	BCR	C15-C16-C17	-2.06	119.25	123.47
34	b	620	BCR	C3-C4-C5	-2.06	110.40	114.08
34	B	619	BCR	C35-C13-C14	-2.06	120.04	122.92
26	3	1621	LUT	C2-C3-C4	-2.06	107.48	110.30
27	R	622	XAT	C31-C30-C29	-2.06	124.37	127.31
25	C	501	CLA	C7-C6-C5	-2.06	107.77	113.36
24	g	601	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
24	R	607	CHL	C7-C6-C5	-2.06	107.77	113.36
25	6	602	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
38	d	401	BCT	O3-C-O1	-2.06	114.21	119.55
26	Y	1620	LUT	C8-C9-C10	-2.06	115.78	118.94
28	5	1623	NEX	O24-C25-C26	-2.06	57.25	58.96
26	S	1620	LUT	C15-C14-C13	-2.06	124.37	127.31
25	C	507	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
25	c	504	CLA	CHB-C1B-NB	2.06	126.44	124.26
26	y	1620	LUT	C8-C9-C10	-2.06	115.78	118.94
25	Y	613	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	b	602	CLA	CHB-C1B-NB	2.06	126.44	124.26
24	Y	601	CHL	C3A-C2A-C1A	-2.06	98.26	101.34
26	s	1620	LUT	C40-C33-C32	2.06	121.32	118.08
25	n	612	CLA	CHA-C1A-NA	-2.06	121.69	126.40
25	b	607	CLA	CMB-C2B-C3B	2.06	131.57	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	502	CLA	O1D-CGD-CBD	2.06	128.69	124.48
25	8	603	CLA	CHC-C4B-NB	2.06	126.43	124.26
34	b	620	BCR	C10-C11-C12	-2.06	116.80	123.22
25	9	610	CLA	C1D-ND-C4D	-2.06	104.88	106.33
24	p	601	CHL	C11-C12-C13	-2.06	109.28	115.92
25	c	511	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	c	511	CLA	CHC-C4B-NB	2.05	126.43	124.26
26	7	1621	LUT	C19-C9-C8	2.05	121.31	118.08
34	c	516	BCR	C30-C25-C26	-2.05	119.72	122.61
24	s	608	CHL	C1C-C2C-C3C	-2.05	105.48	107.11
34	b	620	BCR	C15-C16-C17	-2.05	119.27	123.47
25	b	604	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
24	N	609	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
24	S	607	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
24	y	609	CHL	C6-C7-C8	-2.05	109.28	115.92
25	p	604	CLA	C4-C3-C5	2.05	118.72	115.27
34	B	620	BCR	C10-C11-C12	-2.05	116.81	123.22
28	g	1623	NEX	C28-C29-C30	2.05	122.09	118.94
25	2	613	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	r	601	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	3	1620	LUT	C8-C7-C6	-2.05	121.44	127.20
33	A	409	PHO	CMA-C3A-C4A	-2.05	109.88	114.38
25	c	505	CLA	CHC-C4B-NB	2.05	126.43	124.26
24	N	606	CHL	CHB-C1B-C2B	-2.05	121.44	127.24
25	c	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	q	1622	XAT	O24-C25-C26	-2.05	57.26	58.96
24	4	608	CHL	CMB-C2B-C1B	2.05	128.49	125.37
24	2	608	CHL	CHB-C4A-NA	2.05	127.35	124.51
36	S	2631	LMG	C6-C5-C4	-2.05	108.20	113.00
25	b	615	CLA	C3B-C4B-NB	-2.05	108.61	110.52
29	L	101	LHG	O8-C23-O10	-2.05	118.42	123.59
24	N	607	CHL	C3B-C4B-NB	2.05	112.42	110.52
24	N	607	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
33	A	409	PHO	CBC-CAC-C3C	2.05	115.88	112.88
24	r	608	CHL	CHC-C4B-NB	-2.05	122.09	124.26
28	N	1623	NEX	O24-C25-C26	-2.05	57.26	58.96
26	q	1620	LUT	C3-C4-C5	-2.05	107.77	111.85
24	9	601	CHL	C2A-C3A-C4A	-2.05	98.56	101.87
37	C	518	DGD	C3G-C2G-C1G	-2.05	106.94	111.79
25	2	602	CLA	CMB-C2B-C3B	2.05	131.55	126.59
26	s	1620	LUT	C19-C9-C8	2.05	121.30	118.08
25	C	508	CLA	O1D-CGD-CBD	2.05	128.67	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	O1D-CGD-CBD	-2.05	120.30	124.48
25	B	603	CLA	C3B-C4B-NB	-2.05	108.62	110.52
38	D	401	BCT	O3-C-O1	-2.05	114.24	119.55
26	1	1621	LUT	C30-C31-C32	-2.05	116.83	123.22
27	n	1622	XAT	C31-C32-C33	-2.05	120.67	126.42
25	Y	610	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	8	610	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
25	G	604	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	r	612	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	y	1621	LUT	C36-C21-C26	2.04	112.64	109.55
34	C	516	BCR	C30-C25-C26	-2.04	119.73	122.61
25	q	614	CLA	CHC-C4B-NB	2.04	126.42	124.26
26	0	1620	LUT	C31-C30-C29	-2.04	124.39	127.31
28	p	1623	NEX	C19-C9-C10	-2.04	120.06	122.92
25	c	501	CLA	C7-C6-C5	-2.04	107.81	113.36
25	C	505	CLA	C3B-C4B-NB	-2.04	108.62	110.52
25	S	614	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	N	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	8	609	CHL	CHC-C4B-NB	-2.04	122.09	124.26
25	4	604	CLA	CHB-C1B-NB	2.04	126.42	124.26
24	s	607	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
37	c	518	DGD	C3G-C2G-C1G	-2.04	106.96	111.79
25	A	406	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	a	406	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	n	607	CHL	C4D-C3D-CAD	2.04	110.50	108.10
25	8	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	1	1622	XAT	C35-C15-C14	-2.04	119.29	123.47
25	b	603	CLA	C3B-C4B-NB	-2.04	108.62	110.52
24	4	601	CHL	CHB-C4A-NA	2.04	127.33	124.51
26	1	1620	LUT	C16-C1-C6	-2.04	106.99	110.30
25	p	610	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	C	501	CLA	O2D-CGD-CBD	2.04	114.89	111.27
26	g	1620	LUT	C31-C30-C29	-2.04	124.40	127.31
24	N	608	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
28	g	1623	NEX	C11-C12-C13	-2.04	120.69	126.42
26	S	1620	LUT	C20-C13-C12	2.04	121.29	118.08
25	2	603	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	y	1621	LUT	C18-C5-C6	-2.04	122.24	124.53
25	7	612	CLA	CMB-C2B-C3B	2.04	131.53	126.59
25	G	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	N	1621	LUT	C35-C15-C14	-2.04	119.30	123.47
24	g	607	CHL	CGD-CBD-CAD	-2.04	104.13	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1621	LUT	C18-C5-C6	-2.04	122.24	124.53
25	1	612	CLA	C3B-C4B-NB	-2.04	108.62	110.52
26	y	1620	LUT	C22-C23-C24	-2.04	109.42	111.74
25	a	406	CLA	C1-C2-C3	-2.04	122.52	126.04
24	r	608	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
33	a	409	PHO	CBC-CAC-C3C	2.04	115.86	112.88
25	D	402	CLA	C4-C3-C5	2.04	118.70	115.27
24	3	609	CHL	C4A-NA-C1A	-2.04	105.79	106.71
24	n	605	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
25	4	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
25	7	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	g	602	CLA	C6-C7-C8	-2.04	109.34	115.92
25	3	611	CLA	O2D-CGD-CBD	2.04	114.89	111.27
27	q	1622	XAT	C18-C5-C4	2.04	116.57	114.28
26	G	1620	LUT	C31-C30-C29	-2.04	124.40	127.31
24	g	605	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
25	6	610	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	p	601	CHL	C1-C2-C3	-2.04	122.52	126.04
36	s	2631	LMG	C6-C5-C4	-2.04	108.24	113.00
24	2	605	CHL	CED-O2D-CGD	2.04	120.54	115.94
26	1	1621	LUT	C31-C30-C29	-2.03	124.41	127.31
25	R	610	CLA	C3B-C4B-NB	-2.03	108.63	110.52
25	2	610	CLA	C1-C2-C3	-2.03	122.53	126.04
25	6	612	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	1	2630	LHG	C6-C5-C4	-2.03	106.98	111.79
24	R	608	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
29	D	408	LHG	C5-O7-C7	-2.03	112.79	117.79
24	7	601	CHL	C1-C2-C3	-2.03	122.53	126.04
25	s	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	9	1621	LUT	C15-C35-C34	-2.03	119.31	123.47
24	1	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
25	C	509	CLA	C11-C10-C8	-2.03	109.35	115.92
26	q	1621	LUT	C8-C9-C10	-2.03	115.82	118.94
26	q	1620	LUT	C31-C32-C33	-2.03	120.71	126.42
24	Y	609	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
25	B	604	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
36	h	102	LMG	C4-C3-C2	2.03	114.37	110.82
27	4	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
24	0	601	CHL	C2A-C3A-C4A	-2.03	98.59	101.87
25	C	506	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	6	612	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
25	4	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
24	8	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
24	6	609	CHL	CED-O2D-CGD	2.03	120.53	115.94
25	R	616	CLA	CHC-C4B-NB	2.03	126.41	124.26
33	a	409	PHO	CMA-C3A-C4A	-2.03	109.93	114.38
26	Y	1620	LUT	C8-C7-C6	-2.03	121.50	127.20
26	g	1620	LUT	C2-C3-C4	2.03	113.08	110.30
25	9	602	CLA	CHB-C1B-NB	2.03	126.40	124.26
26	4	1621	LUT	C36-C21-C26	2.03	112.62	109.55
27	r	622	XAT	C15-C35-C34	-2.03	119.32	123.47
25	G	614	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	C	502	CLA	O1D-CGD-CBD	2.03	128.63	124.48
25	c	511	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	Y	602	CLA	CHB-C1B-NB	2.03	126.40	124.26
26	4	1620	LUT	C10-C11-C12	-2.03	116.89	123.22
24	6	608	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
25	b	616	CLA	C2C-C1C-NC	2.03	111.87	109.97
24	3	608	CHL	C4D-C3D-CAD	2.03	110.48	108.10
24	Y	609	CHL	C6-C7-C8	-2.03	109.37	115.92
25	C	509	CLA	C11-C12-C13	-2.03	109.37	115.92
25	3	611	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	S	607	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
27	y	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
40	F	101	HEM	CAC-C3C-C4C	-2.03	120.00	124.90
27	6	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
24	S	607	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
24	7	607	CHL	CAA-CBA-CGA	-2.03	107.33	113.25
25	b	616	CLA	CHA-C1A-NA	-2.03	121.76	126.40
25	B	616	CLA	CHA-C1A-NA	-2.02	121.76	126.40
28	4	1623	NEX	C5-C6-C1	2.02	121.70	119.70
25	c	508	CLA	O1D-CGD-CBD	2.02	128.63	124.48
25	G	611	CLA	CHB-C1B-NB	2.02	126.40	124.26
24	7	606	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
29	l	101	LHG	O8-C23-O10	-2.02	118.48	123.59
34	c	515	BCR	C38-C26-C27	2.02	117.50	113.62
37	C	524	DGD	O5D-C1E-C2E	2.02	111.46	108.30
25	y	602	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	n	613	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	n	605	CHL	CAC-C3C-C4C	2.02	127.44	124.81
24	1	609	CHL	C1-C2-C3	-2.02	122.54	126.04
25	q	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	a	410	CLA	CHC-C1C-NC	2.02	127.27	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	s	601	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
24	y	605	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
37	C	520	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
37	c	520	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
28	4	1623	NEX	C38-C25-C24	2.02	116.56	114.28
25	R	612	CLA	C3B-C4B-NB	-2.02	108.64	110.52
27	3	1622	XAT	O24-C25-C26	-2.02	57.28	58.96
25	A	406	CLA	C1-C2-C3	-2.02	122.55	126.04
25	s	614	CLA	CMB-C2B-C3B	2.02	131.48	126.59
25	C	512	CLA	CHC-C4B-NB	2.02	126.40	124.26
24	9	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
25	s	602	CLA	CMB-C2B-C3B	2.02	131.48	126.59
24	7	607	CHL	C4D-C3D-CAD	2.02	110.48	108.10
27	G	1622	XAT	O4-C5-C6	-2.02	57.29	58.96
24	G	609	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
25	n	604	CLA	CHC-C4B-NB	2.02	126.39	124.26
26	2	1621	LUT	C39-C29-C28	2.02	121.26	118.08
25	c	509	CLA	C11-C10-C8	-2.02	109.39	115.92
25	9	610	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
25	1	604	CLA	C1-C2-C3	-2.02	122.55	126.04
24	0	605	CHL	CED-O2D-CGD	2.02	120.50	115.94
25	y	610	CLA	O1D-CGD-CBD	2.02	128.61	124.48
25	n	602	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
24	9	608	CHL	CHB-C4A-NA	2.02	127.30	124.51
24	3	607	CHL	CHB-C1B-C2B	-2.02	121.54	127.24
25	S	610	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
24	9	605	CHL	CED-O2D-CGD	2.02	120.50	115.94
25	4	610	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	r	616	CLA	CHC-C4B-NB	2.02	126.39	124.26
24	3	607	CHL	C4D-C3D-CAD	2.02	110.47	108.10
25	g	614	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
24	N	609	CHL	C1-C2-C3	-2.02	122.55	126.04
27	5	1622	XAT	O24-C25-C26	-2.02	57.29	58.96
25	n	612	CLA	C2A-C1A-CHA	2.02	127.39	123.86
34	h	101	BCR	C2-C1-C6	2.02	113.59	110.48
25	d	403	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	g	611	CLA	CHB-C1B-NB	2.02	126.39	124.26
28	s	1623	NEX	O24-C25-C26	-2.02	57.29	58.96
25	d	403	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
24	3	601	CHL	CBC-CAC-C3C	-2.02	106.87	112.43
28	q	1623	NEX	C38-C25-C24	2.02	116.55	114.28
24	n	606	CHL	CHB-C1B-C2B	-2.02	121.54	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	601	CHL	C7-C6-C5	-2.02	107.88	113.36
24	7	605	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
25	N	604	CLA	CHC-C4B-NB	2.02	126.39	124.26
25	g	604	CLA	CHC-C4B-NB	2.02	126.39	124.26
26	S	1620	LUT	C19-C9-C8	2.02	121.25	118.08
26	4	1621	LUT	C30-C31-C32	-2.02	116.93	123.22
25	4	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	S	604	CLA	CHC-C4B-NB	2.01	126.39	124.26
27	R	622	XAT	C15-C35-C34	-2.01	119.35	123.47
24	3	605	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
25	r	612	CLA	C3B-C4B-NB	-2.01	108.65	110.52
25	s	613	CLA	CHA-C1A-NA	-2.01	121.79	126.40
27	p	1622	XAT	C11-C12-C13	-2.01	120.76	126.42
26	G	1621	LUT	C10-C11-C12	-2.01	116.93	123.22
24	n	609	CHL	C1-C2-C3	-2.01	122.56	126.04
25	6	613	CLA	C1-C2-C3	-2.01	122.56	126.04
25	g	614	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	2	601	CHL	CHC-C4B-NB	-2.01	122.13	124.26
24	g	606	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
24	G	609	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
28	p	1623	NEX	C17-C1-C6	-2.01	108.67	110.47
24	8	601	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
37	C	523	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
25	S	605	CLA	CHB-C1B-NB	2.01	126.39	124.26
27	g	1622	XAT	O4-C5-C6	-2.01	57.29	58.96
27	Y	1622	XAT	O24-C25-C26	-2.01	57.29	58.96
35	B	623	SQD	O6-C44-C45	-2.01	106.05	110.90
25	Y	610	CLA	C11-C10-C8	-2.01	109.42	115.92
24	0	605	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
25	b	608	CLA	CMB-C2B-C3B	2.01	131.46	126.59
25	1	602	CLA	CHC-C4B-NB	2.01	126.39	124.26
28	7	1623	NEX	O24-C25-C26	-2.01	57.29	58.96
25	7	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	2	608	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
24	6	601	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
29	q	2630	LHG	O7-C7-O9	-2.01	118.84	123.70
27	5	1622	XAT	C26-C27-C28	-2.01	121.74	125.99
25	s	605	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	S	614	CLA	CMB-C2B-C3B	2.01	131.46	126.59
25	2	614	CLA	C3B-C4B-NB	-2.01	108.65	110.52
25	6	610	CLA	C3B-C4B-NB	-2.01	108.65	110.52
29	1	2630	LHG	O8-C23-O10	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	405	PL9	C20-C19-C21	2.01	118.65	115.27
24	Y	607	CHL	CGD-CBD-CAD	-2.01	104.22	110.73
24	1	606	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
27	r	622	XAT	C19-C9-C8	2.01	121.24	118.08
25	R	612	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	5	614	CLA	C3B-C4B-NB	-2.01	108.65	110.52
24	n	601	CHL	CHC-C4B-NB	-2.01	122.13	124.26
24	S	607	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
25	S	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	3	609	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
25	c	509	CLA	C11-C12-C13	-2.01	109.43	115.92
24	Y	605	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
24	G	606	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
25	3	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	R	616	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	c	506	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	1	612	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
25	2	610	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
25	q	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	9	607	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
25	B	616	CLA	CMB-C2B-C3B	2.01	131.45	126.59
25	Y	603	CLA	CMB-C2B-C3B	2.01	131.45	126.59
24	1	601	CHL	C4D-C3D-CAD	2.01	110.46	108.10
25	R	616	CLA	O2D-CGD-CBD	2.01	114.83	111.27
25	0	614	CLA	O2D-CGD-CBD	2.01	114.83	111.27
25	r	616	CLA	O2D-CGD-CBD	2.01	114.83	111.27
26	9	1621	LUT	C30-C31-C32	-2.01	116.96	123.22
24	7	606	CHL	CBC-CAC-C3C	-2.01	106.90	112.43
27	9	1622	XAT	O4-C5-C6	-2.01	57.30	58.96
24	S	601	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
24	y	608	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
25	G	614	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	8	607	CHL	C4D-C3D-CAD	2.00	110.46	108.10
25	0	602	CLA	CHB-C4A-NA	2.00	127.28	124.51
25	9	603	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	g	609	CHL	C2A-C1A-CHA	-2.00	120.35	123.86
28	r	623	NEX	C2-C1-C6	2.00	111.16	109.21
24	8	607	CHL	CED-O2D-CGD	2.00	120.47	115.94
24	5	605	CHL	C11-C12-C13	-2.00	109.44	115.92
25	D	402	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	S	601	CHL	O1D-CGD-CBD	-2.00	120.38	124.48
25	D	403	CLA	CHB-C1B-NB	2.00	126.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	619	BCR	C11-C12-C13	-2.00	120.79	126.42
25	N	604	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
25	B	611	CLA	CHC-C1C-NC	2.00	127.24	124.20
26	8	1620	LUT	C8-C7-C6	-2.00	121.58	127.20
24	n	608	CHL	CHC-C4B-NB	-2.00	122.14	124.26
25	2	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	A	410	CLA	CHC-C1C-NC	2.00	127.24	124.20
26	s	1620	LUT	C20-C13-C12	2.00	121.23	118.08
25	8	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	8	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	b	616	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	G	602	CLA	C6-C7-C8	-2.00	109.45	115.92
28	2	1623	NEX	C16-C1-C6	2.00	112.26	110.47
25	S	603	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	B	616	CLA	C3A-C2A-C1A	2.00	104.34	101.34
28	S	1623	NEX	C28-C29-C30	2.00	122.01	118.94
26	g	1621	LUT	C1-C2-C3	2.00	118.16	113.64
25	C	502	CLA	C11-C12-C13	-2.00	109.45	115.92
24	1	605	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
25	4	612	CLA	O2D-CGD-CBD	2.00	114.82	111.27

There are no chirality outliers.

All (6161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	C1A-C2A-CAA-CBA
24	1	606	CHL	C1C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	607	CHL	C1C-C2C-CMC-OMC
24	1	607	CHL	C3C-C2C-CMC-OMC
24	1	608	CHL	C1A-C2A-CAA-CBA
24	1	608	CHL	C1C-C2C-CMC-OMC
24	1	608	CHL	C3C-C2C-CMC-OMC
24	1	609	CHL	C1C-C2C-CMC-OMC
24	1	609	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	C2-C3-C5-C6
24	2	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	C1C-C2C-CMC-OMC
24	2	605	CHL	C3C-C2C-CMC-OMC
24	2	606	CHL	C1C-C2C-CMC-OMC
24	2	606	CHL	C3C-C2C-CMC-OMC
24	2	607	CHL	C1C-C2C-CMC-OMC
24	2	607	CHL	C3C-C2C-CMC-OMC
24	2	609	CHL	C1C-C2C-CMC-OMC
24	2	609	CHL	C3C-C2C-CMC-OMC
24	3	601	CHL	CHA-CBD-CGD-O1D
24	3	601	CHL	CHA-CBD-CGD-O2D
24	3	601	CHL	C6-C7-C8-C9
24	3	605	CHL	C1C-C2C-CMC-OMC
24	3	605	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C1A-C2A-CAA-CBA
24	3	606	CHL	C2B-C3B-CAB-CBB
24	3	606	CHL	C4B-C3B-CAB-CBB
24	3	607	CHL	C11-C12-C13-C14
24	3	608	CHL	C1C-C2C-CMC-OMC
24	3	608	CHL	C3C-C2C-CMC-OMC
24	3	609	CHL	C1A-C2A-CAA-CBA
24	3	609	CHL	C1C-C2C-CMC-OMC
24	3	609	CHL	C3C-C2C-CMC-OMC
24	4	601	CHL	C1A-C2A-CAA-CBA
24	4	605	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C3A-C2A-CAA-CBA
24	4	607	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	C1C-C2C-CMC-OMC
24	4	608	CHL	C3C-C2C-CMC-OMC
24	4	609	CHL	C3C-C2C-CMC-OMC
24	4	609	CHL	C11-C10-C8-C9
24	5	601	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	CHA-CBD-CGD-O1D
24	5	605	CHL	CHA-CBD-CGD-O2D
24	5	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	C1A-C2A-CAA-CBA
24	5	607	CHL	C3C-C2C-CMC-OMC
24	5	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	5	608	CHL	C3C-C2C-CMC-OMC
24	5	609	CHL	C1C-C2C-CMC-OMC
24	5	609	CHL	C3C-C2C-CMC-OMC
24	6	601	CHL	C3C-C2C-CMC-OMC
24	6	605	CHL	C1C-C2C-CMC-OMC
24	6	605	CHL	C3C-C2C-CMC-OMC
24	6	606	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C3A-C2A-CAA-CBA
24	6	607	CHL	C1C-C2C-CMC-OMC
24	6	607	CHL	C3C-C2C-CMC-OMC
24	6	607	CHL	CBD-CGD-O2D-CED
24	6	607	CHL	C6-C7-C8-C9
24	6	608	CHL	C3C-C2C-CMC-OMC
24	6	609	CHL	C1C-C2C-CMC-OMC
24	6	609	CHL	C3C-C2C-CMC-OMC
24	6	609	CHL	CBD-CGD-O2D-CED
24	G	601	CHL	C1A-C2A-CAA-CBA
24	G	601	CHL	C3A-C2A-CAA-CBA
24	G	601	CHL	C1C-C2C-CMC-OMC
24	G	601	CHL	C3C-C2C-CMC-OMC
24	G	601	CHL	C2-C3-C5-C6
24	G	601	CHL	C4-C3-C5-C6
24	G	605	CHL	C3A-C2A-CAA-CBA
24	G	605	CHL	C2A-CAA-CBA-CGA
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	C3C-C2C-CMC-OMC
24	G	607	CHL	C1A-C2A-CAA-CBA
24	G	607	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C1C-C2C-CMC-OMC
24	N	605	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C11-C12-C13-C14
24	N	605	CHL	C12-C13-C15-C16
24	N	608	CHL	C1C-C2C-CMC-OMC
24	N	608	CHL	C3C-C2C-CMC-OMC
24	N	609	CHL	C1C-C2C-CMC-OMC
24	N	609	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	R	606	CHL	C3C-C2C-CMC-OMC
24	R	607	CHL	C1C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC
24	R	607	CHL	CHA-CBD-CGD-O1D
24	R	607	CHL	CHA-CBD-CGD-O2D
24	R	607	CHL	CAD-CBD-CGD-O1D
24	R	607	CHL	C4-C3-C5-C6
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	601	CHL	CHA-CBD-CGD-O1D
24	S	601	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	C1C-C2C-CMC-OMC
24	S	606	CHL	C3C-C2C-CMC-OMC
24	S	607	CHL	C1C-C2C-CMC-OMC
24	S	607	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	CHA-CBD-CGD-O1D
24	S	608	CHL	CHA-CBD-CGD-O2D
24	S	608	CHL	CAD-CBD-CGD-O1D
24	S	608	CHL	CAD-CBD-CGD-O2D
24	S	608	CHL	CBD-CGD-O2D-CED
24	Y	605	CHL	C1C-C2C-CMC-OMC
24	Y	605	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C1A-C2A-CAA-CBA
24	Y	606	CHL	C2B-C3B-CAB-CBB
24	Y	606	CHL	C4B-C3B-CAB-CBB
24	Y	606	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C3C-C2C-CMC-OMC
24	Y	607	CHL	CHA-CBD-CGD-O1D
24	0	601	CHL	C3C-C2C-CMC-OMC
24	0	605	CHL	C1C-C2C-CMC-OMC
24	0	605	CHL	C3C-C2C-CMC-OMC
24	0	606	CHL	C1A-C2A-CAA-CBA
24	0	606	CHL	C14-C13-C15-C16
24	0	607	CHL	C1A-C2A-CAA-CBA
24	0	607	CHL	C1C-C2C-CMC-OMC
24	0	607	CHL	C3C-C2C-CMC-OMC
24	0	607	CHL	C14-C13-C15-C16
24	7	605	CHL	C1C-C2C-CMC-OMC
24	7	605	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C1C-C2C-CMC-OMC
24	7	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	7	607	CHL	C3C-C2C-CMC-OMC
24	7	608	CHL	C1C-C2C-CMC-OMC
24	7	608	CHL	C3C-C2C-CMC-OMC
24	7	608	CHL	CBD-CGD-O2D-CED
24	8	601	CHL	CHA-CBD-CGD-O1D
24	8	601	CHL	CHA-CBD-CGD-O2D
24	8	605	CHL	C1C-C2C-CMC-OMC
24	8	605	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C1A-C2A-CAA-CBA
24	8	606	CHL	C2B-C3B-CAB-CBB
24	8	606	CHL	C4B-C3B-CAB-CBB
24	8	608	CHL	C1C-C2C-CMC-OMC
24	8	608	CHL	C3C-C2C-CMC-OMC
24	8	609	CHL	C1A-C2A-CAA-CBA
24	8	609	CHL	C1C-C2C-CMC-OMC
24	8	609	CHL	C3C-C2C-CMC-OMC
24	9	601	CHL	C3A-C2A-CAA-CBA
24	9	601	CHL	C1C-C2C-CMC-OMC
24	9	601	CHL	C3C-C2C-CMC-OMC
24	9	605	CHL	C1A-C2A-CAA-CBA
24	9	605	CHL	C3A-C2A-CAA-CBA
24	9	605	CHL	C1C-C2C-CMC-OMC
24	9	605	CHL	C3C-C2C-CMC-OMC
24	9	606	CHL	C1C-C2C-CMC-OMC
24	9	606	CHL	C3C-C2C-CMC-OMC
24	9	607	CHL	C1C-C2C-CMC-OMC
24	9	607	CHL	C3C-C2C-CMC-OMC
24	p	605	CHL	C1C-C2C-CMC-OMC
24	p	605	CHL	C3C-C2C-CMC-OMC
24	p	605	CHL	CHA-CBD-CGD-O1D
24	p	605	CHL	CHA-CBD-CGD-O2D
24	p	605	CHL	C14-C13-C15-C16
24	p	607	CHL	C1A-C2A-CAA-CBA
24	p	607	CHL	C3C-C2C-CMC-OMC
24	p	608	CHL	C1C-C2C-CMC-OMC
24	p	608	CHL	C3C-C2C-CMC-OMC
24	p	609	CHL	C1C-C2C-CMC-OMC
24	p	609	CHL	C3C-C2C-CMC-OMC
24	q	605	CHL	C1C-C2C-CMC-OMC
24	q	605	CHL	C3C-C2C-CMC-OMC
24	q	606	CHL	C1A-C2A-CAA-CBA
24	q	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	q	607	CHL	C1C-C2C-CMC-OMC
24	q	607	CHL	C3C-C2C-CMC-OMC
24	q	608	CHL	C1C-C2C-CMC-OMC
24	q	608	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C1A-C2A-CAA-CBA
24	g	601	CHL	C3A-C2A-CAA-CBA
24	g	601	CHL	C1C-C2C-CMC-OMC
24	g	601	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
24	g	605	CHL	C3A-C2A-CAA-CBA
24	g	605	CHL	C2A-CAA-CBA-CGA
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	g	607	CHL	C1A-C2A-CAA-CBA
24	g	607	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C3C-C2C-CMC-OMC
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	C1C-C2C-CMC-OMC
24	n	605	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	C1C-C2C-CMC-OMC
24	n	608	CHL	C3C-C2C-CMC-OMC
24	n	609	CHL	C1C-C2C-CMC-OMC
24	n	609	CHL	C3C-C2C-CMC-OMC
24	s	601	CHL	C1C-C2C-CMC-OMC
24	s	601	CHL	C3C-C2C-CMC-OMC
24	s	601	CHL	CHA-CBD-CGD-O1D
24	s	601	CHL	CHA-CBD-CGD-O2D
24	s	606	CHL	C1C-C2C-CMC-OMC
24	s	606	CHL	C3C-C2C-CMC-OMC
24	s	607	CHL	C1C-C2C-CMC-OMC
24	s	607	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	CHA-CBD-CGD-O1D
24	s	608	CHL	CHA-CBD-CGD-O2D
24	s	608	CHL	CAD-CBD-CGD-O1D
24	s	608	CHL	CAD-CBD-CGD-O2D
24	s	608	CHL	CBD-CGD-O2D-CED
24	y	605	CHL	C1C-C2C-CMC-OMC
24	y	605	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	y	606	CHL	C2B-C3B-CAB-CBB
24	y	606	CHL	C4B-C3B-CAB-CBB
24	y	606	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C3C-C2C-CMC-OMC
24	y	607	CHL	CHA-CBD-CGD-O1D
24	r	606	CHL	C1C-C2C-CMC-OMC
24	r	606	CHL	C3C-C2C-CMC-OMC
24	r	607	CHL	C1C-C2C-CMC-OMC
24	r	607	CHL	C3C-C2C-CMC-OMC
24	r	607	CHL	CHA-CBD-CGD-O1D
24	r	607	CHL	CHA-CBD-CGD-O2D
24	r	607	CHL	CAD-CBD-CGD-O1D
24	r	607	CHL	C4-C3-C5-C6
25	1	602	CLA	C2-C3-C5-C6
25	1	602	CLA	C4-C3-C5-C6
25	1	603	CLA	C2B-C3B-CAB-CBB
25	1	603	CLA	C4B-C3B-CAB-CBB
25	1	604	CLA	C2B-C3B-CAB-CBB
25	1	604	CLA	C4B-C3B-CAB-CBB
25	1	604	CLA	CBD-CGD-O2D-CED
25	1	611	CLA	C2B-C3B-CAB-CBB
25	1	611	CLA	C4B-C3B-CAB-CBB
25	1	614	CLA	C3A-C2A-CAA-CBA
25	1	614	CLA	CHA-CBD-CGD-O1D
25	1	614	CLA	CHA-CBD-CGD-O2D
25	1	614	CLA	CAD-CBD-CGD-O1D
25	1	614	CLA	CAD-CBD-CGD-O2D
25	1	614	CLA	CBD-CGD-O2D-CED
25	2	603	CLA	C2B-C3B-CAB-CBB
25	2	603	CLA	C4B-C3B-CAB-CBB
25	2	604	CLA	C1A-C2A-CAA-CBA
25	2	604	CLA	C3A-C2A-CAA-CBA
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	C1A-C2A-CAA-CBA
25	2	611	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	C2B-C3B-CAB-CBB
25	2	611	CLA	C4B-C3B-CAB-CBB
25	2	611	CLA	CHA-CBD-CGD-O1D
25	2	612	CLA	CBD-CGD-O2D-CED
25	2	613	CLA	CHA-CBD-CGD-O1D
25	2	613	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	614	CLA	C2B-C3B-CAB-CBB
25	2	614	CLA	C4B-C3B-CAB-CBB
25	3	603	CLA	C2B-C3B-CAB-CBB
25	3	603	CLA	C4B-C3B-CAB-CBB
25	3	604	CLA	C3A-C2A-CAA-CBA
25	3	604	CLA	CBD-CGD-O2D-CED
25	3	604	CLA	C2-C3-C5-C6
25	3	604	CLA	C4-C3-C5-C6
25	3	611	CLA	C2B-C3B-CAB-CBB
25	3	611	CLA	C4B-C3B-CAB-CBB
25	3	611	CLA	CHA-CBD-CGD-O1D
25	3	611	CLA	CAD-CBD-CGD-O1D
25	3	611	CLA	CAD-CBD-CGD-O2D
25	3	612	CLA	C1A-C2A-CAA-CBA
25	3	612	CLA	C2B-C3B-CAB-CBB
25	3	612	CLA	C4B-C3B-CAB-CBB
25	3	613	CLA	C1A-C2A-CAA-CBA
25	3	614	CLA	CBD-CGD-O2D-CED
25	4	603	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	C1A-C2A-CAA-CBA
25	4	604	CLA	C3A-C2A-CAA-CBA
25	4	604	CLA	CHA-CBD-CGD-O1D
25	4	604	CLA	CHA-CBD-CGD-O2D
25	4	604	CLA	CAD-CBD-CGD-O1D
25	4	611	CLA	CBD-CGD-O2D-CED
25	4	613	CLA	CBD-CGD-O2D-CED
25	4	614	CLA	C1A-C2A-CAA-CBA
25	4	614	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	C4B-C3B-CAB-CBB
25	5	603	CLA	CHA-CBD-CGD-O2D
25	5	604	CLA	C3A-C2A-CAA-CBA
25	5	604	CLA	C2B-C3B-CAB-CBB
25	5	604	CLA	C4B-C3B-CAB-CBB
25	5	604	CLA	CBD-CGD-O2D-CED
25	5	611	CLA	C2A-CAA-CBA-CGA
25	5	611	CLA	C2B-C3B-CAB-CBB
25	5	611	CLA	C4B-C3B-CAB-CBB
25	5	611	CLA	CHA-CBD-CGD-O1D
25	5	611	CLA	CHA-CBD-CGD-O2D
25	5	612	CLA	C2B-C3B-CAB-CBB
25	5	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	5	614	CLA	C2B-C3B-CAB-CBB
25	5	614	CLA	C4B-C3B-CAB-CBB
25	6	603	CLA	C2B-C3B-CAB-CBB
25	6	603	CLA	C4B-C3B-CAB-CBB
25	6	604	CLA	CHA-CBD-CGD-O1D
25	6	604	CLA	CHA-CBD-CGD-O2D
25	6	613	CLA	C1A-C2A-CAA-CBA
25	6	613	CLA	CHA-CBD-CGD-O1D
25	6	613	CLA	CHA-CBD-CGD-O2D
25	6	614	CLA	CHA-CBD-CGD-O1D
25	6	614	CLA	CHA-CBD-CGD-O2D
25	6	614	CLA	CAD-CBD-CGD-O1D
25	6	614	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	CBD-CGD-O2D-CED
25	A	406	CLA	CHA-CBD-CGD-O1D
25	A	406	CLA	CHA-CBD-CGD-O2D
25	A	407	CLA	CHA-CBD-CGD-O1D
25	A	407	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	C4B-C3B-CAB-CBB
25	B	603	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C4B-C3B-CAB-CBB
25	B	605	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C14-C13-C15-C16
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	C1A-C2A-CAA-CBA
25	B	613	CLA	C3A-C2A-CAA-CBA
25	B	615	CLA	CHA-CBD-CGD-O1D
25	B	615	CLA	CHA-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O2D
25	B	617	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CHA-CBD-CGD-O1D
25	C	506	CLA	CHA-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C4B-C3B-CAB-CBB
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	402	CLA	C2-C3-C5-C6
25	D	402	CLA	C4-C3-C5-C6
25	D	403	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C3A-C2A-CAA-CBA
25	D	403	CLA	CBD-CGD-O2D-CED
25	G	603	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	G	603	CLA	C4B-C3B-CAB-CBB
25	G	604	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	CHA-CBD-CGD-O1D
25	G	604	CLA	CHA-CBD-CGD-O2D
25	G	604	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	C2B-C3B-CAB-CBB
25	G	611	CLA	C4B-C3B-CAB-CBB
25	G	611	CLA	CHA-CBD-CGD-O1D
25	G	611	CLA	CHA-CBD-CGD-O2D
25	G	612	CLA	C2B-C3B-CAB-CBB
25	G	612	CLA	C4B-C3B-CAB-CBB
25	G	613	CLA	CHA-CBD-CGD-O1D
25	G	613	CLA	CHA-CBD-CGD-O2D
25	G	614	CLA	C2B-C3B-CAB-CBB
25	G	614	CLA	C4B-C3B-CAB-CBB
25	N	603	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C3A-C2A-CAA-CBA
25	N	611	CLA	C1A-C2A-CAA-CBA
25	N	611	CLA	CAD-CBD-CGD-O1D
25	N	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	N	611	CLA	CBD-CGD-O2D-CED
25	N	612	CLA	CBD-CGD-O2D-CED
25	N	613	CLA	C2B-C3B-CAB-CBB
25	N	613	CLA	C4B-C3B-CAB-CBB
25	N	614	CLA	C2B-C3B-CAB-CBB
25	N	614	CLA	C4B-C3B-CAB-CBB
25	R	601	CLA	C2B-C3B-CAB-CBB
25	R	601	CLA	C4B-C3B-CAB-CBB
25	R	601	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	C2B-C3B-CAB-CBB
25	R	602	CLA	C4B-C3B-CAB-CBB
25	R	604	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	C2B-C3B-CAB-CBB
25	R	611	CLA	C4B-C3B-CAB-CBB
25	R	612	CLA	C2B-C3B-CAB-CBB
25	R	612	CLA	C4B-C3B-CAB-CBB
25	R	613	CLA	C1A-C2A-CAA-CBA
25	R	613	CLA	C3A-C2A-CAA-CBA
25	R	613	CLA	CHA-CBD-CGD-O1D
25	R	613	CLA	CHA-CBD-CGD-O2D
25	R	613	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C2-C3-C5-C6
25	R	613	CLA	C4-C3-C5-C6
25	R	616	CLA	C1A-C2A-CAA-CBA
25	R	616	CLA	C3A-C2A-CAA-CBA
25	S	603	CLA	C2B-C3B-CAB-CBB
25	S	603	CLA	C4B-C3B-CAB-CBB
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	604	CLA	CBD-CGD-O2D-CED
25	S	605	CLA	C1A-C2A-CAA-CBA
25	S	605	CLA	C2B-C3B-CAB-CBB
25	S	605	CLA	CHA-CBD-CGD-O1D
25	S	605	CLA	CHA-CBD-CGD-O2D
25	S	609	CLA	C4B-C3B-CAB-CBB
25	S	610	CLA	C4B-C3B-CAB-CBB
25	S	610	CLA	CHA-CBD-CGD-O1D
25	S	610	CLA	CHA-CBD-CGD-O2D
25	S	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	S	613	CLA	C2B-C3B-CAB-CBB
25	S	613	CLA	C4B-C3B-CAB-CBB
25	S	613	CLA	CBD-CGD-O2D-CED
25	S	613	CLA	O1D-CGD-O2D-CED
25	S	614	CLA	CBD-CGD-O2D-CED
25	S	614	CLA	O1D-CGD-O2D-CED
25	Y	603	CLA	CHA-CBD-CGD-O1D
25	Y	603	CLA	CHA-CBD-CGD-O2D
25	Y	611	CLA	C2B-C3B-CAB-CBB
25	Y	611	CLA	C4B-C3B-CAB-CBB
25	Y	613	CLA	C2B-C3B-CAB-CBB
25	Y	613	CLA	C4B-C3B-CAB-CBB
25	Y	614	CLA	CHA-CBD-CGD-O1D
25	Y	614	CLA	CHA-CBD-CGD-O2D
25	0	604	CLA	C2B-C3B-CAB-CBB
25	0	604	CLA	C4B-C3B-CAB-CBB
25	0	604	CLA	CHA-CBD-CGD-O1D
25	0	604	CLA	CHA-CBD-CGD-O2D
25	0	604	CLA	CBD-CGD-O2D-CED
25	0	613	CLA	C4B-C3B-CAB-CBB
25	0	613	CLA	CHA-CBD-CGD-O1D
25	0	613	CLA	CHA-CBD-CGD-O2D
25	0	614	CLA	CHA-CBD-CGD-O1D
25	0	614	CLA	CHA-CBD-CGD-O2D
25	0	614	CLA	CAD-CBD-CGD-O1D
25	0	614	CLA	CBD-CGD-O2D-CED
25	7	602	CLA	C2-C3-C5-C6
25	7	602	CLA	C4-C3-C5-C6
25	7	603	CLA	C2B-C3B-CAB-CBB
25	7	603	CLA	C4B-C3B-CAB-CBB
25	7	604	CLA	CHA-CBD-CGD-O1D
25	7	611	CLA	C1A-C2A-CAA-CBA
25	7	611	CLA	C3A-C2A-CAA-CBA
25	7	611	CLA	C2B-C3B-CAB-CBB
25	7	611	CLA	C4B-C3B-CAB-CBB
25	7	613	CLA	CHA-CBD-CGD-O1D
25	7	613	CLA	CHA-CBD-CGD-O2D
25	7	614	CLA	C3A-C2A-CAA-CBA
25	7	614	CLA	CHA-CBD-CGD-O1D
25	7	614	CLA	CHA-CBD-CGD-O2D
25	7	614	CLA	CAD-CBD-CGD-O1D
25	7	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	7	614	CLA	CBD-CGD-O2D-CED
25	8	603	CLA	C2B-C3B-CAB-CBB
25	8	603	CLA	C4B-C3B-CAB-CBB
25	8	604	CLA	C3A-C2A-CAA-CBA
25	8	604	CLA	CBD-CGD-O2D-CED
25	8	611	CLA	C2B-C3B-CAB-CBB
25	8	611	CLA	C4B-C3B-CAB-CBB
25	8	611	CLA	CHA-CBD-CGD-O1D
25	8	611	CLA	CHA-CBD-CGD-O2D
25	8	611	CLA	CAD-CBD-CGD-O1D
25	8	611	CLA	CAD-CBD-CGD-O2D
25	8	612	CLA	C1A-C2A-CAA-CBA
25	8	612	CLA	C2B-C3B-CAB-CBB
25	8	612	CLA	C4B-C3B-CAB-CBB
25	8	613	CLA	C1A-C2A-CAA-CBA
25	8	614	CLA	CBD-CGD-O2D-CED
25	9	602	CLA	C2-C3-C5-C6
25	9	602	CLA	C4-C3-C5-C6
25	9	603	CLA	C2B-C3B-CAB-CBB
25	9	603	CLA	C4B-C3B-CAB-CBB
25	9	604	CLA	C1A-C2A-CAA-CBA
25	9	604	CLA	C3A-C2A-CAA-CBA
25	9	611	CLA	C1A-C2A-CAA-CBA
25	9	611	CLA	C3A-C2A-CAA-CBA
25	9	611	CLA	C2B-C3B-CAB-CBB
25	9	611	CLA	C4B-C3B-CAB-CBB
25	9	611	CLA	CHA-CBD-CGD-O1D
25	9	611	CLA	CHA-CBD-CGD-O2D
25	9	612	CLA	CBD-CGD-O2D-CED
25	9	613	CLA	CHA-CBD-CGD-O1D
25	9	613	CLA	CHA-CBD-CGD-O2D
25	9	614	CLA	C2B-C3B-CAB-CBB
25	9	614	CLA	C4B-C3B-CAB-CBB
25	p	602	CLA	CBD-CGD-O2D-CED
25	p	603	CLA	C4B-C3B-CAB-CBB
25	p	603	CLA	CHA-CBD-CGD-O1D
25	p	603	CLA	CHA-CBD-CGD-O2D
25	p	604	CLA	C3A-C2A-CAA-CBA
25	p	611	CLA	C4B-C3B-CAB-CBB
25	p	611	CLA	CHA-CBD-CGD-O1D
25	p	611	CLA	CHA-CBD-CGD-O2D
25	p	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	p	613	CLA	C2B-C3B-CAB-CBB
25	p	613	CLA	C4B-C3B-CAB-CBB
25	p	613	CLA	CHA-CBD-CGD-O1D
25	p	613	CLA	CHA-CBD-CGD-O2D
25	p	614	CLA	C2B-C3B-CAB-CBB
25	p	614	CLA	C4B-C3B-CAB-CBB
25	p	614	CLA	CBD-CGD-O2D-CED
25	q	602	CLA	CBD-CGD-O2D-CED
25	q	604	CLA	C3A-C2A-CAA-CBA
25	q	604	CLA	C4B-C3B-CAB-CBB
25	q	604	CLA	CAD-CBD-CGD-O1D
25	q	604	CLA	CAD-CBD-CGD-O2D
25	q	611	CLA	CBD-CGD-O2D-CED
25	q	614	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
25	a	406	CLA	CHA-CBD-CGD-O1D
25	a	406	CLA	CHA-CBD-CGD-O2D
25	a	407	CLA	CHA-CBD-CGD-O1D
25	a	407	CLA	CHA-CBD-CGD-O2D
25	b	603	CLA	C1A-C2A-CAA-CBA
25	b	604	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C4B-C3B-CAB-CBB
25	b	605	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	C4B-C3B-CAB-CBB
25	b	606	CLA	C14-C13-C15-C16
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	b	617	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C2-C3-C5-C6
25	c	503	CLA	C4-C3-C5-C6
25	c	504	CLA	C2B-C3B-CAB-CBB
25	c	504	CLA	C4B-C3B-CAB-CBB
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	c	513	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	C4-C3-C5-C6
25	d	402	CLA	C2-C3-C5-C6
25	d	402	CLA	C4-C3-C5-C6
25	d	403	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	C1A-C2A-CAA-CBA
25	g	603	CLA	C3A-C2A-CAA-CBA
25	g	603	CLA	C2B-C3B-CAB-CBB
25	g	603	CLA	C4B-C3B-CAB-CBB
25	g	604	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	CHA-CBD-CGD-O1D
25	g	604	CLA	CHA-CBD-CGD-O2D
25	g	604	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	C2B-C3B-CAB-CBB
25	g	611	CLA	C4B-C3B-CAB-CBB
25	g	611	CLA	CHA-CBD-CGD-O1D
25	g	611	CLA	CHA-CBD-CGD-O2D
25	g	612	CLA	C2B-C3B-CAB-CBB
25	g	612	CLA	C4B-C3B-CAB-CBB
25	g	614	CLA	C2B-C3B-CAB-CBB
25	g	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	n	603	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C3A-C2A-CAA-CBA
25	n	611	CLA	CAD-CBD-CGD-O1D
25	n	611	CLA	CAD-CBD-CGD-O2D
25	n	611	CLA	CBD-CGD-O2D-CED
25	n	612	CLA	CBD-CGD-O2D-CED
25	n	613	CLA	C2B-C3B-CAB-CBB
25	n	613	CLA	C4B-C3B-CAB-CBB
25	n	614	CLA	C2B-C3B-CAB-CBB
25	n	614	CLA	C4B-C3B-CAB-CBB
25	s	603	CLA	C2B-C3B-CAB-CBB
25	s	603	CLA	C4B-C3B-CAB-CBB
25	s	603	CLA	CHA-CBD-CGD-O1D
25	s	603	CLA	CHA-CBD-CGD-O2D
25	s	604	CLA	CBD-CGD-O2D-CED
25	s	605	CLA	C1A-C2A-CAA-CBA
25	s	605	CLA	CHA-CBD-CGD-O1D
25	s	605	CLA	CHA-CBD-CGD-O2D
25	s	609	CLA	C4B-C3B-CAB-CBB
25	s	610	CLA	C4B-C3B-CAB-CBB
25	s	610	CLA	CHA-CBD-CGD-O1D
25	s	610	CLA	CHA-CBD-CGD-O2D
25	s	612	CLA	CBD-CGD-O2D-CED
25	s	613	CLA	C2B-C3B-CAB-CBB
25	s	613	CLA	C4B-C3B-CAB-CBB
25	s	613	CLA	CBD-CGD-O2D-CED
25	s	613	CLA	O1D-CGD-O2D-CED
25	s	614	CLA	CBD-CGD-O2D-CED
25	s	614	CLA	O1D-CGD-O2D-CED
25	y	603	CLA	CHA-CBD-CGD-O1D
25	y	603	CLA	CHA-CBD-CGD-O2D
25	y	611	CLA	C2B-C3B-CAB-CBB
25	y	611	CLA	C4B-C3B-CAB-CBB
25	y	613	CLA	C2B-C3B-CAB-CBB
25	y	613	CLA	C4B-C3B-CAB-CBB
25	y	614	CLA	CHA-CBD-CGD-O1D
25	y	614	CLA	CHA-CBD-CGD-O2D
25	r	601	CLA	C3A-C2A-CAA-CBA
25	r	601	CLA	C2B-C3B-CAB-CBB
25	r	601	CLA	C4B-C3B-CAB-CBB
25	r	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	r	602	CLA	C2B-C3B-CAB-CBB
25	r	602	CLA	C4B-C3B-CAB-CBB
25	r	603	CLA	C4B-C3B-CAB-CBB
25	r	604	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	C2B-C3B-CAB-CBB
25	r	611	CLA	C4B-C3B-CAB-CBB
25	r	612	CLA	C2B-C3B-CAB-CBB
25	r	612	CLA	C4B-C3B-CAB-CBB
25	r	613	CLA	C1A-C2A-CAA-CBA
25	r	613	CLA	C3A-C2A-CAA-CBA
25	r	613	CLA	CHA-CBD-CGD-O1D
25	r	613	CLA	CHA-CBD-CGD-O2D
25	r	613	CLA	CBD-CGD-O2D-CED
25	r	613	CLA	C2-C3-C5-C6
25	r	613	CLA	C4-C3-C5-C6
25	r	616	CLA	C1A-C2A-CAA-CBA
25	r	616	CLA	C3A-C2A-CAA-CBA
26	2	1621	LUT	C7-C8-C9-C10
26	2	1621	LUT	C7-C8-C9-C19
26	3	1620	LUT	C27-C28-C29-C39
26	4	1620	LUT	C31-C32-C33-C34
26	4	1620	LUT	C31-C32-C33-C40
26	4	1621	LUT	C11-C12-C13-C20
26	6	1620	LUT	C1-C6-C7-C8
26	N	1620	LUT	C1-C6-C7-C8
26	N	1621	LUT	C1-C6-C7-C8
26	9	1621	LUT	C7-C8-C9-C10
26	9	1621	LUT	C7-C8-C9-C19
26	p	1621	LUT	C1-C6-C7-C8
26	p	1621	LUT	C27-C28-C29-C39
26	q	1620	LUT	C1-C6-C7-C8
26	n	1620	LUT	C1-C6-C7-C8
26	n	1621	LUT	C1-C6-C7-C8
27	1	1622	XAT	C31-C32-C33-C40
27	2	1622	XAT	C31-C32-C33-C34
27	2	1622	XAT	C31-C32-C33-C40
27	6	1622	XAT	C31-C32-C33-C34
27	6	1622	XAT	C31-C32-C33-C40
27	7	1622	XAT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
27	9	1622	XAT	C31-C32-C33-C34
27	9	1622	XAT	C31-C32-C33-C40
28	1	1623	NEX	C11-C12-C13-C14
28	1	1623	NEX	C11-C12-C13-C20
28	S	1623	NEX	C11-C12-C13-C14
28	S	1623	NEX	C11-C12-C13-C20
28	Y	1623	NEX	C31-C32-C33-C34
28	Y	1623	NEX	C31-C32-C33-C40
28	7	1623	NEX	C11-C12-C13-C14
28	7	1623	NEX	C11-C12-C13-C20
28	s	1623	NEX	C11-C12-C13-C14
28	s	1623	NEX	C11-C12-C13-C20
28	y	1623	NEX	C31-C32-C33-C34
28	y	1623	NEX	C31-C32-C33-C40
29	1	2630	LHG	C4-O6-P-O3
29	2	2630	LHG	C1-C2-C3-O3
29	2	2630	LHG	C4-O6-P-O5
29	3	2630	LHG	C4-O6-P-O3
29	3	2630	LHG	C4-O6-P-O4
29	3	2630	LHG	C4-O6-P-O5
29	4	2630	LHG	C4-O6-P-O3
29	4	2630	LHG	C4-O6-P-O4
29	4	2630	LHG	C4-O6-P-O5
29	5	2630	LHG	O1-C1-C2-C3
29	5	2630	LHG	C4-O6-P-O4
29	6	2630	LHG	O1-C1-C2-C3
29	6	2630	LHG	C4-O6-P-O5
29	C	2630	LHG	O1-C1-C2-C3
29	D	408	LHG	C3-O3-P-O5
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C4-O6-P-O3
29	D	410	LHG	C3-O3-P-O4
29	D	410	LHG	C3-O3-P-O5
29	D	410	LHG	C3-O3-P-O6
29	L	101	LHG	C3-O3-P-O5
29	L	101	LHG	C4-O6-P-O3
29	L	101	LHG	C4-O6-P-O4
29	L	101	LHG	C4-O6-P-O5
29	N	2630	LHG	C3-O3-P-O4
29	N	2630	LHG	C4-O6-P-O4
29	N	2630	LHG	C4-O6-P-O5
29	N	2630	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
29	R	2630	LHG	C3-O3-P-O4
29	R	2630	LHG	C4-O6-P-O5
29	Y	2630	LHG	C1-C2-C3-O3
29	Y	2630	LHG	C4-O6-P-O3
29	Y	2630	LHG	C4-O6-P-O4
29	Y	2630	LHG	C4-O6-P-O5
29	0	2630	LHG	C4-O6-P-O4
29	0	2630	LHG	C4-O6-P-O5
29	7	2630	LHG	C4-O6-P-O3
29	8	2630	LHG	C4-O6-P-O3
29	8	2630	LHG	C4-O6-P-O4
29	8	2630	LHG	C4-O6-P-O5
29	9	2630	LHG	C1-C2-C3-O3
29	9	2630	LHG	C3-O3-P-O6
29	9	2630	LHG	C4-O6-P-O5
29	p	2630	LHG	O1-C1-C2-C3
29	p	2630	LHG	C4-O6-P-O4
29	q	2630	LHG	C3-O3-P-O5
29	c	2630	LHG	C4-O6-P-O3
29	d	408	LHG	C3-O3-P-O5
29	d	408	LHG	C4-O6-P-O4
29	d	409	LHG	C4-O6-P-O3
29	d	410	LHG	C3-O3-P-O4
29	d	410	LHG	C3-O3-P-O5
29	d	410	LHG	C3-O3-P-O6
29	l	101	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O5
29	n	2630	LHG	C3-O3-P-O4
29	n	2630	LHG	C4-O6-P-O4
29	n	2630	LHG	C4-O6-P-O5
29	n	2630	LHG	O7-C5-C6-O8
29	s	2630	LHG	O1-C1-C2-C3
29	y	2630	LHG	C1-C2-C3-O3
29	y	2630	LHG	C4-O6-P-O3
29	y	2630	LHG	C4-O6-P-O4
29	y	2630	LHG	C4-O6-P-O5
29	r	2630	LHG	C3-O3-P-O4
29	r	2630	LHG	C4-O6-P-O5
34	B	620	BCR	C7-C8-C9-C34
34	C	516	BCR	C7-C8-C9-C10
34	C	516	BCR	C7-C8-C9-C34
34	C	516	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
34	C	516	BCR	C37-C22-C23-C24
34	H	101	BCR	C7-C8-C9-C10
34	H	101	BCR	C7-C8-C9-C34
34	H	101	BCR	C23-C24-C25-C30
34	b	620	BCR	C7-C8-C9-C34
34	c	516	BCR	C7-C8-C9-C10
34	c	516	BCR	C7-C8-C9-C34
34	c	516	BCR	C21-C22-C23-C24
34	c	516	BCR	C37-C22-C23-C24
34	h	101	BCR	C7-C8-C9-C10
34	h	101	BCR	C7-C8-C9-C34
34	h	101	BCR	C23-C24-C25-C30
35	A	412	SQD	O5-C5-C6-S
35	A	412	SQD	C5-C6-S-O8
35	A	412	SQD	C5-C6-S-O9
35	B	621	SQD	C2-C1-O6-C44
35	B	621	SQD	C8-C7-O47-C45
35	a	412	SQD	O5-C5-C6-S
35	a	412	SQD	C5-C6-S-O8
35	a	412	SQD	C5-C6-S-O9
35	b	621	SQD	C2-C1-O6-C44
35	b	621	SQD	C8-C7-O47-C45
36	S	2631	LMG	O7-C8-C9-O8
36	s	2631	LMG	O7-C8-C9-O8
37	C	519	DGD	C2E-C1E-O5D-C6D
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
39	D	405	PL9	C7-C8-C9-C10
39	D	405	PL9	C22-C23-C24-C26
39	D	405	PL9	C37-C38-C39-C40
39	d	405	PL9	C7-C8-C9-C10
39	d	405	PL9	C22-C23-C24-C26
39	d	405	PL9	C37-C38-C39-C40
39	d	405	PL9	C42-C43-C44-C45
24	6	609	CHL	O1D-CGD-O2D-CED
24	0	609	CHL	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	A	405	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	R	613	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	0	604	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	g	612	CLA	O1D-CGD-O2D-CED
25	s	603	CLA	O1D-CGD-O2D-CED
25	r	613	CLA	O1D-CGD-O2D-CED
24	4	607	CHL	O1D-CGD-O2D-CED
24	G	608	CHL	O1D-CGD-O2D-CED
24	q	607	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
25	5	612	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	N	612	CLA	O1D-CGD-O2D-CED
25	p	612	CLA	O1D-CGD-O2D-CED
25	q	604	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	n	612	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	CBD-CGD-O2D-CED
24	1	608	CHL	CBD-CGD-O2D-CED
24	1	609	CHL	CBD-CGD-O2D-CED
24	2	601	CHL	CBD-CGD-O2D-CED
24	3	608	CHL	CBD-CGD-O2D-CED
24	4	607	CHL	CBD-CGD-O2D-CED
24	4	608	CHL	CBD-CGD-O2D-CED
24	4	609	CHL	CBD-CGD-O2D-CED
24	5	608	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	CBD-CGD-O2D-CED
24	6	608	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	CBD-CGD-O2D-CED
24	G	608	CHL	CBD-CGD-O2D-CED
24	N	606	CHL	CBD-CGD-O2D-CED
24	N	608	CHL	CBD-CGD-O2D-CED
24	Y	607	CHL	CBD-CGD-O2D-CED
24	0	606	CHL	CBD-CGD-O2D-CED
24	0	608	CHL	CBD-CGD-O2D-CED
24	0	609	CHL	CBD-CGD-O2D-CED
24	7	607	CHL	CBD-CGD-O2D-CED
24	8	608	CHL	CBD-CGD-O2D-CED
24	9	601	CHL	CBD-CGD-O2D-CED
24	9	608	CHL	CBD-CGD-O2D-CED
24	p	608	CHL	CBD-CGD-O2D-CED
24	q	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	q	608	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	CBD-CGD-O2D-CED
24	g	607	CHL	CBD-CGD-O2D-CED
24	g	608	CHL	CBD-CGD-O2D-CED
24	n	606	CHL	CBD-CGD-O2D-CED
24	n	608	CHL	CBD-CGD-O2D-CED
24	y	607	CHL	CBD-CGD-O2D-CED
25	2	603	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	CBD-CGD-O2D-CED
25	3	602	CLA	CBD-CGD-O2D-CED
25	3	603	CLA	CBD-CGD-O2D-CED
25	3	612	CLA	CBD-CGD-O2D-CED
25	4	602	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	5	612	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	611	CLA	CBD-CGD-O2D-CED
25	6	613	CLA	CBD-CGD-O2D-CED
25	B	602	CLA	CBD-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	612	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	612	CLA	CBD-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	S	605	CLA	CBD-CGD-O2D-CED
25	S	610	CLA	CBD-CGD-O2D-CED
25	Y	614	CLA	CBD-CGD-O2D-CED
25	0	611	CLA	CBD-CGD-O2D-CED
25	8	602	CLA	CBD-CGD-O2D-CED
25	8	612	CLA	CBD-CGD-O2D-CED
25	9	603	CLA	CBD-CGD-O2D-CED
25	9	604	CLA	CBD-CGD-O2D-CED
25	9	611	CLA	CBD-CGD-O2D-CED
25	9	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	p	603	CLA	CBD-CGD-O2D-CED
25	p	612	CLA	CBD-CGD-O2D-CED
25	q	603	CLA	CBD-CGD-O2D-CED
25	q	604	CLA	CBD-CGD-O2D-CED
25	q	613	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
25	g	612	CLA	CBD-CGD-O2D-CED
25	n	614	CLA	CBD-CGD-O2D-CED
25	s	603	CLA	CBD-CGD-O2D-CED
25	s	605	CLA	CBD-CGD-O2D-CED
25	s	610	CLA	CBD-CGD-O2D-CED
25	y	614	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	612	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
25	s	614	CLA	O1A-CGA-O2A-C1
29	C	2630	LHG	O10-C23-O8-C6
29	c	2630	LHG	O10-C23-O8-C6
24	1	608	CHL	O1D-CGD-O2D-CED
24	5	608	CHL	O1D-CGD-O2D-CED
24	6	607	CHL	O1D-CGD-O2D-CED
24	9	601	CHL	O1D-CGD-O2D-CED
25	1	614	CLA	O1D-CGD-O2D-CED
25	3	604	CLA	O1D-CGD-O2D-CED
25	3	612	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	O1D-CGD-O2D-CED
25	6	611	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
25	R	612	CLA	O1D-CGD-O2D-CED
25	0	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	7	614	CLA	O1D-CGD-O2D-CED
25	8	604	CLA	O1D-CGD-O2D-CED
25	p	602	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	r	612	CLA	O1D-CGD-O2D-CED
24	2	601	CHL	O1D-CGD-O2D-CED
24	4	608	CHL	O1D-CGD-O2D-CED
24	7	608	CHL	O1D-CGD-O2D-CED
24	9	608	CHL	O1D-CGD-O2D-CED
24	p	608	CHL	O1D-CGD-O2D-CED
25	1	604	CLA	O1D-CGD-O2D-CED
25	2	604	CLA	O1D-CGD-O2D-CED
25	4	611	CLA	O1D-CGD-O2D-CED
25	4	614	CLA	O1D-CGD-O2D-CED
25	6	614	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	0	614	CLA	O1D-CGD-O2D-CED
25	8	612	CLA	O1D-CGD-O2D-CED
25	p	614	CLA	O1D-CGD-O2D-CED
25	q	611	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
25	S	614	CLA	CBA-CGA-O2A-C1
25	s	614	CLA	CBA-CGA-O2A-C1
29	C	2630	LHG	C24-C23-O8-C6
24	1	605	CHL	CBD-CGD-O2D-CED
24	4	606	CHL	CBD-CGD-O2D-CED
24	0	607	CHL	CBD-CGD-O2D-CED
24	7	605	CHL	CBD-CGD-O2D-CED
24	9	606	CHL	CBD-CGD-O2D-CED
24	p	607	CHL	CBD-CGD-O2D-CED
24	p	609	CHL	CBD-CGD-O2D-CED
24	q	606	CHL	CBD-CGD-O2D-CED
24	q	609	CHL	CBD-CGD-O2D-CED
25	1	612	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	G	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	Y	603	CLA	CBD-CGD-O2D-CED
25	Y	604	CLA	CBD-CGD-O2D-CED
25	Y	612	CLA	CBD-CGD-O2D-CED
25	0	602	CLA	CBD-CGD-O2D-CED
25	8	603	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	CBD-CGD-O2D-CED
25	y	603	CLA	CBD-CGD-O2D-CED
25	y	604	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	CBD-CGD-O2D-CED
24	N	605	CHL	O1A-CGA-O2A-C1
24	n	605	CHL	O1A-CGA-O2A-C1
25	1	614	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	R	612	CLA	O1A-CGA-O2A-C1
25	S	613	CLA	O1A-CGA-O2A-C1
25	0	611	CLA	O1A-CGA-O2A-C1
25	7	614	CLA	O1A-CGA-O2A-C1
25	q	613	CLA	O1A-CGA-O2A-C1
25	s	605	CLA	O1A-CGA-O2A-C1
25	s	613	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
25	r	612	CLA	O1A-CGA-O2A-C1
24	S	608	CHL	O1D-CGD-O2D-CED
24	s	608	CHL	O1D-CGD-O2D-CED
25	4	613	CLA	O1D-CGD-O2D-CED
25	5	604	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED
25	N	611	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	S	604	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
25	s	604	CLA	O1D-CGD-O2D-CED
25	s	612	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	O1D-CGD-O2D-CED
25	r	610	CLA	O1D-CGD-O2D-CED
24	5	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	612	CLA	O1D-CGD-O2D-CED
25	2	613	CLA	O1D-CGD-O2D-CED
25	3	614	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	9	612	CLA	O1D-CGD-O2D-CED
25	q	602	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
24	2	606	CHL	CBD-CGD-O2D-CED
24	5	609	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	Y	606	CHL	CBD-CGD-O2D-CED
24	Y	608	CHL	CBD-CGD-O2D-CED
24	y	606	CHL	CBD-CGD-O2D-CED
24	y	608	CHL	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	5	614	CLA	CBD-CGD-O2D-CED
25	G	614	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
25	9	614	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	CBD-CGD-O2D-CED
33	A	408	PHO	CBD-CGD-O2D-CED
33	a	408	PHO	CBD-CGD-O2D-CED
24	q	608	CHL	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	O1D-CGD-O2D-CED
25	8	614	CLA	O1D-CGD-O2D-CED
25	q	614	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
35	B	621	SQD	O49-C7-O47-C45
35	b	621	SQD	O49-C7-O47-C45
25	S	611	CLA	O1A-CGA-O2A-C1
25	N	614	CLA	O1D-CGD-O2D-CED
24	2	601	CHL	C3-C5-C6-C7
24	3	607	CHL	C3-C5-C6-C7
24	4	601	CHL	C3-C5-C6-C7
24	5	607	CHL	C3-C5-C6-C7
24	6	601	CHL	C3-C5-C6-C7
24	G	601	CHL	C3-C5-C6-C7
24	p	605	CHL	C3-C5-C6-C7
25	1	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	1	604	CLA	C3-C5-C6-C7
25	2	603	CLA	C3-C5-C6-C7
25	3	603	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
25	B	609	CLA	C3-C5-C6-C7
25	B	615	CLA	C3-C5-C6-C7
25	B	617	CLA	C3-C5-C6-C7
25	C	509	CLA	C3-C5-C6-C7
25	N	613	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	613	CLA	C3-C5-C6-C7
25	Y	612	CLA	C3-C5-C6-C7
25	0	602	CLA	C3-C5-C6-C7
25	7	602	CLA	C3-C5-C6-C7
25	9	603	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
25	b	615	CLA	C3-C5-C6-C7
25	b	617	CLA	C3-C5-C6-C7
25	c	509	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
25	y	612	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	613	CLA	C3-C5-C6-C7
25	3	614	CLA	CBA-CGA-O2A-C1
25	B	617	CLA	CBA-CGA-O2A-C1
25	C	505	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBA-CGA-O2A-C1
25	R	616	CLA	CBA-CGA-O2A-C1
25	8	614	CLA	CBA-CGA-O2A-C1
25	b	617	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
25	s	605	CLA	CBA-CGA-O2A-C1
25	r	611	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBA-CGA-O2A-C1
25	r	616	CLA	CBA-CGA-O2A-C1
29	c	2630	LHG	C24-C23-O8-C6
24	g	606	CHL	O1D-CGD-O2D-CED
25	2	611	CLA	O1D-CGD-O2D-CED
25	B	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
24	2	608	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	7	609	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
25	5	613	CLA	CBD-CGD-O2D-CED
25	p	604	CLA	CBD-CGD-O2D-CED
25	g	614	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
25	s	611	CLA	O1A-CGA-O2A-C1
25	8	602	CLA	O1D-CGD-O2D-CED
24	5	607	CHL	C4-C3-C5-C6
25	8	604	CLA	C4-C3-C5-C6
24	R	607	CHL	C2-C3-C5-C6
24	r	607	CHL	C2-C3-C5-C6
25	8	604	CLA	C2-C3-C5-C6
25	c	513	CLA	C2-C3-C5-C6
39	d	405	PL9	C12-C11-C9-C8
24	3	609	CHL	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	N	604	CLA	CBD-CGD-O2D-CED
25	7	604	CLA	CBD-CGD-O2D-CED
25	n	604	CLA	CBD-CGD-O2D-CED
24	1	601	CHL	C2A-CAA-CBA-CGA
24	1	605	CHL	C2A-CAA-CBA-CGA
24	1	607	CHL	C2A-CAA-CBA-CGA
24	2	601	CHL	C2A-CAA-CBA-CGA
24	2	607	CHL	C2A-CAA-CBA-CGA
24	Y	605	CHL	C2A-CAA-CBA-CGA
24	7	601	CHL	C2A-CAA-CBA-CGA
24	7	605	CHL	C2A-CAA-CBA-CGA
24	7	607	CHL	C2A-CAA-CBA-CGA
24	9	601	CHL	C2A-CAA-CBA-CGA
24	9	607	CHL	C2A-CAA-CBA-CGA
24	n	608	CHL	C2A-CAA-CBA-CGA
24	y	605	CHL	C2A-CAA-CBA-CGA
25	3	611	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C2A-CAA-CBA-CGA
25	R	613	CLA	C2A-CAA-CBA-CGA
25	S	613	CLA	C2A-CAA-CBA-CGA
25	7	604	CLA	C2A-CAA-CBA-CGA
25	8	611	CLA	C2A-CAA-CBA-CGA
25	q	613	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
25	b	611	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	s	613	CLA	C2A-CAA-CBA-CGA
25	r	613	CLA	C2A-CAA-CBA-CGA
25	Y	611	CLA	O1A-CGA-O2A-C1
25	g	613	CLA	O1A-CGA-O2A-C1
25	y	611	CLA	O1A-CGA-O2A-C1
25	3	602	CLA	O1D-CGD-O2D-CED
25	Y	614	CLA	O1D-CGD-O2D-CED
25	y	614	CLA	O1D-CGD-O2D-CED
24	5	605	CHL	C3-C5-C6-C7
24	6	607	CHL	C3-C5-C6-C7
24	9	601	CHL	C3-C5-C6-C7
24	g	601	CHL	C3-C5-C6-C7
25	5	602	CLA	C3-C5-C6-C7
25	C	508	CLA	C3-C5-C6-C7
25	G	613	CLA	C3-C5-C6-C7
25	0	613	CLA	C3-C5-C6-C7
25	7	604	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
25	q	612	CLA	C2A-CAA-CBA-CGA
24	N	605	CHL	CBA-CGA-O2A-C1
24	R	607	CHL	CBA-CGA-O2A-C1
24	n	605	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	CBA-CGA-O2A-C1
25	1	614	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	G	613	CLA	CBA-CGA-O2A-C1
25	S	605	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
25	S	613	CLA	CBA-CGA-O2A-C1
25	Y	612	CLA	CBA-CGA-O2A-C1
25	0	611	CLA	CBA-CGA-O2A-C1
25	7	614	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	p	614	CLA	CBA-CGA-O2A-C1
25	q	613	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
25	g	613	CLA	CBA-CGA-O2A-C1
25	s	611	CLA	CBA-CGA-O2A-C1
25	s	613	CLA	CBA-CGA-O2A-C1
25	y	612	CLA	CBA-CGA-O2A-C1
24	1	607	CHL	O1D-CGD-O2D-CED
24	N	606	CHL	O1D-CGD-O2D-CED
24	7	607	CHL	O1D-CGD-O2D-CED
25	S	605	CLA	O1D-CGD-O2D-CED
25	9	604	CLA	O1D-CGD-O2D-CED
39	D	405	PL9	C22-C23-C24-C25
39	D	405	PL9	C42-C43-C44-C45
39	d	405	PL9	C22-C23-C24-C25
24	1	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	CBD-CGD-O2D-CED
24	8	609	CHL	CBD-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	7	612	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
24	3	608	CHL	O1D-CGD-O2D-CED
24	4	609	CHL	O1D-CGD-O2D-CED
24	G	606	CHL	O1D-CGD-O2D-CED
24	0	606	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
25	9	611	CLA	O1D-CGD-O2D-CED
25	9	613	CLA	O1D-CGD-O2D-CED
39	D	405	PL9	C7-C8-C9-C11
39	d	405	PL9	C7-C8-C9-C11
25	A	405	CLA	O1A-CGA-O2A-C1
25	G	613	CLA	O1A-CGA-O2A-C1
25	G	614	CLA	O1A-CGA-O2A-C1
25	S	605	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
24	8	608	CHL	O1D-CGD-O2D-CED
25	q	603	CLA	O1D-CGD-O2D-CED
24	2	609	CHL	CBD-CGD-O2D-CED
24	3	607	CHL	CBD-CGD-O2D-CED
24	5	601	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Y	605	CHL	CBD-CGD-O2D-CED
24	8	607	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
24	s	606	CHL	CBD-CGD-O2D-CED
24	y	605	CHL	CBD-CGD-O2D-CED
25	3	610	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	0	613	CLA	CBD-CGD-O2D-CED
25	8	613	CLA	CBD-CGD-O2D-CED
25	q	612	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	y	610	CLA	CBD-CGD-O2D-CED
24	n	606	CHL	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	C	508	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	p	603	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
25	s	605	CLA	O1D-CGD-O2D-CED
29	Y	2630	LHG	O2-C2-C3-O3
29	y	2630	LHG	O2-C2-C3-O3
24	Y	606	CHL	C3-C5-C6-C7
24	0	601	CHL	C3-C5-C6-C7
24	0	607	CHL	C3-C5-C6-C7
24	y	606	CHL	C3-C5-C6-C7
25	6	612	CLA	C3-C5-C6-C7
25	C	504	CLA	C3-C5-C6-C7
25	0	612	CLA	C3-C5-C6-C7
25	8	603	CLA	C3-C5-C6-C7
25	c	504	CLA	C3-C5-C6-C7
24	1	607	CHL	CBA-CGA-O2A-C1
25	5	614	CLA	CBA-CGA-O2A-C1
25	6	611	CLA	CBA-CGA-O2A-C1
25	S	602	CLA	CBA-CGA-O2A-C1
25	Y	611	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	s	602	CLA	CBA-CGA-O2A-C1
25	y	611	CLA	CBA-CGA-O2A-C1
25	3	614	CLA	O1A-CGA-O2A-C1
25	6	611	CLA	O1A-CGA-O2A-C1
25	R	616	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	8	614	CLA	O1A-CGA-O2A-C1
25	g	614	CLA	O1A-CGA-O2A-C1
25	r	616	CLA	O1A-CGA-O2A-C1
24	Y	607	CHL	O1D-CGD-O2D-CED
24	g	607	CHL	O1D-CGD-O2D-CED
25	4	602	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	O1D-CGD-O2D-CED
25	b	612	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED
24	y	607	CHL	O1D-CGD-O2D-CED
25	s	610	CLA	O1D-CGD-O2D-CED
24	4	601	CHL	CBD-CGD-O2D-CED
24	N	609	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	S	607	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	CBD-CGD-O2D-CED
24	0	605	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	CBD-CGD-O2D-CED
24	s	607	CHL	CBD-CGD-O2D-CED
25	5	611	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	Y	610	CLA	CBD-CGD-O2D-CED
25	8	610	CLA	CBD-CGD-O2D-CED
25	g	611	CLA	CBD-CGD-O2D-CED
36	h	102	LMG	O6-C5-C6-O5
25	b	603	CLA	O1D-CGD-O2D-CED
24	r	607	CHL	O1A-CGA-O2A-C1
24	6	606	CHL	O1D-CGD-O2D-CED
24	6	608	CHL	O1D-CGD-O2D-CED
25	2	603	CLA	O1D-CGD-O2D-CED
25	S	610	CLA	O1D-CGD-O2D-CED
25	q	613	CLA	O1D-CGD-O2D-CED
24	7	606	CHL	CBD-CGD-O2D-CED
25	G	611	CLA	CBD-CGD-O2D-CED
25	p	610	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	C3-C5-C6-C7
25	r	609	CLA	C3-C5-C6-C7
25	A	405	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
24	N	608	CHL	O1D-CGD-O2D-CED
25	9	603	CLA	O1D-CGD-O2D-CED
24	R	607	CHL	O1A-CGA-O2A-C1
25	5	614	CLA	O1A-CGA-O2A-C1
25	S	602	CLA	O1A-CGA-O2A-C1
25	Y	612	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	y	612	CLA	O1A-CGA-O2A-C1
24	S	608	CHL	O2A-C1-C2-C3
24	s	608	CHL	O2A-C1-C2-C3
25	C	504	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	p	604	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	p	604	CLA	C2-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
25	c	501	CLA	CBD-CGD-O2D-CED
24	Y	607	CHL	C2A-CAA-CBA-CGA
24	0	607	CHL	C2A-CAA-CBA-CGA
24	y	607	CHL	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	G	614	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	g	614	CLA	C2A-CAA-CBA-CGA
24	7	607	CHL	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	p	614	CLA	O1A-CGA-O2A-C1
25	s	602	CLA	O1A-CGA-O2A-C1
35	A	412	SQD	O5-C1-O6-C44
35	B	621	SQD	O5-C1-O6-C44
35	a	412	SQD	O5-C1-O6-C44
35	b	621	SQD	O5-C1-O6-C44
24	R	608	CHL	C3-C5-C6-C7
24	r	608	CHL	C3-C5-C6-C7
24	7	607	CHL	CBA-CGA-O2A-C1
25	b	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	n	613	CLA	CBA-CGA-O2A-C1
36	H	102	LMG	O6-C5-C6-O5
24	1	609	CHL	O1D-CGD-O2D-CED
24	0	608	CHL	O1D-CGD-O2D-CED
25	3	603	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	O1D-CGD-O2D-CED
25	Y	604	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
25	y	604	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	O1A-CGA-O2A-C1
24	1	605	CHL	O1D-CGD-O2D-CED
24	7	605	CHL	O1D-CGD-O2D-CED
25	1	612	CLA	O1D-CGD-O2D-CED
25	G	603	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
25	g	603	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
29	6	2630	LHG	C1-C2-C3-O3
29	l	101	LHG	C1-C2-C3-O3
24	3	607	CHL	O1A-CGA-O2A-C1
24	y	601	CHL	C3-C5-C6-C7
25	Y	614	CLA	C3-C5-C6-C7
25	y	613	CLA	C3-C5-C6-C7
25	y	614	CLA	C3-C5-C6-C7
24	4	606	CHL	O1D-CGD-O2D-CED
24	q	606	CHL	O1D-CGD-O2D-CED
25	Y	603	CLA	O1D-CGD-O2D-CED
25	0	602	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	CBA-CGA-O2A-C1
24	3	607	CHL	CBA-CGA-O2A-C1
24	4	607	CHL	CBA-CGA-O2A-C1
24	6	606	CHL	CBA-CGA-O2A-C1
24	Y	607	CHL	CBA-CGA-O2A-C1
24	0	606	CHL	CBA-CGA-O2A-C1
24	8	607	CHL	CBA-CGA-O2A-C1
24	9	607	CHL	CBA-CGA-O2A-C1
24	y	607	CHL	CBA-CGA-O2A-C1
25	2	614	CLA	CBA-CGA-O2A-C1
25	4	614	CLA	CBA-CGA-O2A-C1
25	B	603	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	CBA-CGA-O2A-C1
25	D	402	CLA	CBA-CGA-O2A-C1
25	N	613	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	R	604	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	CBA-CGA-O2A-C1
25	9	614	CLA	CBA-CGA-O2A-C1
25	q	614	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	d	402	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
25	r	613	CLA	CBA-CGA-O2A-C1
25	3	613	CLA	CBD-CGD-O2D-CED
25	R	616	CLA	CBD-CGD-O2D-CED
25	r	616	CLA	CBD-CGD-O2D-CED
24	9	609	CHL	C2C-C3C-CAC-CBC
24	q	601	CHL	C13-C15-C16-C17
24	y	609	CHL	C8-C10-C11-C12
24	R	606	CHL	C15-C16-C17-C18
24	Y	609	CHL	C8-C10-C11-C12
24	Y	609	CHL	C15-C16-C17-C18
24	n	601	CHL	C15-C16-C17-C18
24	n	609	CHL	C8-C10-C11-C12
24	y	607	CHL	C15-C16-C17-C18
25	6	613	CLA	C13-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
24	0	606	CHL	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
24	5	607	CHL	C2-C3-C5-C6
39	D	405	PL9	C12-C11-C9-C8
24	1	609	CHL	C14-C13-C15-C16
24	3	607	CHL	C11-C10-C8-C9
24	5	605	CHL	C11-C10-C8-C9
24	5	609	CHL	C11-C10-C8-C9
24	6	606	CHL	C14-C13-C15-C16
24	6	607	CHL	C14-C13-C15-C16
24	6	609	CHL	C14-C13-C15-C16
24	N	605	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C10-C8-C9
24	N	609	CHL	C14-C13-C15-C16
24	R	608	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	0	609	CHL	C14-C13-C15-C16
24	7	609	CHL	C14-C13-C15-C16
24	8	601	CHL	C6-C7-C8-C9
24	8	607	CHL	C11-C12-C13-C14
24	p	607	CHL	C11-C12-C13-C14
24	p	609	CHL	C11-C10-C8-C9
24	q	609	CHL	C11-C10-C8-C9
24	n	605	CHL	C11-C10-C8-C9
24	n	605	CHL	C11-C12-C13-C14
24	n	609	CHL	C11-C10-C8-C9
24	n	609	CHL	C14-C13-C15-C16
24	r	608	CHL	C6-C7-C8-C9
25	B	602	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C10-C8-C9
25	N	610	CLA	C6-C7-C8-C9
25	R	616	CLA	C14-C13-C15-C16
25	b	602	CLA	C14-C13-C15-C16
25	b	605	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	n	610	CLA	C6-C7-C8-C9
25	r	616	CLA	C14-C13-C15-C16
24	p	607	CHL	O1D-CGD-O2D-CED
25	y	603	CLA	O1D-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
24	4	601	CHL	C13-C15-C16-C17
25	C	502	CLA	C10-C11-C12-C13
25	8	602	CLA	C10-C11-C12-C13
24	0	608	CHL	C2A-CAA-CBA-CGA
24	7	608	CHL	C2A-CAA-CBA-CGA
24	q	609	CHL	C2A-CAA-CBA-CGA
25	1	603	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C2A-CAA-CBA-CGA
25	r	601	CLA	C2A-CAA-CBA-CGA
26	4	1620	LUT	C27-C28-C29-C39
26	Y	1621	LUT	C7-C8-C9-C19
26	8	1620	LUT	C27-C28-C29-C39
26	p	1620	LUT	C27-C28-C29-C39
26	p	1620	LUT	C31-C32-C33-C40
26	y	1621	LUT	C7-C8-C9-C19
27	0	1622	XAT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
27	q	1622	XAT	C11-C12-C13-C20
28	2	1623	NEX	C31-C32-C33-C40
34	C	514	BCR	C37-C22-C23-C24
34	C	515	BCR	C7-C8-C9-C34
34	D	404	BCR	C7-C8-C9-C34
34	c	514	BCR	C37-C22-C23-C24
34	c	515	BCR	C7-C8-C9-C34
34	d	404	BCR	C7-C8-C9-C34
29	9	2630	LHG	C7-C8-C9-C10
24	6	606	CHL	O1A-CGA-O2A-C1
24	Y	607	CHL	O1A-CGA-O2A-C1
24	8	607	CHL	O1A-CGA-O2A-C1
24	y	607	CHL	O1A-CGA-O2A-C1
25	4	614	CLA	O1A-CGA-O2A-C1
25	N	613	CLA	O1A-CGA-O2A-C1
25	R	613	CLA	O1A-CGA-O2A-C1
25	9	614	CLA	O1A-CGA-O2A-C1
25	q	614	CLA	O1A-CGA-O2A-C1
25	r	613	CLA	O1A-CGA-O2A-C1
24	2	609	CHL	C13-C15-C16-C17
24	3	605	CHL	C15-C16-C17-C18
24	3	609	CHL	C5-C6-C7-C8
24	4	609	CHL	C5-C6-C7-C8
24	6	607	CHL	C5-C6-C7-C8
24	N	601	CHL	C15-C16-C17-C18
24	7	607	CHL	C8-C10-C11-C12
24	r	606	CHL	C15-C16-C17-C18
25	1	610	CLA	C13-C15-C16-C17
25	6	604	CLA	C13-C15-C16-C17
25	B	606	CLA	C13-C15-C16-C17
25	B	617	CLA	C15-C16-C17-C18
25	C	510	CLA	C13-C15-C16-C17
25	Y	604	CLA	C10-C11-C12-C13
25	b	606	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
25	y	604	CLA	C10-C11-C12-C13
25	s	609	CLA	CBD-CGD-O2D-CED
37	C	524	DGD	O6E-C5E-C6E-O5E
37	c	524	DGD	O6E-C5E-C6E-O5E
25	C	513	CLA	C3-C5-C6-C7
24	9	608	CHL	C2A-CAA-CBA-CGA
24	q	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	r	604	CLA	CBA-CGA-O2A-C1
24	1	601	CHL	C15-C16-C17-C18
24	1	607	CHL	C13-C15-C16-C17
24	2	609	CHL	C5-C6-C7-C8
24	Y	607	CHL	C8-C10-C11-C12
24	q	609	CHL	C8-C10-C11-C12
24	y	609	CHL	C13-C15-C16-C17
25	2	603	CLA	C15-C16-C17-C18
25	4	613	CLA	C5-C6-C7-C8
25	A	405	CLA	C13-C15-C16-C17
25	C	506	CLA	C8-C10-C11-C12
25	C	512	CLA	C5-C6-C7-C8
25	D	403	CLA	C5-C6-C7-C8
25	G	602	CLA	C10-C11-C12-C13
25	Y	612	CLA	C13-C15-C16-C17
25	7	613	CLA	C10-C11-C12-C13
25	9	603	CLA	C8-C10-C11-C12
25	9	603	CLA	C15-C16-C17-C18
25	p	604	CLA	C13-C15-C16-C17
25	p	604	CLA	C15-C16-C17-C18
25	q	602	CLA	C8-C10-C11-C12
25	a	405	CLA	C13-C15-C16-C17
25	b	605	CLA	C8-C10-C11-C12
25	c	506	CLA	C8-C10-C11-C12
25	c	507	CLA	C15-C16-C17-C18
25	c	512	CLA	C5-C6-C7-C8
25	y	612	CLA	C13-C15-C16-C17
24	1	601	CHL	C10-C11-C12-C13
24	1	607	CHL	C8-C10-C11-C12
24	3	601	CHL	C8-C10-C11-C12
24	3	605	CHL	C5-C6-C7-C8
24	4	609	CHL	C15-C16-C17-C18
24	5	601	CHL	C13-C15-C16-C17
24	6	606	CHL	C10-C11-C12-C13
24	G	609	CHL	C8-C10-C11-C12
24	G	609	CHL	C15-C16-C17-C18
24	N	601	CHL	C8-C10-C11-C12
24	N	605	CHL	C13-C15-C16-C17
24	N	609	CHL	C8-C10-C11-C12
24	R	608	CHL	C5-C6-C7-C8
24	Y	606	CHL	C13-C15-C16-C17
24	Y	609	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	0	601	CHL	C13-C15-C16-C17
24	0	609	CHL	C8-C10-C11-C12
24	7	607	CHL	C13-C15-C16-C17
24	8	601	CHL	C8-C10-C11-C12
24	8	605	CHL	C5-C6-C7-C8
24	9	609	CHL	C5-C6-C7-C8
24	9	609	CHL	C13-C15-C16-C17
24	p	601	CHL	C13-C15-C16-C17
24	p	605	CHL	C13-C15-C16-C17
24	p	607	CHL	C8-C10-C11-C12
24	q	601	CHL	C10-C11-C12-C13
24	q	609	CHL	C15-C16-C17-C18
24	g	609	CHL	C8-C10-C11-C12
24	g	609	CHL	C15-C16-C17-C18
24	n	605	CHL	C8-C10-C11-C12
24	y	606	CHL	C13-C15-C16-C17
24	y	607	CHL	C8-C10-C11-C12
24	y	609	CHL	C15-C16-C17-C18
24	r	608	CHL	C5-C6-C7-C8
25	1	613	CLA	C10-C11-C12-C13
25	2	603	CLA	C8-C10-C11-C12
25	4	602	CLA	C8-C10-C11-C12
25	6	610	CLA	C8-C10-C11-C12
25	B	602	CLA	C13-C15-C16-C17
25	B	603	CLA	C10-C11-C12-C13
25	B	605	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
25	C	507	CLA	C15-C16-C17-C18
25	C	508	CLA	C8-C10-C11-C12
25	R	616	CLA	C13-C15-C16-C17
25	0	604	CLA	C8-C10-C11-C12
25	0	604	CLA	C13-C15-C16-C17
25	0	610	CLA	C8-C10-C11-C12
25	7	610	CLA	C13-C15-C16-C17
25	q	610	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	b	603	CLA	C10-C11-C12-C13
25	b	617	CLA	C15-C16-C17-C18
25	c	508	CLA	C8-C10-C11-C12
25	c	513	CLA	C13-C15-C16-C17
25	d	403	CLA	C5-C6-C7-C8
25	r	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	0	607	CHL	O1D-CGD-O2D-CED
25	Y	612	CLA	O1D-CGD-O2D-CED
25	8	603	CLA	O1D-CGD-O2D-CED
25	y	612	CLA	O1D-CGD-O2D-CED
25	2	614	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
29	1	2630	LHG	C7-C8-C9-C10
29	D	410	LHG	C23-C24-C25-C26
29	d	410	LHG	C23-C24-C25-C26
35	B	623	SQD	C23-C24-C25-C26
35	b	623	SQD	C23-C24-C25-C26
36	B	622	LMG	C28-C29-C30-C31
36	C	521	LMG	C28-C29-C30-C31
36	b	622	LMG	C28-C29-C30-C31
36	c	521	LMG	C28-C29-C30-C31
24	1	607	CHL	C5-C6-C7-C8
24	3	605	CHL	C8-C10-C11-C12
24	3	609	CHL	C13-C15-C16-C17
24	5	607	CHL	C8-C10-C11-C12
24	6	601	CHL	C13-C15-C16-C17
24	Y	601	CHL	C15-C16-C17-C18
24	7	607	CHL	C5-C6-C7-C8
24	p	609	CHL	C15-C16-C17-C18
24	q	601	CHL	C8-C10-C11-C12
24	g	601	CHL	C15-C16-C17-C18
24	n	601	CHL	C8-C10-C11-C12
24	n	607	CHL	C8-C10-C11-C12
25	3	603	CLA	C5-C6-C7-C8
25	3	613	CLA	C15-C16-C17-C18
25	4	602	CLA	C10-C11-C12-C13
25	A	410	CLA	C5-C6-C7-C8
25	B	610	CLA	C5-C6-C7-C8
25	C	505	CLA	C8-C10-C11-C12
25	C	513	CLA	C8-C10-C11-C12
25	G	602	CLA	C8-C10-C11-C12
25	7	602	CLA	C8-C10-C11-C12
25	8	613	CLA	C15-C16-C17-C18
25	9	602	CLA	C8-C10-C11-C12
25	a	410	CLA	C5-C6-C7-C8
25	b	610	CLA	C5-C6-C7-C8
25	c	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	g	602	CLA	C8-C10-C11-C12
25	g	602	CLA	C10-C11-C12-C13
25	n	610	CLA	C10-C11-C12-C13
24	n	607	CHL	CBA-CGA-O2A-C1
25	Y	613	CLA	CBA-CGA-O2A-C1
25	7	604	CLA	CBA-CGA-O2A-C1
25	y	613	CLA	CBA-CGA-O2A-C1
24	2	601	CHL	C15-C16-C17-C18
24	4	601	CHL	C8-C10-C11-C12
24	6	607	CHL	C8-C10-C11-C12
24	G	601	CHL	C15-C16-C17-C18
24	0	607	CHL	C8-C10-C11-C12
24	7	601	CHL	C10-C11-C12-C13
24	8	605	CHL	C15-C16-C17-C18
24	8	609	CHL	C13-C15-C16-C17
24	9	601	CHL	C5-C6-C7-C8
25	1	602	CLA	C8-C10-C11-C12
25	B	608	CLA	C13-C15-C16-C17
25	B	614	CLA	C10-C11-C12-C13
25	C	508	CLA	C5-C6-C7-C8
25	C	513	CLA	C13-C15-C16-C17
25	N	610	CLA	C10-C11-C12-C13
25	0	613	CLA	C13-C15-C16-C17
25	7	604	CLA	C10-C11-C12-C13
25	8	603	CLA	C5-C6-C7-C8
25	q	602	CLA	C10-C11-C12-C13
25	b	608	CLA	C13-C15-C16-C17
25	b	614	CLA	C10-C11-C12-C13
25	c	508	CLA	C5-C6-C7-C8
29	2	2630	LHG	C7-C8-C9-C10
29	6	2630	LHG	C7-C8-C9-C10
29	G	2630	LHG	C7-C8-C9-C10
29	g	2630	LHG	C7-C8-C9-C10
24	8	606	CHL	CBD-CGD-O2D-CED
24	2	608	CHL	C2A-CAA-CBA-CGA
24	S	606	CHL	C2A-CAA-CBA-CGA
24	s	606	CHL	C2A-CAA-CBA-CGA
25	4	612	CLA	C2A-CAA-CBA-CGA
40	f	101	HEM	C3D-CAD-CBD-CGD
25	S	614	CLA	O2A-C1-C2-C3
25	s	614	CLA	O2A-C1-C2-C3
24	8	605	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	9	601	CHL	C15-C16-C17-C18
24	p	601	CHL	C15-C16-C17-C18
25	1	604	CLA	C10-C11-C12-C13
25	3	602	CLA	C10-C11-C12-C13
25	B	612	CLA	C13-C15-C16-C17
25	N	610	CLA	C5-C6-C7-C8
25	b	612	CLA	C13-C15-C16-C17
25	c	502	CLA	C10-C11-C12-C13
24	2	606	CHL	O1D-CGD-O2D-CED
33	A	408	PHO	O1D-CGD-O2D-CED
24	2	601	CHL	C6-C7-C8-C10
24	4	601	CHL	C6-C7-C8-C10
24	5	605	CHL	C6-C7-C8-C10
24	6	606	CHL	C12-C13-C15-C16
24	6	607	CHL	C11-C10-C8-C7
24	6	609	CHL	C12-C13-C15-C16
24	G	601	CHL	C6-C7-C8-C10
24	0	606	CHL	C12-C13-C15-C16
24	7	607	CHL	C11-C10-C8-C7
24	8	609	CHL	C11-C10-C8-C7
24	g	601	CHL	C6-C7-C8-C10
24	n	605	CHL	C12-C13-C15-C16
25	B	613	CLA	C12-C13-C15-C16
25	N	603	CLA	C11-C12-C13-C15
25	Y	610	CLA	C11-C12-C13-C15
25	b	613	CLA	C12-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C10
25	n	603	CLA	C11-C12-C13-C15
25	y	610	CLA	C11-C12-C13-C15
26	q	1621	LUT	C29-C30-C31-C32
29	g	2630	LHG	C24-C23-O8-C6
24	6	607	CHL	C2A-CAA-CBA-CGA
24	6	608	CHL	C2A-CAA-CBA-CGA
25	1	614	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	C2A-CAA-CBA-CGA
25	7	603	CLA	C2A-CAA-CBA-CGA
25	7	614	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
24	5	609	CHL	O1D-CGD-O2D-CED
24	Y	606	CHL	O1D-CGD-O2D-CED
24	Y	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	9	606	CHL	O1D-CGD-O2D-CED
24	p	609	CHL	O1D-CGD-O2D-CED
24	y	606	CHL	O1D-CGD-O2D-CED
24	y	608	CHL	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	5	614	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	r	611	CLA	O1D-CGD-O2D-CED
33	a	408	PHO	O1D-CGD-O2D-CED
24	6	609	CHL	C8-C10-C11-C12
24	N	607	CHL	C8-C10-C11-C12
24	Y	601	CHL	C13-C15-C16-C17
24	0	606	CHL	C10-C11-C12-C13
24	p	605	CHL	C5-C6-C7-C8
24	q	609	CHL	C5-C6-C7-C8
24	y	601	CHL	C15-C16-C17-C18
25	3	613	CLA	C5-C6-C7-C8
25	5	604	CLA	C13-C15-C16-C17
25	6	612	CLA	C10-C11-C12-C13
25	C	503	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	C	513	CLA	C15-C16-C17-C18
25	G	613	CLA	C15-C16-C17-C18
25	N	613	CLA	C10-C11-C12-C13
25	R	613	CLA	C8-C10-C11-C12
25	0	612	CLA	C10-C11-C12-C13
25	8	613	CLA	C5-C6-C7-C8
25	9	603	CLA	C5-C6-C7-C8
25	c	503	CLA	C15-C16-C17-C18
25	g	613	CLA	C15-C16-C17-C18
25	n	603	CLA	C5-C6-C7-C8
25	n	613	CLA	C10-C11-C12-C13
25	r	613	CLA	C8-C10-C11-C12
24	4	607	CHL	O1A-CGA-O2A-C1
25	B	603	CLA	O1A-CGA-O2A-C1
25	D	402	CLA	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1
25	b	603	CLA	O1A-CGA-O2A-C1
25	r	603	CLA	O1A-CGA-O2A-C1
25	C	507	CLA	CBD-CGD-O2D-CED
25	9	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	7	601	CHL	C13-C15-C16-C17
24	8	601	CHL	C5-C6-C7-C8
24	8	607	CHL	C8-C10-C11-C12
24	p	605	CHL	C15-C16-C17-C18
24	g	601	CHL	C13-C15-C16-C17
24	y	601	CHL	C5-C6-C7-C8
24	y	601	CHL	C13-C15-C16-C17
25	R	616	CLA	C15-C16-C17-C18
25	c	507	CLA	C13-C15-C16-C17
25	r	616	CLA	C15-C16-C17-C18
24	R	606	CHL	O1D-CGD-O2D-CED
24	q	609	CHL	O1D-CGD-O2D-CED
24	r	606	CHL	O1D-CGD-O2D-CED
29	0	2630	LHG	C7-C8-C9-C10
29	y	2630	LHG	C7-C8-C9-C10
37	C	518	DGD	C1A-C2A-C3A-C4A
29	6	2630	LHG	O2-C2-C3-O3
29	G	2630	LHG	O2-C2-C3-O3
29	g	2630	LHG	O2-C2-C3-O3
29	l	101	LHG	O2-C2-C3-O3
25	Y	613	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
24	G	608	CHL	C2A-CAA-CBA-CGA
25	9	612	CLA	C2A-CAA-CBA-CGA
24	1	606	CHL	C13-C15-C16-C17
24	1	609	CHL	C8-C10-C11-C12
24	5	609	CHL	C5-C6-C7-C8
24	N	601	CHL	C13-C15-C16-C17
24	N	605	CHL	C8-C10-C11-C12
24	N	607	CHL	C13-C15-C16-C17
24	7	606	CHL	C13-C15-C16-C17
24	7	609	CHL	C8-C10-C11-C12
24	p	601	CHL	C8-C10-C11-C12
24	n	601	CHL	C13-C15-C16-C17
25	1	603	CLA	C10-C11-C12-C13
25	4	610	CLA	C13-C15-C16-C17
25	N	603	CLA	C5-C6-C7-C8
25	Y	604	CLA	C13-C15-C16-C17
25	c	502	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	511	CLA	C15-C16-C17-C18
25	n	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	y	604	CLA	C13-C15-C16-C17
25	y	610	CLA	C5-C6-C7-C8
24	N	607	CHL	CBA-CGA-O2A-C1
24	8	608	CHL	CBA-CGA-O2A-C1
24	p	607	CHL	CBA-CGA-O2A-C1
25	p	604	CLA	O1D-CGD-O2D-CED
24	9	607	CHL	O1A-CGA-O2A-C1
25	R	604	CLA	O1A-CGA-O2A-C1
25	d	402	CLA	O1A-CGA-O2A-C1
25	n	613	CLA	O1A-CGA-O2A-C1
25	2	614	CLA	O1D-CGD-O2D-CED
24	3	607	CHL	C15-C16-C17-C18
24	8	605	CHL	C13-C15-C16-C17
24	p	607	CHL	C5-C6-C7-C8
24	p	609	CHL	C8-C10-C11-C12
24	n	609	CHL	C10-C11-C12-C13
25	6	602	CLA	C5-C6-C7-C8
25	6	612	CLA	C13-C15-C16-C17
25	A	405	CLA	C15-C16-C17-C18
25	C	504	CLA	C8-C10-C11-C12
25	C	507	CLA	C13-C15-C16-C17
25	C	511	CLA	C15-C16-C17-C18
25	G	613	CLA	C13-C15-C16-C17
25	Y	610	CLA	C5-C6-C7-C8
25	0	612	CLA	C13-C15-C16-C17
25	7	603	CLA	C10-C11-C12-C13
25	8	603	CLA	C10-C11-C12-C13
25	p	604	CLA	C10-C11-C12-C13
25	q	602	CLA	C15-C16-C17-C18
25	q	603	CLA	C8-C10-C11-C12
25	a	405	CLA	C15-C16-C17-C18
25	c	504	CLA	C8-C10-C11-C12
25	g	613	CLA	C13-C15-C16-C17
25	G	614	CLA	O1D-CGD-O2D-CED
25	9	614	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	O1A-CGA-O2A-C1
24	n	607	CHL	O1A-CGA-O2A-C1
37	C	524	DGD	C2B-C1B-O2G-C2G
37	c	524	DGD	C2B-C1B-O2G-C2G
24	1	601	CHL	C5-C6-C7-C8
24	2	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	3	607	CHL	C8-C10-C11-C12
24	5	601	CHL	C8-C10-C11-C12
24	5	605	CHL	C13-C15-C16-C17
24	5	605	CHL	C15-C16-C17-C18
24	G	601	CHL	C13-C15-C16-C17
24	N	609	CHL	C10-C11-C12-C13
24	R	606	CHL	C8-C10-C11-C12
24	8	607	CHL	C15-C16-C17-C18
24	q	609	CHL	C10-C11-C12-C13
24	n	607	CHL	C13-C15-C16-C17
24	r	606	CHL	C8-C10-C11-C12
25	2	602	CLA	C8-C10-C11-C12
25	2	603	CLA	C5-C6-C7-C8
25	3	610	CLA	C5-C6-C7-C8
25	5	604	CLA	C15-C16-C17-C18
25	B	606	CLA	C15-C16-C17-C18
25	R	610	CLA	C15-C16-C17-C18
25	8	610	CLA	C5-C6-C7-C8
25	b	606	CLA	C15-C16-C17-C18
29	2	2630	LHG	C3-O3-P-O6
29	2	2630	LHG	C4-O6-P-O3
29	5	2630	LHG	C4-O6-P-O3
29	C	2630	LHG	C4-O6-P-O3
29	D	408	LHG	C4-O6-P-O3
29	N	2630	LHG	C3-O3-P-O6
29	N	2630	LHG	C4-O6-P-O3
29	R	2630	LHG	C3-O3-P-O6
29	R	2630	LHG	C4-O6-P-O3
29	0	2630	LHG	C4-O6-P-O3
29	9	2630	LHG	C4-O6-P-O3
29	p	2630	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O3
29	n	2630	LHG	C3-O3-P-O6
29	n	2630	LHG	C4-O6-P-O3
29	r	2630	LHG	C3-O3-P-O6
29	r	2630	LHG	C4-O6-P-O3
37	C	523	DGD	C1A-C2A-C3A-C4A
37	c	518	DGD	C1A-C2A-C3A-C4A
37	c	523	DGD	C1A-C2A-C3A-C4A
24	6	606	CHL	C3-C5-C6-C7
24	8	607	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C3-C5-C6-C7
33	A	408	PHO	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
24	5	608	CHL	CBA-CGA-O2A-C1
24	n	608	CHL	CBA-CGA-O2A-C1
24	r	606	CHL	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
29	2	2630	LHG	C24-C23-O8-C6
29	G	2630	LHG	C24-C23-O8-C6
29	S	2630	LHG	C24-C23-O8-C6
25	5	613	CLA	O1D-CGD-O2D-CED
24	4	609	CHL	C8-C10-C11-C12
24	8	607	CHL	C13-C15-C16-C17
24	9	609	CHL	C15-C16-C17-C18
24	n	605	CHL	C13-C15-C16-C17
25	B	615	CLA	C10-C11-C12-C13
25	B	616	CLA	C15-C16-C17-C18
25	Y	604	CLA	C8-C10-C11-C12
25	0	604	CLA	C15-C16-C17-C18
25	b	615	CLA	C10-C11-C12-C13
25	b	616	CLA	C15-C16-C17-C18
25	y	604	CLA	C8-C10-C11-C12
25	r	610	CLA	C15-C16-C17-C18
24	7	609	CHL	O1D-CGD-O2D-CED
24	2	609	CHL	C2C-C3C-CAC-CBC
25	2	612	CLA	C2A-CAA-CBA-CGA
29	7	2630	LHG	C7-C8-C9-C10
24	2	608	CHL	O1D-CGD-O2D-CED
24	3	609	CHL	C15-C16-C17-C18
25	C	502	CLA	C5-C6-C7-C8
25	C	502	CLA	C8-C10-C11-C12
25	p	602	CLA	C8-C10-C11-C12
25	c	501	CLA	C15-C16-C17-C18
25	a	407	CLA	CBD-CGD-O2D-CED
24	4	605	CHL	C2A-CAA-CBA-CGA
25	1	610	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	C2A-CAA-CBA-CGA
25	C	505	CLA	C2A-CAA-CBA-CGA
25	C	507	CLA	C2A-CAA-CBA-CGA
25	7	610	CLA	C2A-CAA-CBA-CGA
25	p	610	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	r	604	CLA	C2A-CAA-CBA-CGA
24	3	601	CHL	C16-C17-C18-C20
24	6	609	CHL	C16-C17-C18-C20
24	R	606	CHL	C16-C17-C18-C20
24	8	601	CHL	C16-C17-C18-C20
24	r	606	CHL	C16-C17-C18-C20
37	C	518	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	O6E-C5E-C6E-O5E
25	N	604	CLA	C3-C5-C6-C7
24	1	609	CHL	CBA-CGA-O2A-C1
24	3	608	CHL	CBA-CGA-O2A-C1
24	R	606	CHL	CBA-CGA-O2A-C1
24	Y	606	CHL	CBA-CGA-O2A-C1
24	y	606	CHL	CBA-CGA-O2A-C1
25	6	614	CLA	CBA-CGA-O2A-C1
25	c	501	CLA	CBA-CGA-O2A-C1
29	s	2630	LHG	C24-C23-O8-C6
24	1	607	CHL	C15-C16-C17-C18
25	3	603	CLA	C10-C11-C12-C13
24	3	601	CHL	C5-C6-C7-C8
24	0	607	CHL	C15-C16-C17-C18
24	p	609	CHL	C5-C6-C7-C8
25	5	613	CLA	C13-C15-C16-C17
29	4	2630	LHG	C33-C34-C35-C36
29	6	2630	LHG	C27-C28-C29-C30
36	C	521	LMG	C30-C31-C32-C33
35	D	413	SQD	C8-C7-O47-C45
35	d	413	SQD	C8-C7-O47-C45
24	Y	601	CHL	C5-C6-C7-C8
25	G	612	CLA	C2A-CAA-CBA-CGA
25	g	612	CLA	C2A-CAA-CBA-CGA
29	6	2630	LHG	C14-C15-C16-C17
35	a	412	SQD	C9-C10-C11-C12
36	c	521	LMG	C30-C31-C32-C33
37	C	523	DGD	C6A-C7A-C8A-C9A
37	c	523	DGD	C6A-C7A-C8A-C9A
37	c	524	DGD	C4E-C5E-C6E-O5E
24	1	606	CHL	O1D-CGD-O2D-CED
25	7	604	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	g	614	CLA	O1D-CGD-O2D-CED
24	1	606	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	6	601	CHL	C16-C17-C18-C20
24	6	606	CHL	C16-C17-C18-C19
24	0	601	CHL	C16-C17-C18-C19
24	0	609	CHL	C16-C17-C18-C19
25	4	603	CLA	C16-C17-C18-C20
25	B	607	CLA	C16-C17-C18-C20
25	R	602	CLA	C11-C12-C13-C14
25	a	405	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
25	r	602	CLA	C11-C12-C13-C14
24	3	601	CHL	CBA-CGA-O2A-C1
29	Y	2630	LHG	C32-C33-C34-C35
29	0	2630	LHG	C14-C15-C16-C17
29	r	2630	LHG	C9-C10-C11-C12
35	A	412	SQD	C9-C10-C11-C12
36	s	2631	LMG	C39-C40-C41-C42
24	3	607	CHL	O1D-CGD-O2D-CED
24	3	609	CHL	O1D-CGD-O2D-CED
24	5	607	CHL	O1D-CGD-O2D-CED
25	C	511	CLA	O1D-CGD-O2D-CED
25	7	612	CLA	O1D-CGD-O2D-CED
35	D	413	SQD	O49-C7-O47-C45
35	d	413	SQD	O49-C7-O47-C45
37	C	524	DGD	O1B-C1B-O2G-C2G
37	c	524	DGD	O1B-C1B-O2G-C2G
24	6	607	CHL	C15-C16-C17-C18
37	C	524	DGD	C4E-C5E-C6E-O5E
24	4	605	CHL	CBD-CGD-O2D-CED
29	R	2630	LHG	C9-C10-C11-C12
24	Y	605	CHL	O1D-CGD-O2D-CED
24	y	605	CHL	O1D-CGD-O2D-CED
25	B	611	CLA	O1D-CGD-O2D-CED
25	N	604	CLA	O1D-CGD-O2D-CED
25	n	604	CLA	O1D-CGD-O2D-CED
24	N	607	CHL	O1A-CGA-O2A-C1
25	7	604	CLA	O1A-CGA-O2A-C1
29	y	2630	LHG	C32-C33-C34-C35
37	C	519	DGD	C5A-C6A-C7A-C8A
37	c	523	DGD	C7A-C8A-C9A-CAA
24	1	609	CHL	C15-C16-C17-C18
24	6	609	CHL	C15-C16-C17-C18
24	p	609	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	1	2630	LHG	O2-C2-C3-O3
29	2	2630	LHG	O2-C2-C3-O3
29	7	2630	LHG	O2-C2-C3-O3
29	q	2630	LHG	O2-C2-C3-O3
35	a	412	SQD	C24-C25-C26-C27
37	C	523	DGD	C7A-C8A-C9A-CAA
37	C	524	DGD	CCA-CDA-CEA-CFA
25	7	612	CLA	C3-C5-C6-C7
24	8	607	CHL	O1D-CGD-O2D-CED
36	A	413	LMG	C2-C1-O1-C7
36	a	413	LMG	C2-C1-O1-C7
25	C	501	CLA	CBA-CGA-O2A-C1
29	1	2630	LHG	C14-C15-C16-C17
29	d	409	LHG	C24-C25-C26-C27
35	A	412	SQD	C24-C25-C26-C27
35	B	623	SQD	C15-C16-C17-C18
35	b	623	SQD	C15-C16-C17-C18
37	c	524	DGD	CCA-CDA-CEA-CFA
24	7	601	CHL	C15-C16-C17-C18
24	n	608	CHL	O1A-CGA-O2A-C1
25	Y	613	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
25	y	613	CLA	O1A-CGA-O2A-C1
29	g	2630	LHG	O10-C23-O8-C6
24	5	601	CHL	C16-C17-C18-C19
24	5	607	CHL	C16-C17-C18-C19
24	6	609	CHL	C16-C17-C18-C19
24	8	601	CHL	C16-C17-C18-C19
24	8	605	CHL	C16-C17-C18-C20
24	q	609	CHL	C16-C17-C18-C19
25	2	603	CLA	C16-C17-C18-C19
25	6	604	CLA	C16-C17-C18-C20
25	B	614	CLA	C16-C17-C18-C19
25	Y	611	CLA	C16-C17-C18-C20
25	9	603	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
25	y	611	CLA	C16-C17-C18-C20
25	r	610	CLA	C16-C17-C18-C20
24	R	607	CHL	O1D-CGD-O2D-CED
24	8	609	CHL	O1D-CGD-O2D-CED
25	0	613	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	0	607	CHL	C4-C3-C5-C6
24	r	608	CHL	C4-C3-C5-C6
25	5	603	CLA	C4-C3-C5-C6
39	D	405	PL9	C15-C14-C16-C17
29	D	409	LHG	C24-C25-C26-C27
29	L	101	LHG	C9-C10-C11-C12
29	7	2630	LHG	C14-C15-C16-C17
29	9	2630	LHG	C18-C19-C20-C21
29	l	101	LHG	C9-C10-C11-C12
25	5	603	CLA	C2-C3-C5-C6
24	4	609	CHL	C6-C7-C8-C9
24	Y	607	CHL	C11-C10-C8-C9
24	Y	609	CHL	C11-C12-C13-C14
24	y	609	CHL	C11-C12-C13-C14
25	C	511	CLA	C6-C7-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C10-C8-C9
25	8	604	CLA	C14-C13-C15-C16
25	p	602	CLA	C6-C7-C8-C9
25	q	602	CLA	C14-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	r	610	CLA	C11-C10-C8-C9
25	r	613	CLA	C6-C7-C8-C9
24	5	601	CHL	O1D-CGD-O2D-CED
24	r	607	CHL	O1D-CGD-O2D-CED
25	3	610	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
29	L	101	LHG	C18-C19-C20-C21
29	l	101	LHG	C18-C19-C20-C21
24	0	607	CHL	C13-C15-C16-C17
24	7	601	CHL	C5-C6-C7-C8
24	n	605	CHL	C10-C11-C12-C13
25	C	504	CLA	C10-C11-C12-C13
25	7	612	CLA	C8-C10-C11-C12
25	c	504	CLA	C10-C11-C12-C13
24	1	608	CHL	C2A-CAA-CBA-CGA
24	S	601	CHL	C2A-CAA-CBA-CGA
24	s	601	CHL	C2A-CAA-CBA-CGA
25	5	602	CLA	C2A-CAA-CBA-CGA
25	5	614	CLA	C2A-CAA-CBA-CGA
25	R	601	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	0	610	CLA	C2A-CAA-CBA-CGA
24	Y	606	CHL	O1A-CGA-O2A-C1
24	y	606	CHL	O1A-CGA-O2A-C1
25	r	604	CLA	O1A-CGA-O2A-C1
29	2	2630	LHG	C27-C28-C29-C30
36	A	413	LMG	C11-C12-C13-C14
36	a	413	LMG	C11-C12-C13-C14
29	N	2630	LHG	O1-C1-C2-C3
29	n	2630	LHG	O1-C1-C2-C3
26	p	1621	LUT	C27-C28-C29-C30
24	8	601	CHL	C3-C5-C6-C7
24	p	607	CHL	C3-C5-C6-C7
25	n	604	CLA	C3-C5-C6-C7
24	3	601	CHL	C15-C16-C17-C18
24	Y	607	CHL	C15-C16-C17-C18
24	7	606	CHL	C8-C10-C11-C12
25	0	602	CLA	C5-C6-C7-C8
25	c	502	CLA	C8-C10-C11-C12
24	3	609	CHL	C2C-C3C-CAC-CBC
29	5	2630	LHG	C13-C14-C15-C16
37	C	518	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	C5A-C6A-C7A-C8A
25	C	512	CLA	O1D-CGD-O2D-CED
29	C	2630	LHG	C29-C30-C31-C32
29	S	2630	LHG	C12-C13-C14-C15
29	Y	2630	LHG	C34-C35-C36-C37
29	c	2630	LHG	C29-C30-C31-C32
29	s	2630	LHG	C12-C13-C14-C15
29	y	2630	LHG	C34-C35-C36-C37
37	c	518	DGD	C4A-C5A-C6A-C7A
37	c	518	DGD	CAB-CBB-CCB-CDB
24	N	601	CHL	C4B-C3B-CAB-CBB
24	S	601	CHL	C4B-C3B-CAB-CBB
24	Y	605	CHL	C4B-C3B-CAB-CBB
24	9	601	CHL	C4B-C3B-CAB-CBB
24	n	601	CHL	C4B-C3B-CAB-CBB
24	n	609	CHL	C4B-C3B-CAB-CBB
24	s	601	CHL	C4B-C3B-CAB-CBB
25	1	614	CLA	C4B-C3B-CAB-CBB
25	2	612	CLA	C4B-C3B-CAB-CBB
25	3	614	CLA	C4B-C3B-CAB-CBB
25	4	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	4	614	CLA	C4B-C3B-CAB-CBB
25	5	610	CLA	C4B-C3B-CAB-CBB
25	6	604	CLA	C4B-C3B-CAB-CBB
25	6	610	CLA	C4B-C3B-CAB-CBB
25	6	611	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	C4B-C3B-CAB-CBB
25	B	607	CLA	C4B-C3B-CAB-CBB
25	D	403	CLA	C4B-C3B-CAB-CBB
25	N	603	CLA	C4B-C3B-CAB-CBB
25	N	610	CLA	C4B-C3B-CAB-CBB
25	N	611	CLA	C4B-C3B-CAB-CBB
25	N	612	CLA	C4B-C3B-CAB-CBB
25	R	603	CLA	C4B-C3B-CAB-CBB
25	R	616	CLA	C4B-C3B-CAB-CBB
25	S	602	CLA	C4B-C3B-CAB-CBB
25	S	605	CLA	C4B-C3B-CAB-CBB
25	0	603	CLA	C4B-C3B-CAB-CBB
25	0	610	CLA	C4B-C3B-CAB-CBB
25	0	611	CLA	C4B-C3B-CAB-CBB
25	0	612	CLA	C4B-C3B-CAB-CBB
25	7	604	CLA	C4B-C3B-CAB-CBB
25	7	614	CLA	C4B-C3B-CAB-CBB
25	8	614	CLA	C4B-C3B-CAB-CBB
25	9	604	CLA	C4B-C3B-CAB-CBB
25	9	612	CLA	C4B-C3B-CAB-CBB
25	p	604	CLA	C4B-C3B-CAB-CBB
25	p	610	CLA	C4B-C3B-CAB-CBB
25	q	610	CLA	C4B-C3B-CAB-CBB
25	q	611	CLA	C4B-C3B-CAB-CBB
25	q	614	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	b	607	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	d	403	CLA	C4B-C3B-CAB-CBB
25	n	603	CLA	C4B-C3B-CAB-CBB
25	n	610	CLA	C4B-C3B-CAB-CBB
25	n	611	CLA	C4B-C3B-CAB-CBB
25	n	612	CLA	C4B-C3B-CAB-CBB
25	s	602	CLA	C4B-C3B-CAB-CBB
25	s	605	CLA	C4B-C3B-CAB-CBB
25	r	616	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	3	601	CHL	C16-C17-C18-C19
24	3	605	CHL	C16-C17-C18-C20
24	3	607	CHL	C16-C17-C18-C19
24	3	607	CHL	C16-C17-C18-C20
24	4	609	CHL	C16-C17-C18-C19
24	5	609	CHL	C16-C17-C18-C19
24	G	601	CHL	C16-C17-C18-C20
24	G	609	CHL	C16-C17-C18-C20
24	R	606	CHL	C16-C17-C18-C19
24	0	601	CHL	C16-C17-C18-C20
24	0	609	CHL	C16-C17-C18-C20
24	7	606	CHL	C16-C17-C18-C20
24	p	601	CHL	C16-C17-C18-C19
24	p	609	CHL	C16-C17-C18-C20
24	q	601	CHL	C16-C17-C18-C20
24	g	601	CHL	C16-C17-C18-C20
24	g	609	CHL	C16-C17-C18-C20
24	r	606	CHL	C16-C17-C18-C19
25	A	405	CLA	C16-C17-C18-C20
25	B	607	CLA	C16-C17-C18-C19
25	R	610	CLA	C16-C17-C18-C19
25	R	610	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19
25	r	610	CLA	C16-C17-C18-C19
36	A	413	LMG	O6-C1-O1-C7
36	a	413	LMG	O6-C1-O1-C7
24	4	609	CHL	C10-C11-C12-C13
24	9	609	CHL	C8-C10-C11-C12
25	q	602	CLA	C13-C15-C16-C17
36	S	2631	LMG	C39-C40-C41-C42
37	C	518	DGD	CAB-CBB-CCB-CDB
24	p	601	CHL	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
24	0	605	CHL	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
24	8	609	CHL	C2C-C3C-CAC-CBC
29	y	2630	LHG	C14-C15-C16-C17
35	b	621	SQD	C18-C19-C20-C21
37	C	519	DGD	C8B-C9B-CAB-CBB
36	D	411	LMG	C10-C11-C12-C13
36	d	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	5	601	CHL	C5-C6-C7-C8
24	5	605	CHL	C8-C10-C11-C12
24	5	609	CHL	C8-C10-C11-C12
25	5	604	CLA	C10-C11-C12-C13
25	B	607	CLA	C10-C11-C12-C13
25	C	501	CLA	C15-C16-C17-C18
25	C	508	CLA	C15-C16-C17-C18
25	R	613	CLA	C5-C6-C7-C8
25	b	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C10-C11-C12-C13
25	c	508	CLA	C15-C16-C17-C18
25	r	613	CLA	C5-C6-C7-C8
24	3	608	CHL	O1A-CGA-O2A-C1
29	G	2630	LHG	O10-C23-O8-C6
35	B	621	SQD	C18-C19-C20-C21
24	S	606	CHL	O1D-CGD-O2D-CED
25	8	613	CLA	O1D-CGD-O2D-CED
29	D	409	LHG	C13-C14-C15-C16
29	d	409	LHG	C13-C14-C15-C16
24	G	609	CHL	O1D-CGD-O2D-CED
24	g	609	CHL	O1D-CGD-O2D-CED
24	2	606	CHL	C3A-C2A-CAA-CBA
24	2	607	CHL	C3A-C2A-CAA-CBA
24	3	606	CHL	C3A-C2A-CAA-CBA
24	3	607	CHL	C3A-C2A-CAA-CBA
24	4	601	CHL	C3A-C2A-CAA-CBA
24	4	605	CHL	C3A-C2A-CAA-CBA
24	5	607	CHL	C3A-C2A-CAA-CBA
24	G	607	CHL	C3A-C2A-CAA-CBA
24	N	605	CHL	C3A-C2A-CAA-CBA
24	N	606	CHL	C3A-C2A-CAA-CBA
24	N	607	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	Y	606	CHL	C3A-C2A-CAA-CBA
24	0	607	CHL	C3A-C2A-CAA-CBA
24	8	607	CHL	C3A-C2A-CAA-CBA
24	9	606	CHL	C3A-C2A-CAA-CBA
24	9	607	CHL	C3A-C2A-CAA-CBA
24	p	607	CHL	C3A-C2A-CAA-CBA
24	q	607	CHL	C3A-C2A-CAA-CBA
24	q	609	CHL	C3A-C2A-CAA-CBA
24	g	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	n	605	CHL	C3A-C2A-CAA-CBA
24	n	606	CHL	C3A-C2A-CAA-CBA
24	n	607	CHL	C3A-C2A-CAA-CBA
24	y	606	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA
25	1	603	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	3	603	CLA	C3A-C2A-CAA-CBA
25	3	612	CLA	C3A-C2A-CAA-CBA
25	3	613	CLA	C3A-C2A-CAA-CBA
25	4	603	CLA	C3A-C2A-CAA-CBA
25	4	612	CLA	C3A-C2A-CAA-CBA
25	5	603	CLA	C3A-C2A-CAA-CBA
25	6	603	CLA	C3A-C2A-CAA-CBA
25	A	405	CLA	C3A-C2A-CAA-CBA
25	D	402	CLA	C3A-C2A-CAA-CBA
25	N	603	CLA	C3A-C2A-CAA-CBA
25	R	601	CLA	C3A-C2A-CAA-CBA
25	R	604	CLA	C3A-C2A-CAA-CBA
25	S	605	CLA	C3A-C2A-CAA-CBA
25	Y	603	CLA	C3A-C2A-CAA-CBA
25	0	603	CLA	C3A-C2A-CAA-CBA
25	7	603	CLA	C3A-C2A-CAA-CBA
25	8	603	CLA	C3A-C2A-CAA-CBA
25	8	612	CLA	C3A-C2A-CAA-CBA
25	8	613	CLA	C3A-C2A-CAA-CBA
25	9	603	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	C3A-C2A-CAA-CBA
25	q	603	CLA	C3A-C2A-CAA-CBA
25	q	612	CLA	C3A-C2A-CAA-CBA
25	a	405	CLA	C3A-C2A-CAA-CBA
25	d	402	CLA	C3A-C2A-CAA-CBA
25	n	603	CLA	C3A-C2A-CAA-CBA
25	s	605	CLA	C3A-C2A-CAA-CBA
25	y	603	CLA	C3A-C2A-CAA-CBA
25	r	604	CLA	C3A-C2A-CAA-CBA
33	A	409	PHO	C3A-C2A-CAA-CBA
33	a	409	PHO	C3A-C2A-CAA-CBA
24	3	605	CHL	C13-C15-C16-C17
24	5	609	CHL	C13-C15-C16-C17
25	B	607	CLA	C8-C10-C11-C12
29	p	2630	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	Y	2630	LHG	C7-C8-C9-C10
24	s	606	CHL	O1D-CGD-O2D-CED
36	h	102	LMG	C4-C5-C6-O5
24	5	608	CHL	O1A-CGA-O2A-C1
24	p	607	CHL	O1A-CGA-O2A-C1
24	3	605	CHL	C16-C17-C18-C19
24	5	609	CHL	C16-C17-C18-C20
24	6	601	CHL	C16-C17-C18-C19
24	G	601	CHL	C16-C17-C18-C19
24	g	601	CHL	C16-C17-C18-C19
24	g	609	CHL	C16-C17-C18-C19
25	4	603	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	R	602	CLA	C11-C12-C13-C15
25	Y	604	CLA	C16-C17-C18-C19
25	Y	604	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	y	604	CLA	C16-C17-C18-C19
25	y	604	CLA	C16-C17-C18-C20
25	r	602	CLA	C11-C12-C13-C15
29	Y	2630	LHG	C13-C14-C15-C16
36	A	413	LMG	C14-C15-C16-C17
36	a	413	LMG	C14-C15-C16-C17
37	C	519	DGD	CAB-CBB-CCB-CDB
24	2	609	CHL	O1D-CGD-O2D-CED
24	Y	609	CHL	O1D-CGD-O2D-CED
25	q	612	CLA	O1D-CGD-O2D-CED
29	6	2630	LHG	C4-C5-C6-O8
36	H	102	LMG	C7-C8-C9-O8
37	C	523	DGD	C1G-C2G-C3G-O3G
37	c	523	DGD	C1G-C2G-C3G-O3G
24	y	609	CHL	CBD-CGD-O2D-CED
24	8	605	CHL	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
24	8	601	CHL	C15-C16-C17-C18
24	6	607	CHL	C4-C3-C5-C6
25	2	603	CLA	C4-C3-C5-C6
25	6	611	CLA	C4-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	9	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
39	d	405	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
24	6	607	CHL	C2-C3-C5-C6
24	R	608	CHL	C2-C3-C5-C6
24	0	607	CHL	C2-C3-C5-C6
24	p	607	CHL	C2-C3-C5-C6
24	r	608	CHL	C2-C3-C5-C6
25	2	603	CLA	C2-C3-C5-C6
25	6	611	CLA	C2-C3-C5-C6
25	9	603	CLA	C2-C3-C5-C6
39	D	405	PL9	C13-C14-C16-C17
39	d	405	PL9	C13-C14-C16-C17
36	B	622	LMG	C11-C10-O7-C8
36	D	412	LMG	C11-C10-O7-C8
36	b	622	LMG	C11-C10-O7-C8
36	d	412	LMG	C11-C10-O7-C8
25	5	611	CLA	O1D-CGD-O2D-CED
24	9	609	CHL	C4C-C3C-CAC-CBC
24	p	606	CHL	C2A-CAA-CBA-CGA
24	q	607	CHL	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
29	5	2630	LHG	O1-C1-C2-O2
29	6	2630	LHG	O1-C1-C2-O2
29	C	2630	LHG	O1-C1-C2-O2
29	Y	2630	LHG	C9-C10-C11-C12
25	y	610	CLA	O1D-CGD-O2D-CED
24	8	608	CHL	O1A-CGA-O2A-C1
25	R	601	CLA	O1A-CGA-O2A-C1
29	s	2630	LHG	O10-C23-O8-C6
24	1	601	CHL	C16-C17-C18-C19
24	2	609	CHL	C16-C17-C18-C20
24	G	609	CHL	C16-C17-C18-C19
24	8	605	CHL	C16-C17-C18-C19
25	C	508	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
24	2	606	CHL	C2B-C3B-CAB-CBB
24	3	601	CHL	C2B-C3B-CAB-CBB
24	N	601	CHL	C2B-C3B-CAB-CBB
24	N	609	CHL	C2B-C3B-CAB-CBB
24	S	601	CHL	C2B-C3B-CAB-CBB
24	Y	605	CHL	C2B-C3B-CAB-CBB
24	9	601	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	9	606	CHL	C2B-C3B-CAB-CBB
24	n	601	CHL	C2B-C3B-CAB-CBB
24	n	609	CHL	C2B-C3B-CAB-CBB
24	s	601	CHL	C2B-C3B-CAB-CBB
24	y	605	CHL	C2B-C3B-CAB-CBB
25	1	614	CLA	C2B-C3B-CAB-CBB
25	3	614	CLA	C2B-C3B-CAB-CBB
25	4	610	CLA	C2B-C3B-CAB-CBB
25	4	611	CLA	C2B-C3B-CAB-CBB
25	4	614	CLA	C2B-C3B-CAB-CBB
25	5	603	CLA	C2B-C3B-CAB-CBB
25	5	610	CLA	C2B-C3B-CAB-CBB
25	6	604	CLA	C2B-C3B-CAB-CBB
25	6	610	CLA	C2B-C3B-CAB-CBB
25	6	611	CLA	C2B-C3B-CAB-CBB
25	B	602	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	C	501	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
25	C	506	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	D	403	CLA	C2B-C3B-CAB-CBB
25	G	603	CLA	C2B-C3B-CAB-CBB
25	N	603	CLA	C2B-C3B-CAB-CBB
25	N	610	CLA	C2B-C3B-CAB-CBB
25	N	611	CLA	C2B-C3B-CAB-CBB
25	N	612	CLA	C2B-C3B-CAB-CBB
25	R	603	CLA	C2B-C3B-CAB-CBB
25	R	616	CLA	C2B-C3B-CAB-CBB
25	S	609	CLA	C2B-C3B-CAB-CBB
25	S	610	CLA	C2B-C3B-CAB-CBB
25	0	603	CLA	C2B-C3B-CAB-CBB
25	0	610	CLA	C2B-C3B-CAB-CBB
25	0	611	CLA	C2B-C3B-CAB-CBB
25	0	613	CLA	C2B-C3B-CAB-CBB
25	7	604	CLA	C2B-C3B-CAB-CBB
25	7	614	CLA	C2B-C3B-CAB-CBB
25	8	614	CLA	C2B-C3B-CAB-CBB
25	9	604	CLA	C2B-C3B-CAB-CBB
25	p	603	CLA	C2B-C3B-CAB-CBB
25	p	604	CLA	C2B-C3B-CAB-CBB
25	p	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	p	611	CLA	C2B-C3B-CAB-CBB
25	p	612	CLA	C2B-C3B-CAB-CBB
25	q	604	CLA	C2B-C3B-CAB-CBB
25	q	610	CLA	C2B-C3B-CAB-CBB
25	q	611	CLA	C2B-C3B-CAB-CBB
25	q	614	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
25	c	502	CLA	C2B-C3B-CAB-CBB
25	c	506	CLA	C2B-C3B-CAB-CBB
25	c	512	CLA	C2B-C3B-CAB-CBB
25	d	403	CLA	C2B-C3B-CAB-CBB
25	n	603	CLA	C2B-C3B-CAB-CBB
25	n	610	CLA	C2B-C3B-CAB-CBB
25	n	611	CLA	C2B-C3B-CAB-CBB
25	n	612	CLA	C2B-C3B-CAB-CBB
25	s	605	CLA	C2B-C3B-CAB-CBB
25	s	609	CLA	C2B-C3B-CAB-CBB
25	s	610	CLA	C2B-C3B-CAB-CBB
25	r	603	CLA	C2B-C3B-CAB-CBB
25	r	616	CLA	C2B-C3B-CAB-CBB
29	9	2630	LHG	O2-C2-C3-O3
24	3	609	CHL	C8-C10-C11-C12
24	g	609	CHL	C5-C6-C7-C8
25	B	606	CLA	C10-C11-C12-C13
25	Y	611	CLA	C13-C15-C16-C17
25	8	610	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13
36	s	2631	LMG	C20-C21-C22-C23
25	c	502	CLA	C3-C5-C6-C7
35	a	412	SQD	C30-C31-C32-C33
24	1	609	CHL	O1A-CGA-O2A-C1
24	3	601	CHL	O1A-CGA-O2A-C1
24	R	606	CHL	O1A-CGA-O2A-C1
24	r	606	CHL	O1A-CGA-O2A-C1
25	6	614	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	O1A-CGA-O2A-C1
29	2	2630	LHG	O10-C23-O8-C6
29	S	2630	LHG	O10-C23-O8-C6
24	2	609	CHL	C8-C10-C11-C12
25	y	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	C	523	DGD	CEA-CFA-CGA-CHA
37	c	523	DGD	CEA-CFA-CGA-CHA
36	B	622	LMG	O9-C10-O7-C8
36	D	412	LMG	O9-C10-O7-C8
36	b	622	LMG	O9-C10-O7-C8
36	d	412	LMG	O9-C10-O7-C8
24	Y	607	CHL	C2-C1-O2A-CGA
24	y	607	CHL	C2-C1-O2A-CGA
29	D	409	LHG	C12-C13-C14-C15
29	q	2630	LHG	C28-C29-C30-C31
29	d	409	LHG	C12-C13-C14-C15
36	D	411	LMG	C31-C32-C33-C34
37	c	519	DGD	C6A-C7A-C8A-C9A
25	5	610	CLA	C8-C10-C11-C12
25	Y	611	CLA	C15-C16-C17-C18
25	7	604	CLA	C5-C6-C7-C8
25	y	602	CLA	C15-C16-C17-C18
25	y	611	CLA	C15-C16-C17-C18
29	q	2630	LHG	C9-C10-C11-C12
29	y	2630	LHG	C9-C10-C11-C12
37	C	519	DGD	C6A-C7A-C8A-C9A
24	5	607	CHL	C16-C17-C18-C20
24	0	606	CHL	C16-C17-C18-C19
25	6	604	CLA	C16-C17-C18-C19
37	C	519	DGD	C1B-C2B-C3B-C4B
37	c	519	DGD	C1B-C2B-C3B-C4B
24	3	601	CHL	C3-C5-C6-C7
26	1	1620	LUT	C1-C6-C7-C8
26	3	1620	LUT	C1-C6-C7-C8
26	3	1620	LUT	C5-C6-C7-C8
26	4	1621	LUT	C1-C6-C7-C8
26	4	1621	LUT	C5-C6-C7-C8
26	5	1620	LUT	C1-C6-C7-C8
26	5	1620	LUT	C5-C6-C7-C8
26	6	1620	LUT	C5-C6-C7-C8
26	G	1620	LUT	C1-C6-C7-C8
26	G	1620	LUT	C5-C6-C7-C8
26	N	1620	LUT	C5-C6-C7-C8
26	N	1621	LUT	C5-C6-C7-C8
26	0	1620	LUT	C1-C6-C7-C8
26	0	1620	LUT	C5-C6-C7-C8
26	8	1620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	8	1620	LUT	C5-C6-C7-C8
26	p	1620	LUT	C1-C6-C7-C8
26	p	1620	LUT	C5-C6-C7-C8
26	p	1621	LUT	C5-C6-C7-C8
26	q	1620	LUT	C5-C6-C7-C8
26	q	1621	LUT	C1-C6-C7-C8
26	q	1621	LUT	C5-C6-C7-C8
26	g	1620	LUT	C1-C6-C7-C8
26	g	1620	LUT	C5-C6-C7-C8
26	n	1620	LUT	C5-C6-C7-C8
26	n	1621	LUT	C5-C6-C7-C8
34	A	411	BCR	C23-C24-C25-C26
34	A	411	BCR	C23-C24-C25-C30
34	B	618	BCR	C1-C6-C7-C8
34	B	618	BCR	C5-C6-C7-C8
34	C	514	BCR	C1-C6-C7-C8
34	C	514	BCR	C5-C6-C7-C8
34	C	515	BCR	C5-C6-C7-C8
34	C	516	BCR	C23-C24-C25-C26
34	C	516	BCR	C23-C24-C25-C30
34	H	101	BCR	C23-C24-C25-C26
34	a	411	BCR	C23-C24-C25-C26
34	a	411	BCR	C23-C24-C25-C30
34	b	618	BCR	C1-C6-C7-C8
34	b	618	BCR	C5-C6-C7-C8
34	c	514	BCR	C1-C6-C7-C8
34	c	514	BCR	C5-C6-C7-C8
34	c	516	BCR	C23-C24-C25-C26
34	c	516	BCR	C23-C24-C25-C30
34	h	101	BCR	C23-C24-C25-C26
29	2	2630	LHG	C18-C19-C20-C21
36	d	411	LMG	C31-C32-C33-C34
24	p	601	CHL	CBA-CGA-O2A-C1
24	q	607	CHL	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
24	2	601	CHL	C8-C10-C11-C12
24	G	609	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	Y	607	CHL	C5-C6-C7-C8
24	7	609	CHL	C15-C16-C17-C18
24	p	605	CHL	C8-C10-C11-C12
25	4	613	CLA	C15-C16-C17-C18
25	B	602	CLA	C15-C16-C17-C18
25	C	507	CLA	C8-C10-C11-C12
25	D	402	CLA	C10-C11-C12-C13
25	Y	602	CLA	C15-C16-C17-C18
25	Y	612	CLA	C10-C11-C12-C13
25	7	610	CLA	C5-C6-C7-C8
25	b	602	CLA	C15-C16-C17-C18
25	y	612	CLA	C10-C11-C12-C13
29	1	2630	LHG	C24-C25-C26-C27
35	A	412	SQD	C26-C27-C28-C29
35	a	412	SQD	C26-C27-C28-C29
36	S	2631	LMG	C19-C20-C21-C22
36	S	2631	LMG	C20-C21-C22-C23
29	D	409	LHG	C7-C8-C9-C10
24	6	601	CHL	C10-C11-C12-C13
24	0	601	CHL	C10-C11-C12-C13
25	B	611	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
33	A	408	PHO	C15-C16-C17-C18
33	a	408	PHO	C15-C16-C17-C18
35	A	412	SQD	C30-C31-C32-C33
36	s	2631	LMG	C16-C17-C18-C19
25	4	613	CLA	C4-C3-C5-C6
25	5	604	CLA	C4-C3-C5-C6
25	7	612	CLA	C4-C3-C5-C6
24	S	601	CHL	O1D-CGD-O2D-CED
25	p	610	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	C11-C10-C8-C7
24	1	609	CHL	C11-C12-C13-C15
24	1	609	CHL	C12-C13-C15-C16
24	N	605	CHL	C6-C7-C8-C10
24	N	605	CHL	C11-C10-C8-C7
24	R	608	CHL	C6-C7-C8-C10
24	Y	601	CHL	C11-C10-C8-C7
24	Y	607	CHL	C11-C10-C8-C7
24	0	609	CHL	C2-C3-C5-C6
24	7	609	CHL	C11-C12-C13-C15
24	p	607	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	q	609	CHL	C2-C3-C5-C6
24	q	609	CHL	C11-C10-C8-C7
24	n	605	CHL	C6-C7-C8-C10
24	y	607	CHL	C11-C10-C8-C7
24	r	608	CHL	C6-C7-C8-C10
25	1	604	CLA	C12-C13-C15-C16
25	1	610	CLA	C11-C12-C13-C15
25	1	611	CLA	C2-C3-C5-C6
25	3	603	CLA	C11-C10-C8-C7
25	4	610	CLA	C11-C12-C13-C15
25	6	604	CLA	C11-C12-C13-C15
25	B	607	CLA	C11-C12-C13-C15
25	B	613	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	506	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	D	402	CLA	C11-C10-C8-C7
25	G	613	CLA	C12-C13-C15-C16
25	R	610	CLA	C11-C10-C8-C7
25	R	616	CLA	C6-C7-C8-C10
25	R	616	CLA	C11-C12-C13-C15
25	Y	604	CLA	C12-C13-C15-C16
25	0	604	CLA	C2-C3-C5-C6
25	7	604	CLA	C12-C13-C15-C16
25	7	610	CLA	C11-C12-C13-C15
25	7	612	CLA	C12-C13-C15-C16
25	8	603	CLA	C11-C10-C8-C7
25	8	604	CLA	C12-C13-C15-C16
25	p	602	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15
25	b	613	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	d	403	CLA	C11-C12-C13-C15
25	g	613	CLA	C12-C13-C15-C16
25	y	604	CLA	C12-C13-C15-C16
25	r	610	CLA	C11-C10-C8-C7
25	r	616	CLA	C6-C7-C8-C10
25	r	616	CLA	C11-C12-C13-C15
33	A	408	PHO	C2-C3-C5-C6
33	a	408	PHO	C2-C3-C5-C6
25	B	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	b	622	LMG	C12-C13-C14-C15
24	1	606	CHL	C8-C10-C11-C12
24	p	601	CHL	C10-C11-C12-C13
24	y	609	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
25	4	613	CLA	C13-C15-C16-C17
25	B	614	CLA	C5-C6-C7-C8
25	b	614	CLA	C5-C6-C7-C8
26	7	1621	LUT	C29-C30-C31-C32
24	5	605	CHL	C16-C17-C18-C19
29	d	409	LHG	C7-C8-C9-C10
35	B	621	SQD	C7-C8-C9-C10
35	b	621	SQD	C7-C8-C9-C10
36	s	2631	LMG	C28-C29-C30-C31
24	7	609	CHL	CBA-CGA-O2A-C1
24	8	601	CHL	CBA-CGA-O2A-C1
24	p	608	CHL	CBA-CGA-O2A-C1
25	1	613	CLA	CBA-CGA-O2A-C1
25	S	610	CLA	CBA-CGA-O2A-C1
25	0	614	CLA	CBA-CGA-O2A-C1
25	7	613	CLA	CBA-CGA-O2A-C1
25	8	613	CLA	CBA-CGA-O2A-C1
25	s	610	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
24	1	606	CHL	C2A-CAA-CBA-CGA
24	6	606	CHL	C2A-CAA-CBA-CGA
24	8	605	CHL	C2A-CAA-CBA-CGA
25	2	611	CLA	C2A-CAA-CBA-CGA
25	3	614	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	Y	610	CLA	C2A-CAA-CBA-CGA
25	8	614	CLA	C2A-CAA-CBA-CGA
25	9	611	CLA	C2A-CAA-CBA-CGA
25	b	604	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
25	s	602	CLA	C2A-CAA-CBA-CGA
24	R	607	CHL	C5-C6-C7-C8
29	C	2630	LHG	C33-C34-C35-C36
29	n	2630	LHG	C26-C27-C28-C29
35	B	621	SQD	C9-C10-C11-C12
36	a	413	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	4	601	CHL	O1D-CGD-O2D-CED
29	0	2630	LHG	C27-C28-C29-C30
35	b	621	SQD	C9-C10-C11-C12
36	A	413	LMG	C30-C31-C32-C33
24	S	607	CHL	O1D-CGD-O2D-CED
24	7	606	CHL	O1D-CGD-O2D-CED
24	s	607	CHL	O1D-CGD-O2D-CED
25	8	610	CLA	O1D-CGD-O2D-CED
24	7	607	CHL	C15-C16-C17-C18
24	8	609	CHL	C15-C16-C17-C18
24	y	607	CHL	C5-C6-C7-C8
25	4	610	CLA	C5-C6-C7-C8
29	C	2630	LHG	C11-C10-C9-C8
29	N	2630	LHG	C11-C10-C9-C8
36	B	622	LMG	C12-C13-C14-C15
24	q	607	CHL	O1A-CGA-O2A-C1
25	1	603	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
24	N	605	CHL	CBD-CGD-O2D-CED
25	A	407	CLA	CBD-CGD-O2D-CED
25	7	611	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBA-CGA-O2A-C1
24	Y	606	CHL	C16-C17-C18-C20
24	0	607	CHL	C16-C17-C18-C20
24	p	605	CHL	C16-C17-C18-C19
24	y	606	CHL	C16-C17-C18-C20
25	Y	611	CLA	C16-C17-C18-C19
25	q	603	CLA	C16-C17-C18-C20
25	y	611	CLA	C16-C17-C18-C19
24	3	607	CHL	C13-C15-C16-C17
25	3	610	CLA	C10-C11-C12-C13
25	C	501	CLA	O1D-CGD-O2D-CED
29	d	409	LHG	C14-C15-C16-C17
29	C	2630	LHG	C8-C7-O7-C5
29	c	2630	LHG	C8-C7-O7-C5
35	A	412	SQD	C8-C7-O47-C45
35	a	412	SQD	C8-C7-O47-C45
29	C	2630	LHG	C32-C33-C34-C35
29	y	2630	LHG	C26-C27-C28-C29
25	B	614	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
24	8	601	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	9	609	CHL	CBD-CGD-O2D-CED
29	D	409	LHG	C14-C15-C16-C17
36	B	622	LMG	C10-C11-C12-C13
37	c	519	DGD	CAB-CBB-CCB-CDB
25	b	602	CLA	C5-C6-C7-C8
37	C	519	DGD	O1G-C1G-C2G-O2G
37	C	524	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	O1G-C1G-C2G-O2G
37	c	524	DGD	O1G-C1G-C2G-O2G
36	S	2631	LMG	O6-C5-C6-O5
36	s	2631	LMG	O6-C5-C6-O5
36	D	411	LMG	C17-C18-C19-C20
36	d	411	LMG	C17-C18-C19-C20
37	c	519	DGD	C8B-C9B-CAB-CBB
25	G	610	CLA	CBD-CGD-O2D-CED
25	g	610	CLA	CBD-CGD-O2D-CED
24	s	601	CHL	O1D-CGD-O2D-CED
24	q	609	CHL	C16-C17-C18-C20
25	1	610	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
29	0	2630	LHG	C32-C33-C34-C35
24	G	601	CHL	C10-C11-C12-C13
24	N	601	CHL	C10-C11-C12-C13
24	R	606	CHL	C13-C15-C16-C17
24	n	601	CHL	C10-C11-C12-C13
25	q	603	CLA	C15-C16-C17-C18
24	p	607	CHL	C4-C3-C5-C6
24	q	609	CHL	C4-C3-C5-C6
25	2	602	CLA	C4-C3-C5-C6
25	0	604	CLA	C4-C3-C5-C6
25	7	613	CLA	C4-C3-C5-C6
33	A	408	PHO	C4-C3-C5-C6
33	a	408	PHO	C4-C3-C5-C6
39	D	405	PL9	C30-C29-C31-C32
39	d	405	PL9	C30-C29-C31-C32
25	4	613	CLA	C2-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
37	C	523	DGD	CBA-CCA-CDA-CEA
37	c	523	DGD	CBA-CCA-CDA-CEA
24	1	607	CHL	C11-C10-C8-C9
24	1	609	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	2	601	CHL	C6-C7-C8-C9
24	3	609	CHL	C11-C12-C13-C14
24	6	607	CHL	C11-C10-C8-C9
24	G	601	CHL	C6-C7-C8-C9
24	N	607	CHL	C14-C13-C15-C16
24	Y	601	CHL	C11-C10-C8-C9
24	7	607	CHL	C11-C10-C8-C9
24	7	609	CHL	C11-C12-C13-C14
24	8	609	CHL	C11-C12-C13-C14
24	g	601	CHL	C6-C7-C8-C9
24	n	607	CHL	C14-C13-C15-C16
24	y	601	CHL	C11-C10-C8-C9
24	y	607	CHL	C11-C10-C8-C9
25	1	604	CLA	C14-C13-C15-C16
25	1	610	CLA	C11-C12-C13-C14
25	1	612	CLA	C14-C13-C15-C16
25	3	603	CLA	C11-C10-C8-C9
25	4	610	CLA	C11-C12-C13-C14
25	6	604	CLA	C11-C10-C8-C9
25	6	604	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	D	402	CLA	C11-C10-C8-C9
25	G	613	CLA	C14-C13-C15-C16
25	R	616	CLA	C6-C7-C8-C9
25	R	616	CLA	C11-C12-C13-C14
25	Y	604	CLA	C14-C13-C15-C16
25	Y	610	CLA	C11-C12-C13-C14
25	0	604	CLA	C11-C10-C8-C9
25	7	604	CLA	C14-C13-C15-C16
25	7	610	CLA	C11-C12-C13-C14
25	8	603	CLA	C11-C10-C8-C9
25	q	613	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9
25	d	402	CLA	C11-C10-C8-C9
25	g	613	CLA	C14-C13-C15-C16
25	y	604	CLA	C14-C13-C15-C16
25	r	616	CLA	C6-C7-C8-C9
25	r	616	CLA	C11-C12-C13-C14
25	Y	610	CLA	O1D-CGD-O2D-CED
25	g	611	CLA	O1D-CGD-O2D-CED
25	1	611	CLA	CBD-CGD-O2D-CED
29	6	2630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
36	h	102	LMG	C32-C33-C34-C35
24	3	605	CHL	C2A-CAA-CBA-CGA
24	3	608	CHL	C2A-CAA-CBA-CGA
24	R	606	CHL	C2A-CAA-CBA-CGA
24	7	606	CHL	C2A-CAA-CBA-CGA
24	8	608	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
25	B	604	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
25	N	613	CLA	C2A-CAA-CBA-CGA
25	Y	602	CLA	C2A-CAA-CBA-CGA
25	Y	603	CLA	C2A-CAA-CBA-CGA
25	p	602	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
25	y	602	CLA	C2A-CAA-CBA-CGA
36	H	102	LMG	C32-C33-C34-C35
24	3	609	CHL	CBA-CGA-O2A-C1
24	N	605	CHL	C10-C11-C12-C13
24	p	601	CHL	C5-C6-C7-C8
25	2	610	CLA	C10-C11-C12-C13
25	3	604	CLA	C13-C15-C16-C17
25	B	602	CLA	C5-C6-C7-C8
26	3	1620	LUT	C27-C28-C29-C30
27	0	1622	XAT	C31-C32-C33-C34
27	7	1622	XAT	C31-C32-C33-C34
24	8	601	CHL	O1A-CGA-O2A-C1
24	p	601	CHL	O1A-CGA-O2A-C1
25	B	602	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
24	1	609	CHL	C1A-C2A-CAA-CBA
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	606	CHL	C1A-C2A-CAA-CBA
24	2	607	CHL	C1A-C2A-CAA-CBA
24	2	608	CHL	C1A-C2A-CAA-CBA
24	3	607	CHL	C1A-C2A-CAA-CBA
24	G	605	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	609	CHL	C1A-C2A-CAA-CBA
24	N	605	CHL	C1A-C2A-CAA-CBA
24	N	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	N	607	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1A-C2A-CAA-CBA
24	Y	609	CHL	C1A-C2A-CAA-CBA
24	7	608	CHL	C1A-C2A-CAA-CBA
24	8	607	CHL	C1A-C2A-CAA-CBA
24	9	601	CHL	C1A-C2A-CAA-CBA
24	9	606	CHL	C1A-C2A-CAA-CBA
24	9	607	CHL	C1A-C2A-CAA-CBA
24	9	608	CHL	C1A-C2A-CAA-CBA
24	q	607	CHL	C1A-C2A-CAA-CBA
24	q	609	CHL	C1A-C2A-CAA-CBA
24	g	605	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	609	CHL	C1A-C2A-CAA-CBA
24	n	605	CHL	C1A-C2A-CAA-CBA
24	n	606	CHL	C1A-C2A-CAA-CBA
24	n	607	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1A-C2A-CAA-CBA
24	y	609	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	C1A-C2A-CAA-CBA
25	1	603	CLA	C1A-C2A-CAA-CBA
25	1	604	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	614	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	C1A-C2A-CAA-CBA
25	3	603	CLA	C1A-C2A-CAA-CBA
25	3	604	CLA	C1A-C2A-CAA-CBA
25	3	611	CLA	C1A-C2A-CAA-CBA
25	3	614	CLA	C1A-C2A-CAA-CBA
25	4	603	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	C1A-C2A-CAA-CBA
25	5	603	CLA	C1A-C2A-CAA-CBA
25	5	604	CLA	C1A-C2A-CAA-CBA
25	5	611	CLA	C1A-C2A-CAA-CBA
25	5	614	CLA	C1A-C2A-CAA-CBA
25	6	603	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	C1A-C2A-CAA-CBA
25	A	405	CLA	C1A-C2A-CAA-CBA
25	A	406	CLA	C1A-C2A-CAA-CBA
25	A	407	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	511	CLA	C1A-C2A-CAA-CBA
25	D	402	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	N	614	CLA	C1A-C2A-CAA-CBA
25	R	601	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	S	610	CLA	C1A-C2A-CAA-CBA
25	S	611	CLA	C1A-C2A-CAA-CBA
25	Y	603	CLA	C1A-C2A-CAA-CBA
25	Y	604	CLA	C1A-C2A-CAA-CBA
25	Y	610	CLA	C1A-C2A-CAA-CBA
25	Y	614	CLA	C1A-C2A-CAA-CBA
25	0	603	CLA	C1A-C2A-CAA-CBA
25	0	604	CLA	C1A-C2A-CAA-CBA
25	0	610	CLA	C1A-C2A-CAA-CBA
25	7	603	CLA	C1A-C2A-CAA-CBA
25	7	610	CLA	C1A-C2A-CAA-CBA
25	7	614	CLA	C1A-C2A-CAA-CBA
25	8	603	CLA	C1A-C2A-CAA-CBA
25	8	604	CLA	C1A-C2A-CAA-CBA
25	8	611	CLA	C1A-C2A-CAA-CBA
25	8	614	CLA	C1A-C2A-CAA-CBA
25	9	603	CLA	C1A-C2A-CAA-CBA
25	9	610	CLA	C1A-C2A-CAA-CBA
25	9	614	CLA	C1A-C2A-CAA-CBA
25	p	603	CLA	C1A-C2A-CAA-CBA
25	p	604	CLA	C1A-C2A-CAA-CBA
25	p	610	CLA	C1A-C2A-CAA-CBA
25	p	611	CLA	C1A-C2A-CAA-CBA
25	p	614	CLA	C1A-C2A-CAA-CBA
25	q	603	CLA	C1A-C2A-CAA-CBA
25	q	604	CLA	C1A-C2A-CAA-CBA
25	q	610	CLA	C1A-C2A-CAA-CBA
25	q	614	CLA	C1A-C2A-CAA-CBA
25	a	405	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	a	407	CLA	C1A-C2A-CAA-CBA
25	b	602	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	d	402	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	n	611	CLA	C1A-C2A-CAA-CBA
25	n	614	CLA	C1A-C2A-CAA-CBA
25	s	604	CLA	C1A-C2A-CAA-CBA
25	s	610	CLA	C1A-C2A-CAA-CBA
25	s	611	CLA	C1A-C2A-CAA-CBA
25	y	603	CLA	C1A-C2A-CAA-CBA
25	y	604	CLA	C1A-C2A-CAA-CBA
25	y	610	CLA	C1A-C2A-CAA-CBA
25	y	614	CLA	C1A-C2A-CAA-CBA
25	r	601	CLA	C1A-C2A-CAA-CBA
24	2	609	CHL	C16-C17-C18-C19
24	4	609	CHL	C16-C17-C18-C20
24	5	601	CHL	C16-C17-C18-C20
24	6	607	CHL	C16-C17-C18-C19
24	Y	606	CHL	C16-C17-C18-C19
24	0	606	CHL	C16-C17-C18-C20
24	0	607	CHL	C16-C17-C18-C19
24	p	601	CHL	C16-C17-C18-C20
24	q	601	CHL	C16-C17-C18-C19
24	y	606	CHL	C16-C17-C18-C19
25	2	603	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C19
25	C	508	CLA	C16-C17-C18-C20
25	9	603	CLA	C16-C17-C18-C20
25	q	603	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
29	q	2630	LHG	C27-C28-C29-C30
26	1	1621	LUT	C29-C30-C31-C32
25	G	611	CLA	O1D-CGD-O2D-CED
24	1	601	CHL	C8-C10-C11-C12
24	g	601	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C13-C15-C16-C17
25	6	602	CLA	C10-C11-C12-C13
29	6	2630	LHG	C4-O6-P-O3
29	D	408	LHG	C3-O3-P-O6
29	d	409	LHG	C3-O3-P-O6
29	l	101	LHG	C3-O3-P-O6
29	c	2630	LHG	C33-C34-C35-C36
35	D	413	SQD	C11-C10-C9-C8
24	0	606	CHL	C3-C5-C6-C7
29	Y	2630	LHG	C16-C17-C18-C19
35	d	413	SQD	C11-C10-C9-C8
24	Y	609	CHL	C5-C6-C7-C8
25	1	603	CLA	C8-C10-C11-C12
25	5	602	CLA	C8-C10-C11-C12
25	R	610	CLA	C13-C15-C16-C17
25	7	603	CLA	C8-C10-C11-C12
29	4	2630	LHG	O6-C4-C5-C6
24	n	609	CHL	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED
36	b	622	LMG	C10-C11-C12-C13
24	9	601	CHL	C13-C15-C16-C17
25	1	612	CLA	C8-C10-C11-C12
25	r	610	CLA	C13-C15-C16-C17
24	7	606	CHL	C16-C17-C18-C19
24	p	609	CHL	C16-C17-C18-C19
25	A	405	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C20
29	3	2630	LHG	C18-C19-C20-C21
37	C	524	DGD	C6A-C7A-C8A-C9A
24	4	601	CHL	C5-C6-C7-C8
24	G	609	CHL	C13-C15-C16-C17
29	9	2630	LHG	C27-C28-C29-C30
24	5	607	CHL	CBA-CGA-O2A-C1
24	q	601	CHL	CBA-CGA-O2A-C1
29	c	2630	LHG	O9-C7-O7-C5
24	3	607	CHL	C4-C3-C5-C6
24	4	609	CHL	C4-C3-C5-C6
24	0	609	CHL	C4-C3-C5-C6
25	1	611	CLA	C4-C3-C5-C6
25	1	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	1	613	CLA	C4-C3-C5-C6
25	5	604	CLA	C2-C3-C5-C6
25	7	612	CLA	C2-C3-C5-C6
29	2	2630	LHG	C9-C10-C11-C12
29	9	2630	LHG	C13-C14-C15-C16
29	d	409	LHG	C34-C35-C36-C37
29	s	2630	LHG	C25-C26-C27-C28
35	B	623	SQD	C16-C17-C18-C19
37	C	519	DGD	CAA-CBA-CCA-CDA
37	c	524	DGD	C6A-C7A-C8A-C9A
25	c	501	CLA	O1D-CGD-O2D-CED
29	S	2630	LHG	C25-C26-C27-C28
24	p	608	CHL	O1A-CGA-O2A-C1
25	0	614	CLA	O1A-CGA-O2A-C1
29	4	2630	LHG	O2-C2-C3-O3
24	Y	607	CHL	C10-C11-C12-C13
25	6	611	CLA	C2A-CAA-CBA-CGA
24	6	606	CHL	C16-C17-C18-C20
24	9	609	CHL	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	D	403	CLA	C16-C17-C18-C20
25	7	610	CLA	C16-C17-C18-C19
24	Y	601	CHL	C3-C5-C6-C7
29	1	2630	LHG	C4-C5-C6-O8
29	2	2630	LHG	C11-C12-C13-C14
29	G	2630	LHG	C17-C18-C19-C20
29	N	2630	LHG	C4-C5-C6-O8
29	7	2630	LHG	C4-C5-C6-O8
29	n	2630	LHG	C4-C5-C6-O8
29	y	2630	LHG	C4-C5-C6-O8
29	y	2630	LHG	C11-C10-C9-C8
36	S	2631	LMG	C7-C8-C9-O8
36	h	102	LMG	C7-C8-C9-O8
36	s	2631	LMG	C7-C8-C9-O8
37	C	524	DGD	O1G-C1G-C2G-C3G
37	c	524	DGD	O1G-C1G-C2G-C3G
24	g	609	CHL	C13-C15-C16-C17
25	N	602	CLA	C5-C6-C7-C8
35	A	412	SQD	C11-C12-C13-C14
24	7	609	CHL	O1A-CGA-O2A-C1
25	S	610	CLA	O1A-CGA-O2A-C1
25	s	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	r	601	CLA	O1A-CGA-O2A-C1
24	N	601	CHL	C5-C6-C7-C8
24	N	607	CHL	C15-C16-C17-C18
25	D	403	CLA	C8-C10-C11-C12
29	9	2630	LHG	C9-C10-C11-C12
35	a	412	SQD	C11-C12-C13-C14
37	C	520	DGD	C9B-CAB-CBB-CCB
37	c	520	DGD	C9B-CAB-CBB-CCB
36	D	412	LMG	O6-C5-C6-O5
36	d	412	LMG	O6-C5-C6-O5
24	q	601	CHL	O1A-CGA-O2A-C1
25	8	613	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	C16-C17-C18-C20
24	N	609	CHL	O1D-CGD-O2D-CED
29	C	2630	LHG	C10-C11-C12-C13
29	0	2630	LHG	C24-C25-C26-C27
29	N	2630	LHG	O1-C1-C2-O2
29	p	2630	LHG	O1-C1-C2-O2
29	n	2630	LHG	O1-C1-C2-O2
29	s	2630	LHG	O1-C1-C2-O2
25	1	613	CLA	O1A-CGA-O2A-C1
29	8	2630	LHG	C18-C19-C20-C21
29	9	2630	LHG	C11-C12-C13-C14
24	N	605	CHL	O1D-CGD-O2D-CED
24	n	601	CHL	C5-C6-C7-C8
24	n	607	CHL	C15-C16-C17-C18
25	c	513	CLA	C15-C16-C17-C18
25	d	403	CLA	C8-C10-C11-C12
36	D	411	LMG	O6-C5-C6-O5
36	d	411	LMG	O6-C5-C6-O5
24	6	609	CHL	C4-C3-C5-C6
25	3	603	CLA	C4-C3-C5-C6
25	6	604	CLA	C4-C3-C5-C6
29	p	2630	LHG	C15-C16-C17-C18
37	C	523	DGD	CAA-CBA-CCA-CDA
37	c	523	DGD	CAA-CBA-CCA-CDA
25	6	604	CLA	C2-C3-C5-C6
25	7	613	CLA	C2-C3-C5-C6
24	1	606	CHL	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	0	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C20
24	5	601	CHL	CBA-CGA-O2A-C1
25	2	613	CLA	CBA-CGA-O2A-C1
25	7	603	CLA	CBA-CGA-O2A-C1
25	9	613	CLA	CBA-CGA-O2A-C1
29	D	410	LHG	C24-C23-O8-C6
29	d	410	LHG	C24-C23-O8-C6
29	q	2630	LHG	C33-C34-C35-C36
25	g	604	CLA	CBD-CGD-O2D-CED
24	2	601	CHL	C13-C15-C16-C17
24	5	601	CHL	C15-C16-C17-C18
25	0	602	CLA	C10-C11-C12-C13
29	D	410	LHG	C34-C35-C36-C37
24	8	606	CHL	O1D-CGD-O2D-CED
25	6	602	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	C2A-CAA-CBA-CGA
24	6	607	CHL	C13-C15-C16-C17
25	b	613	CLA	C13-C15-C16-C17
25	C	513	CLA	C2-C1-O2A-CGA
25	6	614	CLA	C6-C7-C8-C9
29	R	2630	LHG	C24-C25-C26-C27
29	d	410	LHG	C34-C35-C36-C37
25	0	614	CLA	C6-C7-C8-C9
25	9	602	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
25	n	602	CLA	C5-C6-C7-C8
29	y	2630	LHG	C13-C14-C15-C16
24	1	606	CHL	CBA-CGA-O2A-C1
24	8	609	CHL	CBA-CGA-O2A-C1
24	q	605	CHL	CBA-CGA-O2A-C1
25	1	612	CLA	CBA-CGA-O2A-C1
29	5	2630	LHG	C24-C23-O8-C6
29	5	2630	LHG	O6-C4-C5-O7
24	6	607	CHL	C16-C17-C18-C20
24	9	609	CHL	C16-C17-C18-C19
24	p	605	CHL	C16-C17-C18-C20
29	y	2630	LHG	C27-C28-C29-C30
25	B	612	CLA	C10-C11-C12-C13
29	3	2630	LHG	O2-C2-C3-O3
24	4	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	R	616	CLA	O1D-CGD-O2D-CED
24	3	609	CHL	O1A-CGA-O2A-C1
24	5	607	CHL	O1A-CGA-O2A-C1
25	3	613	CLA	O1A-CGA-O2A-C1
25	7	613	CLA	O1A-CGA-O2A-C1
29	r	2630	LHG	C24-C25-C26-C27
25	B	607	CLA	C15-C16-C17-C18
25	B	609	CLA	C10-C11-C12-C13
25	r	616	CLA	O1D-CGD-O2D-CED
35	B	621	SQD	C33-C34-C35-C36
35	b	621	SQD	C33-C34-C35-C36
24	q	607	CHL	CAA-CBA-CGA-O2A
29	6	2630	LHG	O7-C5-C6-O8
29	Y	2630	LHG	O7-C5-C6-O8
29	y	2630	LHG	O7-C5-C6-O8
36	H	102	LMG	O7-C8-C9-O8
36	h	102	LMG	O7-C8-C9-O8
25	C	507	CLA	O1D-CGD-O2D-CED
29	N	2630	LHG	C26-C27-C28-C29
29	C	2630	LHG	O9-C7-O7-C5
24	5	609	CHL	C15-C16-C17-C18
24	0	606	CHL	C13-C15-C16-C17
25	Y	602	CLA	C8-C10-C11-C12
25	b	607	CLA	C15-C16-C17-C18
25	y	602	CLA	C8-C10-C11-C12
33	A	409	PHO	CHA-CBD-CGD-O1D
33	A	409	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O1D
33	a	409	PHO	CHA-CBD-CGD-O2D
29	D	409	LHG	C34-C35-C36-C37
25	7	603	CLA	C4-C3-C5-C6
25	p	603	CLA	C4-C3-C5-C6
39	d	405	PL9	C12-C13-C14-C15
24	2	609	CHL	C4C-C3C-CAC-CBC
36	c	521	LMG	C29-C30-C31-C32
37	C	523	DGD	C8A-C9A-CAA-CBA
37	c	523	DGD	C8A-C9A-CAA-CBA
25	b	609	CLA	C10-C11-C12-C13
24	1	601	CHL	C6-C7-C8-C10
24	1	607	CHL	C11-C12-C13-C15
24	3	601	CHL	C12-C13-C15-C16
24	3	609	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	4	609	CHL	C2-C3-C5-C6
24	5	605	CHL	C11-C12-C13-C15
24	5	605	CHL	C12-C13-C15-C16
24	6	609	CHL	C2-C3-C5-C6
24	N	601	CHL	C11-C10-C8-C7
24	N	609	CHL	C11-C10-C8-C7
24	0	607	CHL	C11-C10-C8-C7
24	0	607	CHL	C12-C13-C15-C16
24	0	609	CHL	C12-C13-C15-C16
24	8	601	CHL	C6-C7-C8-C10
24	8	601	CHL	C11-C12-C13-C15
24	8	601	CHL	C12-C13-C15-C16
24	8	607	CHL	C6-C7-C8-C10
24	8	609	CHL	C11-C12-C13-C15
24	9	601	CHL	C6-C7-C8-C10
24	p	609	CHL	C11-C12-C13-C15
24	p	609	CHL	C12-C13-C15-C16
24	q	601	CHL	C12-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C7
24	n	605	CHL	C11-C10-C8-C7
24	n	609	CHL	C11-C12-C13-C15
24	y	601	CHL	C11-C10-C8-C7
24	y	607	CHL	C11-C12-C13-C15
25	1	603	CLA	C12-C13-C15-C16
25	1	611	CLA	C11-C12-C13-C15
25	1	612	CLA	C11-C10-C8-C7
25	1	612	CLA	C12-C13-C15-C16
25	1	613	CLA	C6-C7-C8-C10
25	1	613	CLA	C12-C13-C15-C16
25	4	603	CLA	C12-C13-C15-C16
25	5	603	CLA	C11-C10-C8-C7
25	5	613	CLA	C6-C7-C8-C10
25	6	602	CLA	C6-C7-C8-C10
25	6	604	CLA	C11-C10-C8-C7
25	6	612	CLA	C12-C13-C15-C16
25	6	613	CLA	C6-C7-C8-C10
25	6	613	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	602	CLA	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	C	512	CLA	C12-C13-C15-C16
25	N	613	CLA	C12-C13-C15-C16
25	R	602	CLA	C6-C7-C8-C10
25	0	602	CLA	C6-C7-C8-C10
25	0	604	CLA	C11-C10-C8-C7
25	0	612	CLA	C12-C13-C15-C16
25	0	613	CLA	C11-C10-C8-C7
25	7	603	CLA	C12-C13-C15-C16
25	7	613	CLA	C12-C13-C15-C16
25	8	602	CLA	C11-C12-C13-C15
25	p	610	CLA	C11-C10-C8-C7
25	p	613	CLA	C12-C13-C15-C16
25	q	602	CLA	C6-C7-C8-C10
25	q	613	CLA	C6-C7-C8-C10
25	q	613	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C12-C13-C15
25	d	402	CLA	C11-C10-C8-C7
25	n	613	CLA	C12-C13-C15-C16
25	r	602	CLA	C6-C7-C8-C10
29	c	2630	LHG	C32-C33-C34-C35
24	1	607	CHL	C11-C12-C13-C14
24	5	605	CHL	C11-C12-C13-C14
24	Y	607	CHL	C11-C12-C13-C14
24	0	607	CHL	C11-C10-C8-C9
24	0	609	CHL	C11-C12-C13-C14
24	8	609	CHL	C11-C10-C8-C9
24	n	605	CHL	C14-C13-C15-C16
24	y	607	CHL	C11-C12-C13-C14
25	1	602	CLA	C11-C12-C13-C14
25	1	603	CLA	C11-C12-C13-C14
25	1	612	CLA	C11-C10-C8-C9
25	1	613	CLA	C14-C13-C15-C16
25	2	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	3	602	CLA	C6-C7-C8-C9
25	3	602	CLA	C11-C12-C13-C14
25	4	603	CLA	C14-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C9
25	5	604	CLA	C6-C7-C8-C9
25	5	613	CLA	C6-C7-C8-C9
25	6	603	CLA	C14-C13-C15-C16
25	6	613	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	603	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C10-C8-C9
25	B	615	CLA	C6-C7-C8-C9
25	B	617	CLA	C6-C7-C8-C9
25	C	502	CLA	C11-C10-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C10-C8-C9
25	N	613	CLA	C11-C10-C8-C9
25	N	613	CLA	C14-C13-C15-C16
25	R	602	CLA	C6-C7-C8-C9
25	Y	602	CLA	C6-C7-C8-C9
25	Y	602	CLA	C11-C12-C13-C14
25	Y	603	CLA	C14-C13-C15-C16
25	Y	612	CLA	C11-C10-C8-C9
25	0	602	CLA	C6-C7-C8-C9
25	0	611	CLA	C14-C13-C15-C16
25	7	602	CLA	C11-C12-C13-C14
25	7	610	CLA	C6-C7-C8-C9
25	7	611	CLA	C11-C12-C13-C14
25	7	612	CLA	C14-C13-C15-C16
25	7	613	CLA	C14-C13-C15-C16
25	8	602	CLA	C6-C7-C8-C9
25	8	602	CLA	C11-C12-C13-C14
25	9	603	CLA	C14-C13-C15-C16
25	p	604	CLA	C6-C7-C8-C9
25	p	613	CLA	C6-C7-C8-C9
25	q	602	CLA	C6-C7-C8-C9
25	q	613	CLA	C6-C7-C8-C9
25	q	613	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	b	603	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C11-C10-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	b	617	CLA	C6-C7-C8-C9
25	c	502	CLA	C11-C10-C8-C9
25	c	507	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	n	613	CLA	C11-C10-C8-C9
25	n	613	CLA	C14-C13-C15-C16
25	y	602	CLA	C6-C7-C8-C9
25	y	602	CLA	C11-C12-C13-C14
25	y	610	CLA	C11-C12-C13-C14
25	y	612	CLA	C11-C10-C8-C9
25	r	602	CLA	C6-C7-C8-C9
24	7	606	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	C15-C16-C17-C18
25	7	613	CLA	C5-C6-C7-C8
25	q	610	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	7	602	CLA	C2A-CAA-CBA-CGA
25	y	610	CLA	C2A-CAA-CBA-CGA
29	S	2630	LHG	C11-C10-C9-C8
24	5	601	CHL	O1A-CGA-O2A-C1
26	3	1620	LUT	C31-C32-C33-C40
34	D	404	BCR	C37-C22-C23-C24
34	d	404	BCR	C37-C22-C23-C24
24	5	605	CHL	C16-C17-C18-C20
25	B	616	CLA	C16-C17-C18-C20
25	b	616	CLA	C16-C17-C18-C20
26	4	1621	LUT	C11-C12-C13-C14
27	1	1622	XAT	C31-C32-C33-C34
34	D	404	BCR	C21-C22-C23-C24
34	b	620	BCR	C7-C8-C9-C10
34	d	404	BCR	C21-C22-C23-C24
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	518	DGD	O6D-C5D-C6D-O5D
24	p	607	CHL	C13-C15-C16-C17
25	4	603	CLA	C13-C15-C16-C17
25	B	608	CLA	C15-C16-C17-C18
29	Y	2630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
29	g	2630	LHG	C17-C18-C19-C20
29	s	2630	LHG	C11-C10-C9-C8
36	C	521	LMG	C29-C30-C31-C32
25	4	613	CLA	CBA-CGA-O2A-C1
24	6	606	CHL	C13-C15-C16-C17
25	6	604	CLA	C15-C16-C17-C18
25	b	610	CLA	C13-C15-C16-C17
29	7	2630	LHG	C24-C25-C26-C27
35	B	623	SQD	C24-C25-C26-C27
35	b	623	SQD	C16-C17-C18-C19
37	C	520	DGD	C7B-C8B-C9B-CAB
24	2	606	CHL	C4B-C3B-CAB-CBB
24	3	601	CHL	C4B-C3B-CAB-CBB
24	G	607	CHL	C4B-C3B-CAB-CBB
24	N	609	CHL	C4B-C3B-CAB-CBB
24	9	606	CHL	C4B-C3B-CAB-CBB
24	g	607	CHL	C4B-C3B-CAB-CBB
24	s	606	CHL	C4B-C3B-CAB-CBB
24	y	605	CHL	C4B-C3B-CAB-CBB
25	1	602	CLA	C4B-C3B-CAB-CBB
25	1	612	CLA	C4B-C3B-CAB-CBB
25	2	604	CLA	C4B-C3B-CAB-CBB
25	3	610	CLA	C4B-C3B-CAB-CBB
25	4	604	CLA	C4B-C3B-CAB-CBB
25	4	610	CLA	C4B-C3B-CAB-CBB
25	5	613	CLA	C4B-C3B-CAB-CBB
25	C	501	CLA	C4B-C3B-CAB-CBB
25	C	502	CLA	C4B-C3B-CAB-CBB
25	C	506	CLA	C4B-C3B-CAB-CBB
25	D	402	CLA	C4B-C3B-CAB-CBB
25	G	610	CLA	C4B-C3B-CAB-CBB
25	N	602	CLA	C4B-C3B-CAB-CBB
25	R	609	CLA	C4B-C3B-CAB-CBB
25	R	610	CLA	C4B-C3B-CAB-CBB
25	S	611	CLA	C4B-C3B-CAB-CBB
25	Y	603	CLA	C4B-C3B-CAB-CBB
25	Y	604	CLA	C4B-C3B-CAB-CBB
25	Y	612	CLA	C4B-C3B-CAB-CBB
25	Y	614	CLA	C4B-C3B-CAB-CBB
25	7	602	CLA	C4B-C3B-CAB-CBB
25	7	612	CLA	C4B-C3B-CAB-CBB
25	8	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	c	501	CLA	C4B-C3B-CAB-CBB
25	c	502	CLA	C4B-C3B-CAB-CBB
25	d	402	CLA	C4B-C3B-CAB-CBB
25	g	610	CLA	C4B-C3B-CAB-CBB
25	n	602	CLA	C4B-C3B-CAB-CBB
25	s	611	CLA	C4B-C3B-CAB-CBB
25	y	604	CLA	C4B-C3B-CAB-CBB
25	y	612	CLA	C4B-C3B-CAB-CBB
25	y	614	CLA	C4B-C3B-CAB-CBB
25	r	609	CLA	C4B-C3B-CAB-CBB
25	r	610	CLA	C4B-C3B-CAB-CBB
25	0	604	CLA	C16-C17-C18-C19
25	B	610	CLA	C13-C15-C16-C17
25	9	613	CLA	C5-C6-C7-C8
29	1	2630	LHG	O6-C4-C5-C6
29	7	2630	LHG	O6-C4-C5-C6
29	p	2630	LHG	O6-C4-C5-C6
29	y	2630	LHG	C12-C13-C14-C15
29	1	2630	LHG	C23-C24-C25-C26
29	7	2630	LHG	C23-C24-C25-C26
25	N	604	CLA	CBA-CGA-O2A-C1
24	r	608	CHL	CBD-CGD-O2D-CED
24	2	609	CHL	C10-C11-C12-C13
24	0	609	CHL	C13-C15-C16-C17
24	r	608	CHL	C10-C11-C12-C13
24	y	609	CHL	O1D-CGD-O2D-CED
24	q	601	CHL	C4-C3-C5-C6
25	B	612	CLA	C4-C3-C5-C6
25	C	512	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
25	1	613	CLA	C2-C3-C5-C6
25	7	603	CLA	C2-C3-C5-C6
25	p	603	CLA	C2-C3-C5-C6
29	Y	2630	LHG	C23-C24-C25-C26
25	B	612	CLA	C5-C6-C7-C8
25	b	612	CLA	C5-C6-C7-C8
29	8	2630	LHG	O2-C2-C3-O3
25	7	603	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	C7B-C8B-C9B-CAB
25	C	502	CLA	C3-C5-C6-C7
25	D	402	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C16-C17-C18-C20
25	B	617	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C19
25	S	609	CLA	O1D-CGD-O2D-CED
25	D	402	CLA	C2A-CAA-CBA-CGA
24	G	601	CHL	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
24	5	607	CHL	CAA-CBA-CGA-O2A
24	R	608	CHL	CBD-CGD-O2D-CED
25	s	609	CLA	O1D-CGD-O2D-CED
24	1	608	CHL	C3A-C2A-CAA-CBA
24	0	606	CHL	C3A-C2A-CAA-CBA
24	7	608	CHL	C3A-C2A-CAA-CBA
25	6	613	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
36	A	413	LMG	C35-C36-C37-C38
36	a	413	LMG	C35-C36-C37-C38
26	6	1621	LUT	C29-C30-C31-C32
26	0	1621	LUT	C29-C30-C31-C32
37	C	518	DGD	CDB-CEB-CFB-CGB
29	S	2630	LHG	C23-C24-C25-C26
24	3	605	CHL	C3-C5-C6-C7
25	d	402	CLA	C3-C5-C6-C7
25	1	604	CLA	C5-C6-C7-C8
25	0	613	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	n	604	CLA	CBA-CGA-O2A-C1
24	3	609	CHL	C4C-C3C-CAC-CBC
25	r	604	CLA	O2A-C1-C2-C3
24	9	609	CHL	C10-C11-C12-C13
25	4	610	CLA	C10-C11-C12-C13
25	B	614	CLA	C8-C10-C11-C12
25	8	610	CLA	C15-C16-C17-C18
25	b	614	CLA	C8-C10-C11-C12
25	c	505	CLA	C10-C11-C12-C13
25	c	506	CLA	C5-C6-C7-C8
25	c	507	CLA	C8-C10-C11-C12
29	Y	2630	LHG	C4-C5-C6-O8
35	B	621	SQD	O6-C44-C45-C46
35	b	621	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
36	A	413	LMG	C7-C8-C9-O8
36	a	413	LMG	C7-C8-C9-O8
37	C	520	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
35	a	412	SQD	O49-C7-O47-C45
29	s	2630	LHG	C23-C24-C25-C26
29	r	2630	LHG	C23-C24-C25-C26
36	S	2631	LMG	C28-C29-C30-C31
37	c	519	DGD	CAA-CBA-CCA-CDA
24	y	606	CHL	C15-C16-C17-C18
35	b	621	SQD	C11-C12-C13-C14
25	1	612	CLA	C3-C5-C6-C7
35	B	621	SQD	C11-C12-C13-C14
37	c	518	DGD	CDB-CEB-CFB-CGB
25	C	505	CLA	C10-C11-C12-C13
25	b	605	CLA	C5-C6-C7-C8
25	C	505	CLA	C4-C3-C5-C6
24	1	601	CHL	C16-C17-C18-C20
25	1	612	CLA	C2-C3-C5-C6
29	9	2630	LHG	C10-C11-C12-C13
25	1	603	CLA	CBD-CGD-O2D-CED
29	Y	2630	LHG	C11-C10-C9-C8
29	r	2630	LHG	C11-C10-C9-C8
24	Y	606	CHL	C15-C16-C17-C18
24	0	609	CHL	C15-C16-C17-C18
24	3	601	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C3C-C2C-CMC-OMC
24	4	601	CHL	C3C-C2C-CMC-OMC
24	4	605	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	C3C-C2C-CMC-OMC
24	N	606	CHL	C3C-C2C-CMC-OMC
24	N	607	CHL	C3C-C2C-CMC-OMC
24	R	608	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C3C-C2C-CMC-OMC
24	0	609	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C3C-C2C-CMC-OMC
24	7	609	CHL	C3C-C2C-CMC-OMC
24	8	607	CHL	C3C-C2C-CMC-OMC
24	q	601	CHL	C3C-C2C-CMC-OMC
24	n	606	CHL	C3C-C2C-CMC-OMC
24	n	607	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	r	608	CHL	C3C-C2C-CMC-OMC
29	D	409	LHG	C3-O3-P-O6
29	R	2630	LHG	C23-C24-C25-C26
24	1	606	CHL	O1A-CGA-O2A-C1
24	q	605	CHL	O1A-CGA-O2A-C1
24	g	601	CHL	O1A-CGA-O2A-C1
25	2	613	CLA	O1A-CGA-O2A-C1
24	p	601	CHL	O1D-CGD-O2D-CED
25	B	613	CLA	O1D-CGD-O2D-CED
25	a	407	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	C3-C5-C6-C7
24	0	605	CHL	C2A-CAA-CBA-CGA
25	2	602	CLA	C2A-CAA-CBA-CGA
25	p	614	CLA	C2A-CAA-CBA-CGA
25	r	612	CLA	C2A-CAA-CBA-CGA
24	n	609	CHL	C13-C15-C16-C17
25	B	605	CLA	C5-C6-C7-C8
29	1	2630	LHG	O6-C4-C5-O7
37	C	518	DGD	C4D-C5D-C6D-O5D
37	c	518	DGD	C4D-C5D-C6D-O5D
35	A	412	SQD	O49-C7-O47-C45
25	S	604	CLA	CBA-CGA-O2A-C1
39	D	405	PL9	C12-C13-C14-C15
24	8	609	CHL	O1A-CGA-O2A-C1
29	d	410	LHG	O10-C23-O8-C6
37	C	520	DGD	O6D-C5D-C6D-O5D
37	c	520	DGD	O6D-C5D-C6D-O5D
24	8	607	CHL	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
24	R	608	CHL	C10-C11-C12-C13
25	b	603	CLA	C13-C15-C16-C17
29	R	2630	LHG	C11-C10-C9-C8
24	2	608	CHL	C2B-C3B-CAB-CBB
24	6	605	CHL	C2B-C3B-CAB-CBB
24	G	607	CHL	C2B-C3B-CAB-CBB
24	8	601	CHL	C2B-C3B-CAB-CBB
24	g	607	CHL	C2B-C3B-CAB-CBB
25	1	602	CLA	C2B-C3B-CAB-CBB
25	2	604	CLA	C2B-C3B-CAB-CBB
25	2	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	6	612	CLA	C2B-C3B-CAB-CBB
25	B	607	CLA	C2B-C3B-CAB-CBB
25	N	602	CLA	C2B-C3B-CAB-CBB
25	S	602	CLA	C2B-C3B-CAB-CBB
25	Y	604	CLA	C2B-C3B-CAB-CBB
25	Y	614	CLA	C2B-C3B-CAB-CBB
25	0	612	CLA	C2B-C3B-CAB-CBB
25	9	612	CLA	C2B-C3B-CAB-CBB
25	b	607	CLA	C2B-C3B-CAB-CBB
25	n	602	CLA	C2B-C3B-CAB-CBB
25	s	602	CLA	C2B-C3B-CAB-CBB
25	s	611	CLA	C2B-C3B-CAB-CBB
25	y	604	CLA	C2B-C3B-CAB-CBB
25	y	614	CLA	C2B-C3B-CAB-CBB
25	r	609	CLA	C2B-C3B-CAB-CBB
24	8	609	CHL	C4C-C3C-CAC-CBC
35	b	623	SQD	C32-C33-C34-C35
25	1	612	CLA	O1A-CGA-O2A-C1
25	9	613	CLA	O1A-CGA-O2A-C1
29	5	2630	LHG	O10-C23-O8-C6
29	D	410	LHG	O10-C23-O8-C6
29	Y	2630	LHG	C14-C15-C16-C17
29	1	2630	LHG	O7-C5-C6-O8
29	7	2630	LHG	O7-C5-C6-O8
36	D	411	LMG	O1-C7-C8-O7
37	C	519	DGD	O2G-C2G-C3G-O3G
37	C	520	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	O2G-C2G-C3G-O3G
37	c	520	DGD	O1G-C1G-C2G-O2G
25	s	604	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	O1D-CGD-O2D-CED
24	p	609	CHL	C2C-C3C-CAC-CBC
29	r	2630	LHG	C12-C13-C14-C15
29	4	2630	LHG	C23-C24-C25-C26
25	1	610	CLA	C16-C17-C18-C20
25	N	613	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C19
25	n	613	CLA	C16-C17-C18-C20
29	R	2630	LHG	C12-C13-C14-C15
29	p	2630	LHG	C16-C17-C18-C19
35	b	623	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	2	613	CLA	C5-C6-C7-C8
25	B	606	CLA	C5-C6-C7-C8
25	b	606	CLA	C5-C6-C7-C8
25	d	402	CLA	C10-C11-C12-C13
24	3	607	CHL	C2-C1-O2A-CGA
24	4	607	CHL	C2-C1-O2A-CGA
24	8	607	CHL	C2-C1-O2A-CGA
25	C	511	CLA	C2-C1-O2A-CGA
25	R	612	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
29	s	2630	LHG	C28-C29-C30-C31
25	C	506	CLA	C5-C6-C7-C8
25	8	604	CLA	C13-C15-C16-C17
24	2	609	CHL	C11-C12-C13-C14
24	5	605	CHL	C14-C13-C15-C16
24	6	606	CHL	C11-C10-C8-C9
24	6	609	CHL	C11-C12-C13-C14
24	N	605	CHL	C14-C13-C15-C16
24	N	607	CHL	C11-C12-C13-C14
24	R	606	CHL	C11-C12-C13-C14
24	7	607	CHL	C11-C12-C13-C14
24	9	609	CHL	C11-C12-C13-C14
24	9	609	CHL	C14-C13-C15-C16
24	p	605	CHL	C6-C7-C8-C9
24	p	607	CHL	C11-C10-C8-C9
24	r	606	CHL	C11-C12-C13-C14
25	1	611	CLA	C11-C12-C13-C14
25	5	613	CLA	C14-C13-C15-C16
25	6	602	CLA	C6-C7-C8-C9
25	6	602	CLA	C11-C12-C13-C14
25	6	613	CLA	C11-C10-C8-C9
25	6	613	CLA	C14-C13-C15-C16
25	B	613	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	D	402	CLA	C11-C12-C13-C14
25	G	613	CLA	C11-C10-C8-C9
25	N	602	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C12-C13-C14
25	R	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	0	602	CLA	C11-C12-C13-C14
25	7	603	CLA	C11-C12-C13-C14
25	p	613	CLA	C14-C13-C15-C16
25	q	603	CLA	C11-C12-C13-C14
25	b	613	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C12-C13-C14
25	g	613	CLA	C11-C10-C8-C9
25	y	603	CLA	C14-C13-C15-C16
25	r	610	CLA	C11-C12-C13-C14
25	1	613	CLA	C5-C6-C7-C8
25	6	612	CLA	C8-C10-C11-C12
25	7	610	CLA	C15-C16-C17-C18
25	y	603	CLA	C5-C6-C7-C8
33	A	409	PHO	C1A-C2A-CAA-CBA
25	D	403	CLA	O1A-CGA-O2A-C1
29	s	2630	LHG	C11-C12-C13-C14
36	h	102	LMG	C16-C17-C18-C19
24	p	608	CHL	C2A-CAA-CBA-CGA
25	R	612	CLA	C2A-CAA-CBA-CGA
25	Y	613	CLA	C2A-CAA-CBA-CGA
25	0	602	CLA	C2A-CAA-CBA-CGA
25	8	613	CLA	C2A-CAA-CBA-CGA
25	9	602	CLA	C2A-CAA-CBA-CGA
25	q	602	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
25	y	603	CLA	C2A-CAA-CBA-CGA
25	y	613	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C16-C17-C18-C19
25	B	617	CLA	C16-C17-C18-C20
35	a	412	SQD	C23-C24-C25-C26
25	4	604	CLA	O2A-C1-C2-C3
25	B	608	CLA	C3-C5-C6-C7
26	1	1620	LUT	C5-C6-C7-C8
26	2	1620	LUT	C1-C6-C7-C8
26	2	1620	LUT	C5-C6-C7-C8
26	4	1620	LUT	C5-C6-C7-C8
26	5	1621	LUT	C5-C6-C7-C8
26	S	1620	LUT	C5-C6-C7-C8
26	Y	1621	LUT	C5-C6-C7-C8
26	0	1621	LUT	C5-C6-C7-C8
26	7	1620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	7	1620	LUT	C5-C6-C7-C8
26	7	1621	LUT	C1-C6-C7-C8
26	7	1621	LUT	C5-C6-C7-C8
26	9	1620	LUT	C5-C6-C7-C8
26	s	1620	LUT	C5-C6-C7-C8
26	y	1621	LUT	C5-C6-C7-C8
34	B	620	BCR	C23-C24-C25-C26
34	B	620	BCR	C23-C24-C25-C30
34	C	515	BCR	C1-C6-C7-C8
34	b	620	BCR	C23-C24-C25-C26
34	b	620	BCR	C23-C24-C25-C30
34	c	515	BCR	C1-C6-C7-C8
34	c	515	BCR	C5-C6-C7-C8
27	n	1622	XAT	C31-C32-C33-C40
35	B	623	SQD	C32-C33-C34-C35
25	1	611	CLA	O1D-CGD-O2D-CED
26	4	1620	LUT	C27-C28-C29-C30
26	Y	1621	LUT	C7-C8-C9-C10
26	8	1620	LUT	C27-C28-C29-C30
26	p	1620	LUT	C27-C28-C29-C30
26	y	1621	LUT	C7-C8-C9-C10
27	n	1622	XAT	C31-C32-C33-C34
28	2	1623	NEX	C31-C32-C33-C34
34	B	620	BCR	C7-C8-C9-C10
34	C	515	BCR	C7-C8-C9-C10
34	D	404	BCR	C7-C8-C9-C10
34	d	404	BCR	C7-C8-C9-C10
24	1	606	CHL	C15-C16-C17-C18
24	3	601	CHL	C10-C11-C12-C13
24	7	609	CHL	C13-C15-C16-C17
29	9	2630	LHG	C23-C24-C25-C26
37	C	523	DGD	C3B-C4B-C5B-C6B
37	c	523	DGD	C3B-C4B-C5B-C6B
29	S	2630	LHG	C11-C12-C13-C14
35	A	412	SQD	C31-C32-C33-C34
36	s	2631	LMG	C42-C43-C44-C45
25	B	616	CLA	C16-C17-C18-C19
25	7	610	CLA	C16-C17-C18-C20
25	b	616	CLA	C16-C17-C18-C19
35	A	412	SQD	C23-C24-C25-C26
35	b	623	SQD	C25-C26-C27-C28
25	1	611	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C5-C6-C7-C8
25	0	612	CLA	C8-C10-C11-C12
24	p	607	CHL	CAA-CBA-CGA-O2A
35	B	623	SQD	C25-C26-C27-C28
24	1	606	CHL	C11-C12-C13-C15
24	2	601	CHL	C11-C12-C13-C15
24	2	609	CHL	C11-C12-C13-C15
24	3	601	CHL	C6-C7-C8-C10
24	3	601	CHL	C11-C10-C8-C7
24	3	605	CHL	C12-C13-C15-C16
24	4	601	CHL	C11-C10-C8-C7
24	4	609	CHL	C11-C10-C8-C7
24	5	601	CHL	C11-C10-C8-C7
24	5	607	CHL	C11-C12-C13-C15
24	5	609	CHL	C12-C13-C15-C16
24	6	606	CHL	C11-C12-C13-C15
24	6	607	CHL	C6-C7-C8-C10
24	6	609	CHL	C11-C12-C13-C15
24	G	609	CHL	C11-C12-C13-C15
24	N	605	CHL	C11-C12-C13-C15
24	N	609	CHL	C11-C12-C13-C15
24	R	606	CHL	C11-C12-C13-C15
24	Y	601	CHL	C11-C12-C13-C15
24	Y	606	CHL	C11-C12-C13-C15
24	Y	607	CHL	C11-C12-C13-C15
24	0	609	CHL	C11-C12-C13-C15
24	7	606	CHL	C11-C12-C13-C15
24	7	607	CHL	C11-C12-C13-C15
24	7	609	CHL	C12-C13-C15-C16
24	8	605	CHL	C11-C12-C13-C15
24	9	601	CHL	C11-C10-C8-C7
24	9	609	CHL	C11-C12-C13-C15
24	9	609	CHL	C12-C13-C15-C16
24	p	605	CHL	C12-C13-C15-C16
24	q	601	CHL	C11-C10-C8-C7
24	q	609	CHL	C11-C12-C13-C15
24	g	609	CHL	C11-C12-C13-C15
24	n	605	CHL	C11-C12-C13-C15
24	n	609	CHL	C11-C10-C8-C7
24	y	601	CHL	C11-C12-C13-C15
24	y	606	CHL	C11-C12-C13-C15
24	r	606	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	1	602	CLA	C6-C7-C8-C10
25	1	602	CLA	C11-C12-C13-C15
25	1	610	CLA	C6-C7-C8-C10
25	2	603	CLA	C12-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C10
25	3	602	CLA	C11-C12-C13-C15
25	4	602	CLA	C6-C7-C8-C10
25	4	610	CLA	C12-C13-C15-C16
25	4	613	CLA	C11-C10-C8-C7
25	4	613	CLA	C12-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C10
25	5	604	CLA	C6-C7-C8-C10
25	5	613	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C12-C13-C15
25	6	603	CLA	C12-C13-C15-C16
25	6	611	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C12-C13-C15
25	B	606	CLA	C12-C13-C15-C16
25	B	607	CLA	C11-C10-C8-C7
25	B	607	CLA	C12-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C10
25	B	617	CLA	C6-C7-C8-C10
25	C	505	CLA	C2-C3-C5-C6
25	C	512	CLA	C11-C10-C8-C7
25	D	402	CLA	C11-C12-C13-C15
25	D	403	CLA	C11-C12-C13-C15
25	G	603	CLA	C11-C10-C8-C7
25	G	610	CLA	C12-C13-C15-C16
25	G	613	CLA	C11-C10-C8-C7
25	N	602	CLA	C11-C12-C13-C15
25	N	613	CLA	C11-C10-C8-C7
25	Y	602	CLA	C6-C7-C8-C10
25	Y	602	CLA	C11-C12-C13-C15
25	Y	603	CLA	C12-C13-C15-C16
25	Y	604	CLA	C6-C7-C8-C10
25	Y	612	CLA	C11-C10-C8-C7
25	0	602	CLA	C11-C12-C13-C15
25	0	611	CLA	C12-C13-C15-C16
25	7	602	CLA	C6-C7-C8-C10
25	7	602	CLA	C11-C12-C13-C15
25	7	610	CLA	C6-C7-C8-C10
25	7	611	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	8	602	CLA	C6-C7-C8-C10
25	9	603	CLA	C12-C13-C15-C16
25	p	603	CLA	C12-C13-C15-C16
25	p	604	CLA	C6-C7-C8-C10
25	p	613	CLA	C6-C7-C8-C10
25	p	613	CLA	C11-C10-C8-C7
25	q	613	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C7
25	b	607	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10
25	b	617	CLA	C6-C7-C8-C10
25	c	504	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	d	402	CLA	C11-C12-C13-C15
25	g	603	CLA	C11-C10-C8-C7
25	g	610	CLA	C12-C13-C15-C16
25	g	613	CLA	C11-C10-C8-C7
25	n	613	CLA	C11-C10-C8-C7
25	y	602	CLA	C6-C7-C8-C10
25	y	602	CLA	C11-C12-C13-C15
25	y	603	CLA	C12-C13-C15-C16
25	y	604	CLA	C6-C7-C8-C10
25	y	612	CLA	C11-C10-C8-C7
24	7	606	CHL	O1A-CGA-O2A-C1
35	a	412	SQD	C31-C32-C33-C34
36	S	2631	LMG	C42-C43-C44-C45
24	N	609	CHL	C13-C15-C16-C17
26	G	1621	LUT	C29-C30-C31-C32
26	g	1621	LUT	C29-C30-C31-C32
34	H	101	BCR	C9-C10-C11-C12
34	h	101	BCR	C9-C10-C11-C12
25	b	617	CLA	C16-C17-C18-C20
36	H	102	LMG	C16-C17-C18-C19
29	S	2630	LHG	C28-C29-C30-C31
25	1	610	CLA	C8-C10-C11-C12
25	b	616	CLA	C5-C6-C7-C8
25	4	613	CLA	O1A-CGA-O2A-C1
24	6	605	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	3	613	CLA	C2A-CAA-CBA-CGA
25	d	402	CLA	C2A-CAA-CBA-CGA
25	n	604	CLA	C2A-CAA-CBA-CGA
24	p	606	CHL	CBD-CGD-O2D-CED
25	6	613	CLA	C15-C16-C17-C18
25	g	603	CLA	C15-C16-C17-C18
24	2	609	CHL	C3-C5-C6-C7
24	y	609	CHL	C3-C5-C6-C7
25	R	616	CLA	C3-C5-C6-C7
25	r	616	CLA	C3-C5-C6-C7
37	C	523	DGD	CDB-CEB-CFB-CGB
37	c	523	DGD	CDB-CEB-CFB-CGB
24	Y	601	CHL	C16-C17-C18-C19
24	9	601	CHL	C8-C10-C11-C12
25	C	504	CLA	CBA-CGA-O2A-C1
25	q	604	CLA	CBA-CGA-O2A-C1
29	9	2630	LHG	C24-C23-O8-C6
29	D	408	LHG	C29-C30-C31-C32
29	d	408	LHG	C29-C30-C31-C32
29	4	2630	LHG	C10-C11-C12-C13
36	D	412	LMG	C15-C16-C17-C18
36	H	102	LMG	C17-C18-C19-C20
24	8	601	CHL	O1D-CGD-O2D-CED
24	3	607	CHL	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	G	603	CLA	C15-C16-C17-C18
25	Y	603	CLA	C5-C6-C7-C8
25	7	610	CLA	C8-C10-C11-C12
24	3	606	CHL	CBD-CGD-O2D-CED
29	4	2630	LHG	C11-C12-C13-C14
29	p	2630	LHG	C14-C15-C16-C17
29	c	2630	LHG	C14-C15-C16-C17
36	d	412	LMG	C15-C16-C17-C18
24	1	605	CHL	CAD-CBD-CGD-O2D
24	2	601	CHL	CAD-CBD-CGD-O2D
24	G	605	CHL	CAD-CBD-CGD-O2D
24	N	606	CHL	CAD-CBD-CGD-O2D
24	R	607	CHL	CAD-CBD-CGD-O2D
24	0	601	CHL	CAD-CBD-CGD-O2D
24	7	605	CHL	CAD-CBD-CGD-O2D
24	7	608	CHL	CAD-CBD-CGD-O2D
24	9	607	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	q	608	CHL	CAD-CBD-CGD-O2D
24	g	605	CHL	CAD-CBD-CGD-O2D
24	n	606	CHL	CAD-CBD-CGD-O2D
24	r	607	CHL	CAD-CBD-CGD-O2D
25	1	603	CLA	CAD-CBD-CGD-O2D
25	1	604	CLA	CAD-CBD-CGD-O2D
25	2	602	CLA	CAD-CBD-CGD-O2D
25	3	602	CLA	CAD-CBD-CGD-O2D
25	3	612	CLA	CAD-CBD-CGD-O2D
25	3	614	CLA	CAD-CBD-CGD-O2D
25	4	604	CLA	CAD-CBD-CGD-O2D
25	4	613	CLA	CAD-CBD-CGD-O2D
25	5	610	CLA	CAD-CBD-CGD-O2D
25	5	614	CLA	CAD-CBD-CGD-O2D
25	A	410	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	G	610	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	N	610	CLA	CAD-CBD-CGD-O2D
25	N	614	CLA	CAD-CBD-CGD-O2D
25	R	603	CLA	CAD-CBD-CGD-O2D
25	R	609	CLA	CAD-CBD-CGD-O2D
25	R	610	CLA	CAD-CBD-CGD-O2D
25	R	611	CLA	CAD-CBD-CGD-O2D
25	S	614	CLA	CAD-CBD-CGD-O2D
25	Y	602	CLA	CAD-CBD-CGD-O2D
25	0	603	CLA	CAD-CBD-CGD-O2D
25	0	614	CLA	CAD-CBD-CGD-O2D
25	8	602	CLA	CAD-CBD-CGD-O2D
25	8	612	CLA	CAD-CBD-CGD-O2D
25	8	614	CLA	CAD-CBD-CGD-O2D
25	p	602	CLA	CAD-CBD-CGD-O2D
25	p	610	CLA	CAD-CBD-CGD-O2D
25	q	610	CLA	CAD-CBD-CGD-O2D
25	q	614	CLA	CAD-CBD-CGD-O2D
25	a	410	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	c	501	CLA	CAD-CBD-CGD-O2D
25	g	610	CLA	CAD-CBD-CGD-O2D
25	g	614	CLA	CAD-CBD-CGD-O2D
25	n	610	CLA	CAD-CBD-CGD-O2D
25	n	613	CLA	CAD-CBD-CGD-O2D
25	n	614	CLA	CAD-CBD-CGD-O2D
25	s	614	CLA	CAD-CBD-CGD-O2D
25	y	602	CLA	CAD-CBD-CGD-O2D
25	r	603	CLA	CAD-CBD-CGD-O2D
25	r	609	CLA	CAD-CBD-CGD-O2D
25	r	610	CLA	CAD-CBD-CGD-O2D
25	r	611	CLA	CAD-CBD-CGD-O2D
33	A	408	PHO	CAD-CBD-CGD-O2D
33	a	408	PHO	CAD-CBD-CGD-O2D
24	5	607	CHL	C5-C6-C7-C8
25	G	610	CLA	C13-C15-C16-C17
25	c	504	CLA	CBA-CGA-O2A-C1
24	N	605	CHL	C4-C3-C5-C6
24	n	605	CHL	C4-C3-C5-C6
25	Y	603	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	C	512	CLA	C16-C17-C18-C20
25	c	506	CLA	C2-C3-C5-C6
36	S	2631	LMG	C18-C19-C20-C21
29	R	2630	LHG	C4-C5-C6-O8
29	q	2630	LHG	C4-C5-C6-O8
29	r	2630	LHG	C4-C5-C6-O8
36	D	411	LMG	O1-C7-C8-C9
36	d	411	LMG	O1-C7-C8-C9
37	C	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	C1G-C2G-C3G-O3G
25	G	602	CLA	CBD-CGD-O2D-CED
25	S	604	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
29	4	2630	LHG	C9-C10-C11-C12
29	C	2630	LHG	O6-C4-C5-O7
29	L	101	LHG	O6-C4-C5-O7
29	7	2630	LHG	O6-C4-C5-O7
29	p	2630	LHG	O6-C4-C5-O7
24	1	606	CHL	C5-C6-C7-C8
25	C	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	g	610	CLA	C13-C15-C16-C17
25	g	610	CLA	C15-C16-C17-C18
25	G	614	CLA	O2A-C1-C2-C3
25	N	611	CLA	O2A-C1-C2-C3
25	S	602	CLA	O2A-C1-C2-C3
25	n	611	CLA	O2A-C1-C2-C3
25	s	602	CLA	O2A-C1-C2-C3
25	G	610	CLA	O1D-CGD-O2D-CED
36	h	102	LMG	C17-C18-C19-C20
24	0	606	CHL	C2A-CAA-CBA-CGA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C2A-CAA-CBA-CGA
25	N	604	CLA	C2A-CAA-CBA-CGA
25	9	602	CLA	C15-C16-C17-C18
25	c	506	CLA	C13-C15-C16-C17
36	d	411	LMG	C14-C15-C16-C17
24	Y	601	CHL	C16-C17-C18-C20
24	7	601	CHL	C16-C17-C18-C20
24	8	607	CHL	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
25	g	610	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	CHA-CBD-CGD-O1D
24	R	608	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	CHA-CBD-CGD-O1D
24	S	606	CHL	CHA-CBD-CGD-O2D
24	Y	607	CHL	CHA-CBD-CGD-O2D
24	s	606	CHL	CHA-CBD-CGD-O1D
24	s	606	CHL	CHA-CBD-CGD-O2D
24	y	607	CHL	CHA-CBD-CGD-O2D
24	r	608	CHL	CHA-CBD-CGD-O1D
24	r	608	CHL	CHA-CBD-CGD-O2D
25	1	602	CLA	CHA-CBD-CGD-O1D
25	1	602	CLA	CHA-CBD-CGD-O2D
25	1	613	CLA	CHA-CBD-CGD-O1D
25	1	613	CLA	CHA-CBD-CGD-O2D
25	2	611	CLA	CHA-CBD-CGD-O2D
25	3	611	CLA	CHA-CBD-CGD-O2D
25	4	611	CLA	CHA-CBD-CGD-O1D
25	4	611	CLA	CHA-CBD-CGD-O2D
25	4	612	CLA	CHA-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O2D
25	5	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	CHA-CBD-CGD-O1D
25	C	511	CLA	CHA-CBD-CGD-O2D
25	N	611	CLA	CHA-CBD-CGD-O1D
25	R	616	CLA	CHA-CBD-CGD-O1D
25	7	602	CLA	CHA-CBD-CGD-O1D
25	7	602	CLA	CHA-CBD-CGD-O2D
25	7	604	CLA	CHA-CBD-CGD-O2D
25	9	602	CLA	CHA-CBD-CGD-O1D
25	q	611	CLA	CHA-CBD-CGD-O1D
25	b	603	CLA	CHA-CBD-CGD-O1D
25	b	603	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	r	616	CLA	CHA-CBD-CGD-O1D
25	p	602	CLA	C3-C5-C6-C7
24	G	601	CHL	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
25	n	604	CLA	O1A-CGA-O2A-C1
29	l	101	LHG	C17-C18-C19-C20
36	D	411	LMG	C14-C15-C16-C17
29	q	2630	LHG	O7-C5-C6-O8
29	r	2630	LHG	O7-C5-C6-O8
36	d	411	LMG	O1-C7-C8-O7
37	C	523	DGD	O2G-C2G-C3G-O3G
37	c	523	DGD	O2G-C2G-C3G-O3G
25	A	407	CLA	O1D-CGD-O2D-CED
24	7	601	CHL	C8-C10-C11-C12
24	7	606	CHL	C5-C6-C7-C8
25	G	610	CLA	C15-C16-C17-C18
29	L	101	LHG	C17-C18-C19-C20
24	N	609	CHL	C16-C17-C18-C20
24	9	609	CHL	O1D-CGD-O2D-CED
25	G	602	CLA	O1D-CGD-O2D-CED
29	d	408	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	b	610	CLA	C15-C16-C17-C18
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
25	y	603	CLA	C4-C3-C5-C6
29	D	408	LHG	C31-C32-C33-C34
29	y	2630	LHG	C18-C19-C20-C21
25	N	604	CLA	O1A-CGA-O2A-C1
25	s	604	CLA	O1A-CGA-O2A-C1
25	3	603	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
29	s	2630	LHG	O9-C7-O7-C5
25	B	610	CLA	C15-C16-C17-C18
25	Y	610	CLA	C15-C16-C17-C18
24	1	606	CHL	C11-C12-C13-C14
24	2	609	CHL	C14-C13-C15-C16
24	4	601	CHL	C14-C13-C15-C16
24	4	609	CHL	C11-C12-C13-C14
24	Y	606	CHL	C11-C12-C13-C14
24	7	606	CHL	C11-C12-C13-C14
24	9	601	CHL	C11-C10-C8-C9
24	q	601	CHL	C11-C10-C8-C9
24	y	606	CHL	C11-C12-C13-C14
25	4	602	CLA	C6-C7-C8-C9
25	4	603	CLA	C11-C10-C8-C9
25	4	610	CLA	C14-C13-C15-C16
25	4	613	CLA	C14-C13-C15-C16
25	5	613	CLA	C11-C10-C8-C9
25	6	611	CLA	C14-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C12-C13-C14
25	G	610	CLA	C14-C13-C15-C16
25	0	613	CLA	C14-C13-C15-C16
25	b	610	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C12-C13-C14
25	d	402	CLA	C11-C12-C13-C14
25	g	610	CLA	C14-C13-C15-C16
24	p	606	CHL	O1D-CGD-O2D-CED
29	2	2630	LHG	C10-C11-C12-C13
29	s	2630	LHG	C29-C30-C31-C32
25	C	504	CLA	O1A-CGA-O2A-C1
25	q	604	CLA	O1A-CGA-O2A-C1
25	g	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	Y	612	CLA	C8-C10-C11-C12
25	y	612	CLA	C8-C10-C11-C12
35	A	412	SQD	C4-C5-C6-S
35	a	412	SQD	C4-C5-C6-S
24	5	601	CHL	C3-C5-C6-C7
24	9	609	CHL	C3-C5-C6-C7
29	L	101	LHG	C34-C35-C36-C37
29	Y	2630	LHG	C26-C27-C28-C29
29	7	2630	LHG	C35-C36-C37-C38
25	5	613	CLA	C2A-CAA-CBA-CGA
26	1	1621	LUT	C11-C12-C13-C20
27	4	1622	XAT	C11-C12-C13-C20
28	3	1623	NEX	C31-C32-C33-C40
28	0	1623	NEX	C11-C12-C13-C20
29	1	2630	LHG	C35-C36-C37-C38
35	b	621	SQD	C10-C11-C12-C13
34	c	515	BCR	C7-C8-C9-C10
29	G	2630	LHG	C25-C26-C27-C28
24	7	609	CHL	C1A-C2A-CAA-CBA
24	9	609	CHL	C1A-C2A-CAA-CBA
24	q	601	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	C1A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	4	612	CLA	C1A-C2A-CAA-CBA
25	5	602	CLA	C1A-C2A-CAA-CBA
25	5	610	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C1A-C2A-CAA-CBA
25	B	610	CLA	C1A-C2A-CAA-CBA
25	C	505	CLA	C1A-C2A-CAA-CBA
25	G	602	CLA	C1A-C2A-CAA-CBA
25	N	602	CLA	C1A-C2A-CAA-CBA
25	N	610	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	q	612	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	n	602	CLA	C1A-C2A-CAA-CBA
25	n	610	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
29	y	2630	LHG	C23-C24-C25-C26
24	y	601	CHL	C16-C17-C18-C20
29	R	2630	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	C15-C16-C17-C18
25	C	513	CLA	C5-C6-C7-C8
29	s	2630	LHG	C8-C7-O7-C5
29	S	2630	LHG	C29-C30-C31-C32
24	N	609	CHL	CBA-CGA-O2A-C1
35	B	621	SQD	C10-C11-C12-C13
24	3	606	CHL	O1D-CGD-O2D-CED
29	3	2630	LHG	C3-O3-P-O6
29	8	2630	LHG	C3-O3-P-O6
29	q	2630	LHG	C3-O3-P-O6
29	d	408	LHG	C3-O3-P-O6
29	l	101	LHG	C34-C35-C36-C37
36	B	622	LMG	C36-C37-C38-C39
36	b	622	LMG	C36-C37-C38-C39
29	g	2630	LHG	C25-C26-C27-C28
24	7	609	CHL	C4-C3-C5-C6
25	B	608	CLA	C4-C3-C5-C6
24	3	607	CHL	C2-C3-C5-C6
25	2	602	CLA	C2-C3-C5-C6
25	y	603	CLA	C2-C3-C5-C6
25	0	613	CLA	O1A-CGA-O2A-C1
24	1	601	CHL	C4B-C3B-CAB-CBB
24	1	605	CHL	C4B-C3B-CAB-CBB
24	1	607	CHL	C4B-C3B-CAB-CBB
24	2	601	CHL	C4B-C3B-CAB-CBB
24	2	605	CHL	C4B-C3B-CAB-CBB
24	2	607	CHL	C4B-C3B-CAB-CBB
24	2	608	CHL	C4B-C3B-CAB-CBB
24	2	609	CHL	C4B-C3B-CAB-CBB
24	4	607	CHL	C4B-C3B-CAB-CBB
24	5	601	CHL	C4B-C3B-CAB-CBB
24	5	605	CHL	C4B-C3B-CAB-CBB
24	5	608	CHL	C4B-C3B-CAB-CBB
24	6	601	CHL	C4B-C3B-CAB-CBB
24	6	605	CHL	C4B-C3B-CAB-CBB
24	6	607	CHL	C4B-C3B-CAB-CBB
24	6	608	CHL	C4B-C3B-CAB-CBB
24	6	609	CHL	C4B-C3B-CAB-CBB
24	G	609	CHL	C4B-C3B-CAB-CBB
24	N	605	CHL	C4B-C3B-CAB-CBB
24	R	606	CHL	C4B-C3B-CAB-CBB
24	R	607	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	S	606	CHL	C4B-C3B-CAB-CBB
24	S	608	CHL	C4B-C3B-CAB-CBB
24	Y	601	CHL	C4B-C3B-CAB-CBB
24	Y	609	CHL	C4B-C3B-CAB-CBB
24	0	601	CHL	C4B-C3B-CAB-CBB
24	0	605	CHL	C4B-C3B-CAB-CBB
24	0	608	CHL	C4B-C3B-CAB-CBB
24	0	609	CHL	C4B-C3B-CAB-CBB
24	7	601	CHL	C4B-C3B-CAB-CBB
24	7	605	CHL	C4B-C3B-CAB-CBB
24	7	607	CHL	C4B-C3B-CAB-CBB
24	7	608	CHL	C4B-C3B-CAB-CBB
24	8	601	CHL	C4B-C3B-CAB-CBB
24	8	607	CHL	C4B-C3B-CAB-CBB
24	9	605	CHL	C4B-C3B-CAB-CBB
24	9	607	CHL	C4B-C3B-CAB-CBB
24	9	608	CHL	C4B-C3B-CAB-CBB
24	9	609	CHL	C4B-C3B-CAB-CBB
24	p	601	CHL	C4B-C3B-CAB-CBB
24	q	606	CHL	C4B-C3B-CAB-CBB
24	q	607	CHL	C4B-C3B-CAB-CBB
24	g	609	CHL	C4B-C3B-CAB-CBB
24	n	607	CHL	C4B-C3B-CAB-CBB
24	s	608	CHL	C4B-C3B-CAB-CBB
24	y	601	CHL	C4B-C3B-CAB-CBB
24	y	609	CHL	C4B-C3B-CAB-CBB
24	r	606	CHL	C4B-C3B-CAB-CBB
24	r	607	CHL	C4B-C3B-CAB-CBB
25	B	611	CLA	C4B-C3B-CAB-CBB
25	b	611	CLA	C4B-C3B-CAB-CBB
29	1	2630	LHG	C4-O6-P-O4
29	2	2630	LHG	C3-O3-P-O4
29	2	2630	LHG	C4-O6-P-O4
29	6	2630	LHG	C4-O6-P-O4
29	C	2630	LHG	C4-O6-P-O5
29	D	408	LHG	C3-O3-P-O4
29	D	409	LHG	C4-O6-P-O4
29	R	2630	LHG	C4-O6-P-O4
29	7	2630	LHG	C4-O6-P-O4
29	9	2630	LHG	C3-O3-P-O4
29	9	2630	LHG	C4-O6-P-O4
29	c	2630	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
29	d	408	LHG	C3-O3-P-O4
29	d	409	LHG	C4-O6-P-O4
29	l	101	LHG	C3-O3-P-O4
29	l	101	LHG	C4-O6-P-O4
29	r	2630	LHG	C4-O6-P-O4
25	3	611	CLA	O2A-C1-C2-C3
25	5	611	CLA	O2A-C1-C2-C3
25	A	407	CLA	O2A-C1-C2-C3
25	R	612	CLA	O2A-C1-C2-C3
25	S	613	CLA	O2A-C1-C2-C3
25	8	611	CLA	O2A-C1-C2-C3
25	a	407	CLA	O2A-C1-C2-C3
25	g	614	CLA	O2A-C1-C2-C3
25	s	613	CLA	O2A-C1-C2-C3
25	r	612	CLA	O2A-C1-C2-C3
24	7	606	CHL	C15-C16-C17-C18
24	g	609	CHL	C10-C11-C12-C13
25	c	512	CLA	C15-C16-C17-C18
25	y	610	CLA	C15-C16-C17-C18
29	Y	2630	LHG	C24-C23-O8-C6
33	a	409	PHO	CBA-CGA-O2A-C1
29	5	2630	LHG	O6-C4-C5-C6
29	L	101	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
36	H	102	LMG	C13-C14-C15-C16
25	c	504	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	C2A-CAA-CBA-CGA
25	p	613	CLA	C2A-CAA-CBA-CGA
25	s	614	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C3-C5-C6-C7
40	F	101	HEM	C2A-CAA-CBA-CGA
25	c	505	CLA	C5-C6-C7-C8
29	d	409	LHG	C25-C26-C27-C28
35	a	412	SQD	C12-C13-C14-C15
37	c	519	DGD	C2B-C1B-O2G-C2G
25	q	602	CLA	C16-C17-C18-C19
24	S	606	CHL	CAD-CBD-CGD-O1D
24	s	606	CHL	CAD-CBD-CGD-O1D
25	2	611	CLA	CAD-CBD-CGD-O1D
25	4	611	CLA	CAD-CBD-CGD-O1D
25	5	611	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	CAD-CBD-CGD-O1D
25	S	603	CLA	CAD-CBD-CGD-O1D
25	Y	614	CLA	CAD-CBD-CGD-O1D
25	0	604	CLA	CAD-CBD-CGD-O1D
25	7	604	CLA	CAD-CBD-CGD-O1D
25	9	602	CLA	CAD-CBD-CGD-O1D
25	9	611	CLA	CAD-CBD-CGD-O1D
25	p	611	CLA	CAD-CBD-CGD-O1D
25	q	611	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	CAD-CBD-CGD-O1D
25	s	603	CLA	CAD-CBD-CGD-O1D
25	s	604	CLA	CAD-CBD-CGD-O1D
25	y	614	CLA	CAD-CBD-CGD-O1D
29	q	2630	LHG	O8-C23-C24-C25
25	R	610	CLA	C10-C11-C12-C13
25	r	610	CLA	C10-C11-C12-C13
25	5	602	CLA	C15-C16-C17-C18
37	C	523	DGD	C1B-C2B-C3B-C4B
37	c	523	DGD	C1B-C2B-C3B-C4B
29	C	2630	LHG	C15-C16-C17-C18
24	n	609	CHL	CBA-CGA-O2A-C1
25	c	503	CLA	CBA-CGA-O2A-C1
33	A	409	PHO	CBA-CGA-O2A-C1
29	G	2630	LHG	C1-C2-C3-O3
29	g	2630	LHG	C1-C2-C3-O3
29	C	2630	LHG	C34-C35-C36-C37
35	A	412	SQD	C12-C13-C14-C15
24	R	607	CHL	C6-C7-C8-C10
24	y	609	CHL	C16-C17-C18-C19
24	r	607	CHL	C6-C7-C8-C10
24	2	609	CHL	C12-C13-C15-C16
24	3	601	CHL	C11-C12-C13-C15
24	3	605	CHL	C11-C12-C13-C15
24	4	601	CHL	C11-C12-C13-C15
24	4	601	CHL	C12-C13-C15-C16
24	4	609	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	5	609	CHL	C11-C12-C13-C15
24	6	601	CHL	C12-C13-C15-C16
24	6	607	CHL	C12-C13-C15-C16
24	R	606	CHL	C11-C10-C8-C7
24	R	606	CHL	C12-C13-C15-C16
24	0	601	CHL	C12-C13-C15-C16
24	0	606	CHL	C11-C12-C13-C15
24	8	601	CHL	C11-C10-C8-C7
24	8	605	CHL	C12-C13-C15-C16
24	8	606	CHL	C3A-C2A-CAA-CBA
24	p	609	CHL	C11-C10-C8-C7
24	q	601	CHL	C2-C3-C5-C6
24	r	606	CHL	C11-C10-C8-C7
24	r	606	CHL	C12-C13-C15-C16
25	1	604	CLA	C6-C7-C8-C10
25	2	602	CLA	C11-C12-C13-C15
25	3	603	CLA	C12-C13-C15-C16
25	3	613	CLA	C11-C10-C8-C7
25	4	603	CLA	C11-C10-C8-C7
25	5	603	CLA	C12-C13-C15-C16
25	5	613	CLA	C11-C10-C8-C7
25	6	612	CLA	C6-C7-C8-C10
25	B	605	CLA	C6-C7-C8-C10
25	B	608	CLA	C12-C13-C15-C16
25	B	616	CLA	C12-C13-C15-C16
25	C	502	CLA	C12-C13-C15-C16
25	C	505	CLA	C11-C12-C13-C15
25	C	505	CLA	C12-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
25	C	511	CLA	C11-C12-C13-C15
25	Y	612	CLA	C6-C7-C8-C10
25	Y	613	CLA	C11-C10-C8-C7
25	0	612	CLA	C6-C7-C8-C10
25	7	604	CLA	C6-C7-C8-C10
25	7	613	CLA	C6-C7-C8-C10
25	8	603	CLA	C12-C13-C15-C16
25	8	613	CLA	C11-C10-C8-C7
25	p	603	CLA	C11-C10-C8-C7
25	q	603	CLA	C11-C10-C8-C7
25	q	603	CLA	C12-C13-C15-C16
25	q	610	CLA	C6-C7-C8-C10
25	q	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C6-C7-C8-C10
25	b	608	CLA	C6-C7-C8-C10
25	b	608	CLA	C12-C13-C15-C16
25	b	616	CLA	C12-C13-C15-C16
25	c	505	CLA	C11-C12-C13-C15
25	c	505	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	y	612	CLA	C6-C7-C8-C10
25	y	613	CLA	C11-C10-C8-C7
29	c	2630	LHG	O6-C4-C5-O7
29	l	101	LHG	O6-C4-C5-O7
39	D	405	PL9	C28-C29-C31-C32
39	d	405	PL9	C28-C29-C31-C32
29	2	2630	LHG	C13-C14-C15-C16
24	2	605	CHL	CAA-CBA-CGA-O2A
24	G	607	CHL	CAA-CBA-CGA-O2A
25	y	602	CLA	C10-C11-C12-C13
29	R	2630	LHG	C8-C7-O7-C5
37	C	519	DGD	C2B-C1B-O2G-C2G
29	G	2630	LHG	C24-C25-C26-C27
29	g	2630	LHG	C24-C25-C26-C27
24	5	609	CHL	C2C-C3C-CAC-CBC
25	p	610	CLA	C8-C10-C11-C12
24	p	605	CHL	CBD-CGD-O2D-CED
24	r	608	CHL	C2A-CAA-CBA-CGA
25	4	602	CLA	C2A-CAA-CBA-CGA
25	5	603	CLA	C2A-CAA-CBA-CGA
25	R	602	CLA	C2A-CAA-CBA-CGA
25	R	616	CLA	C2A-CAA-CBA-CGA
25	p	603	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
25	r	616	CLA	C2A-CAA-CBA-CGA
24	1	607	CHL	C16-C17-C18-C19
24	0	609	CHL	C2C-C3C-CAC-CBC
24	3	601	CHL	C1C-C2C-CMC-OMC
24	3	606	CHL	C1C-C2C-CMC-OMC
24	4	601	CHL	C1C-C2C-CMC-OMC
24	4	605	CHL	C1C-C2C-CMC-OMC
24	4	609	CHL	C1C-C2C-CMC-OMC
24	5	601	CHL	C1C-C2C-CMC-OMC
24	5	605	CHL	C1C-C2C-CMC-OMC
24	5	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	5	607	CHL	C1C-C2C-CMC-OMC
24	5	608	CHL	C1C-C2C-CMC-OMC
24	6	601	CHL	C1C-C2C-CMC-OMC
24	6	608	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C1C-C2C-CMC-OMC
24	N	606	CHL	C1C-C2C-CMC-OMC
24	N	607	CHL	C1C-C2C-CMC-OMC
24	R	608	CHL	C1C-C2C-CMC-OMC
24	S	608	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C1C-C2C-CMC-OMC
24	0	601	CHL	C1C-C2C-CMC-OMC
24	0	609	CHL	C1C-C2C-CMC-OMC
24	7	609	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C1C-C2C-CMC-OMC
24	p	607	CHL	C1C-C2C-CMC-OMC
24	n	606	CHL	C1C-C2C-CMC-OMC
24	n	607	CHL	C1C-C2C-CMC-OMC
24	s	608	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C1C-C2C-CMC-OMC
24	r	608	CHL	C1C-C2C-CMC-OMC
37	C	519	DGD	C1G-C2G-C3G-O3G
29	R	2630	LHG	O7-C5-C6-O8
35	B	621	SQD	O6-C44-C45-O47
35	b	621	SQD	O6-C44-C45-O47
36	A	413	LMG	O7-C8-C9-O8
36	a	413	LMG	O7-C8-C9-O8
25	1	610	CLA	C15-C16-C17-C18
24	p	609	CHL	C4C-C3C-CAC-CBC
29	D	409	LHG	C25-C26-C27-C28
29	n	2630	LHG	C11-C10-C9-C8
36	A	413	LMG	C15-C16-C17-C18
36	a	413	LMG	C15-C16-C17-C18
37	C	519	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C5D-C6D-O5D-C1E
25	Y	602	CLA	C10-C11-C12-C13
24	Y	609	CHL	C3-C5-C6-C7
29	9	2630	LHG	O10-C23-O8-C6
33	A	409	PHO	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
25	Y	604	CLA	C4-C3-C5-C6
25	y	604	CLA	C4-C3-C5-C6
29	4	2630	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	9	605	CHL	CAA-CBA-CGA-O2A
24	g	607	CHL	CAA-CBA-CGA-O2A
24	G	609	CHL	C10-C11-C12-C13
25	p	604	CLA	C5-C6-C7-C8
24	2	601	CHL	C11-C12-C13-C14
24	3	601	CHL	C11-C10-C8-C9
24	3	601	CHL	C11-C12-C13-C14
24	3	605	CHL	C14-C13-C15-C16
24	4	601	CHL	C6-C7-C8-C9
24	5	605	CHL	C6-C7-C8-C9
24	G	609	CHL	C11-C12-C13-C14
24	N	605	CHL	C6-C7-C8-C9
24	R	606	CHL	C14-C13-C15-C16
24	Y	601	CHL	C11-C12-C13-C14
24	Y	601	CHL	C14-C13-C15-C16
24	0	606	CHL	C11-C10-C8-C9
24	8	601	CHL	C11-C10-C8-C9
24	8	601	CHL	C11-C12-C13-C14
24	8	605	CHL	C11-C12-C13-C14
24	p	609	CHL	C11-C12-C13-C14
24	p	609	CHL	C14-C13-C15-C16
24	q	609	CHL	C11-C12-C13-C14
24	g	609	CHL	C11-C12-C13-C14
24	y	601	CHL	C11-C12-C13-C14
24	r	606	CHL	C6-C7-C8-C9
24	r	606	CHL	C14-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C9
25	1	610	CLA	C6-C7-C8-C9
25	4	613	CLA	C11-C10-C8-C9
25	5	603	CLA	C11-C10-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	G	603	CLA	C11-C10-C8-C9
25	Y	604	CLA	C6-C7-C8-C9
25	7	602	CLA	C6-C7-C8-C9
25	7	612	CLA	C11-C10-C8-C9
25	7	613	CLA	C6-C7-C8-C9
25	p	613	CLA	C11-C10-C8-C9
25	q	603	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	g	603	CLA	C11-C10-C8-C9
25	n	603	CLA	C11-C12-C13-C14
25	y	604	CLA	C6-C7-C8-C9
25	y	613	CLA	C11-C10-C8-C9
25	c	503	CLA	O1A-CGA-O2A-C1
25	R	609	CLA	C2C-C3C-CAC-CBC
29	2	2630	LHG	C16-C17-C18-C19
35	b	623	SQD	C11-C12-C13-C14
24	7	607	CHL	C16-C17-C18-C19
24	y	601	CHL	C16-C17-C18-C19
25	n	613	CLA	C16-C17-C18-C19
24	8	609	CHL	C8-C10-C11-C12
25	r	609	CLA	C2C-C3C-CAC-CBC
40	f	101	HEM	C2A-CAA-CBA-CGA
24	R	608	CHL	C2A-CAA-CBA-CGA
25	5	604	CLA	C3-C5-C6-C7
35	B	623	SQD	C11-C12-C13-C14
24	N	605	CHL	C16-C17-C18-C19
24	N	609	CHL	C16-C17-C18-C19
25	N	613	CLA	C16-C17-C18-C19
25	q	602	CLA	C16-C17-C18-C20
27	q	1622	XAT	C11-C12-C13-C14
24	1	605	CHL	C2B-C3B-CAB-CBB
24	1	607	CHL	C2B-C3B-CAB-CBB
24	2	601	CHL	C2B-C3B-CAB-CBB
24	4	607	CHL	C2B-C3B-CAB-CBB
24	5	601	CHL	C2B-C3B-CAB-CBB
24	5	608	CHL	C2B-C3B-CAB-CBB
24	6	607	CHL	C2B-C3B-CAB-CBB
24	6	609	CHL	C2B-C3B-CAB-CBB
24	G	609	CHL	C2B-C3B-CAB-CBB
24	R	606	CHL	C2B-C3B-CAB-CBB
24	S	606	CHL	C2B-C3B-CAB-CBB
24	S	608	CHL	C2B-C3B-CAB-CBB
24	0	605	CHL	C2B-C3B-CAB-CBB
24	7	605	CHL	C2B-C3B-CAB-CBB
24	7	607	CHL	C2B-C3B-CAB-CBB
24	7	608	CHL	C2B-C3B-CAB-CBB
24	9	607	CHL	C2B-C3B-CAB-CBB
24	9	608	CHL	C2B-C3B-CAB-CBB
24	p	601	CHL	C2B-C3B-CAB-CBB
24	p	605	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	q	606	CHL	C2B-C3B-CAB-CBB
24	g	609	CHL	C2B-C3B-CAB-CBB
24	s	606	CHL	C2B-C3B-CAB-CBB
24	s	608	CHL	C2B-C3B-CAB-CBB
24	y	601	CHL	C2B-C3B-CAB-CBB
24	r	606	CHL	C2B-C3B-CAB-CBB
25	1	612	CLA	C2B-C3B-CAB-CBB
25	3	610	CLA	C2B-C3B-CAB-CBB
25	4	602	CLA	C2B-C3B-CAB-CBB
25	4	604	CLA	C2B-C3B-CAB-CBB
25	5	613	CLA	C2B-C3B-CAB-CBB
25	6	602	CLA	C2B-C3B-CAB-CBB
25	B	608	CLA	C2B-C3B-CAB-CBB
25	D	402	CLA	C2B-C3B-CAB-CBB
25	G	604	CLA	C2B-C3B-CAB-CBB
25	G	610	CLA	C2B-C3B-CAB-CBB
25	N	604	CLA	C2B-C3B-CAB-CBB
25	R	609	CLA	C2B-C3B-CAB-CBB
25	R	610	CLA	C2B-C3B-CAB-CBB
25	R	613	CLA	C2B-C3B-CAB-CBB
25	S	611	CLA	C2B-C3B-CAB-CBB
25	Y	612	CLA	C2B-C3B-CAB-CBB
25	0	602	CLA	C2B-C3B-CAB-CBB
25	0	614	CLA	C2B-C3B-CAB-CBB
25	7	602	CLA	C2B-C3B-CAB-CBB
25	7	612	CLA	C2B-C3B-CAB-CBB
25	8	610	CLA	C2B-C3B-CAB-CBB
25	9	610	CLA	C2B-C3B-CAB-CBB
25	p	602	CLA	C2B-C3B-CAB-CBB
25	q	602	CLA	C2B-C3B-CAB-CBB
25	c	513	CLA	C2B-C3B-CAB-CBB
25	d	402	CLA	C2B-C3B-CAB-CBB
25	g	604	CLA	C2B-C3B-CAB-CBB
25	g	610	CLA	C2B-C3B-CAB-CBB
25	n	604	CLA	C2B-C3B-CAB-CBB
25	s	612	CLA	C2B-C3B-CAB-CBB
25	y	612	CLA	C2B-C3B-CAB-CBB
25	r	610	CLA	C2B-C3B-CAB-CBB
25	r	613	CLA	C2B-C3B-CAB-CBB
29	r	2630	LHG	O9-C7-O7-C5
25	C	505	CLA	C5-C6-C7-C8
36	h	102	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	1	603	CLA	O1D-CGD-O2D-CED
24	7	609	CHL	C2-C3-C5-C6
24	n	605	CHL	C2-C3-C5-C6
25	b	608	CLA	C2-C3-C5-C6
24	y	607	CHL	C10-C11-C12-C13
25	G	610	CLA	C16-C17-C18-C20
25	g	610	CLA	C16-C17-C18-C20
36	b	622	LMG	C18-C19-C20-C21
36	H	102	LMG	C35-C36-C37-C38
24	1	608	CHL	C1-C2-C3-C4
24	2	606	CHL	C1-C2-C3-C4
24	2	607	CHL	C1-C2-C3-C4
24	3	608	CHL	C1-C2-C3-C4
24	4	606	CHL	C1-C2-C3-C4
24	4	607	CHL	C1-C2-C3-C4
24	5	608	CHL	C1-C2-C3-C4
24	6	608	CHL	C1-C2-C3-C4
24	G	606	CHL	C1-C2-C3-C4
24	G	607	CHL	C1-C2-C3-C4
24	N	608	CHL	C1-C2-C3-C4
24	Y	608	CHL	C1-C2-C3-C4
24	0	608	CHL	C1-C2-C3-C4
24	7	608	CHL	C1-C2-C3-C4
24	8	608	CHL	C1-C2-C3-C4
24	9	606	CHL	C1-C2-C3-C4
24	9	607	CHL	C1-C2-C3-C4
24	p	608	CHL	C1-C2-C3-C4
24	q	606	CHL	C1-C2-C3-C4
24	q	607	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	g	607	CHL	C1-C2-C3-C4
24	n	608	CHL	C1-C2-C3-C4
24	y	608	CHL	C1-C2-C3-C4
25	2	604	CLA	C1-C2-C3-C4
25	2	614	CLA	C1-C2-C3-C4
25	3	611	CLA	C1-C2-C3-C4
25	3	614	CLA	C1-C2-C3-C4
25	4	604	CLA	C1-C2-C3-C4
25	4	614	CLA	C1-C2-C3-C4
25	5	611	CLA	C1-C2-C3-C4
25	5	614	CLA	C1-C2-C3-C4
25	G	604	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	G	614	CLA	C1-C2-C3-C4
25	N	611	CLA	C1-C2-C3-C4
25	N	614	CLA	C1-C2-C3-C4
25	R	601	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	R	612	CLA	C1-C2-C3-C4
25	S	602	CLA	C1-C2-C3-C4
25	S	604	CLA	C1-C2-C3-C4
25	S	610	CLA	C1-C2-C3-C4
25	S	611	CLA	C1-C2-C3-C4
25	S	613	CLA	C1-C2-C3-C4
25	8	611	CLA	C1-C2-C3-C4
25	8	614	CLA	C1-C2-C3-C4
25	9	604	CLA	C1-C2-C3-C4
25	9	614	CLA	C1-C2-C3-C4
25	p	611	CLA	C1-C2-C3-C4
25	p	614	CLA	C1-C2-C3-C4
25	q	604	CLA	C1-C2-C3-C4
25	q	614	CLA	C1-C2-C3-C4
25	g	604	CLA	C1-C2-C3-C4
25	g	614	CLA	C1-C2-C3-C4
25	n	611	CLA	C1-C2-C3-C4
25	n	614	CLA	C1-C2-C3-C4
25	s	602	CLA	C1-C2-C3-C4
25	s	604	CLA	C1-C2-C3-C4
25	s	610	CLA	C1-C2-C3-C4
25	s	611	CLA	C1-C2-C3-C4
25	s	613	CLA	C1-C2-C3-C4
25	r	601	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4
25	r	612	CLA	C1-C2-C3-C4
36	B	622	LMG	C18-C19-C20-C21
25	2	602	CLA	C15-C16-C17-C18
35	D	413	SQD	C44-C45-O47-C7
35	d	413	SQD	C44-C45-O47-C7
29	C	2630	LHG	O6-C4-C5-C6
29	c	2630	LHG	O6-C4-C5-C6
25	3	612	CLA	C2A-CAA-CBA-CGA
25	0	613	CLA	C2A-CAA-CBA-CGA
25	8	612	CLA	C2A-CAA-CBA-CGA
29	S	2630	LHG	O9-C7-O7-C5
29	3	2630	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	1	607	CHL	C2-C1-O2A-CGA
24	3	605	CHL	C2-C1-O2A-CGA
24	4	609	CHL	C2-C1-O2A-CGA
24	7	607	CHL	C2-C1-O2A-CGA
24	8	605	CHL	C2-C1-O2A-CGA
24	p	601	CHL	C2-C1-O2A-CGA
24	p	607	CHL	C2-C1-O2A-CGA
25	C	505	CLA	C2-C1-O2A-CGA
25	R	611	CLA	C2-C1-O2A-CGA
25	p	604	CLA	C2-C1-O2A-CGA
25	c	503	CLA	C2-C1-O2A-CGA
25	r	611	CLA	C2-C1-O2A-CGA
25	r	612	CLA	C2-C1-O2A-CGA
35	A	412	SQD	C14-C15-C16-C17
36	h	102	LMG	C35-C36-C37-C38
29	D	409	LHG	C28-C29-C30-C31
24	N	609	CHL	O1A-CGA-O2A-C1
25	A	410	CLA	C3-C5-C6-C7
29	N	2630	LHG	C27-C28-C29-C30
35	a	412	SQD	C14-C15-C16-C17
24	3	607	CHL	C2C-C3C-CAC-CBC
29	4	2630	LHG	O6-C4-C5-O7
24	n	605	CHL	O1D-CGD-O2D-CED
25	g	602	CLA	O1D-CGD-O2D-CED
26	4	1620	LUT	C1-C6-C7-C8
26	5	1621	LUT	C1-C6-C7-C8
26	6	1621	LUT	C1-C6-C7-C8
26	6	1621	LUT	C5-C6-C7-C8
26	S	1620	LUT	C1-C6-C7-C8
26	Y	1621	LUT	C1-C6-C7-C8
26	9	1620	LUT	C1-C6-C7-C8
26	s	1620	LUT	C1-C6-C7-C8
26	y	1621	LUT	C1-C6-C7-C8
24	N	605	CHL	C2-C3-C5-C6
25	Y	603	CLA	C2-C3-C5-C6
29	Y	2630	LHG	O10-C23-O8-C6
33	A	409	PHO	C8-C10-C11-C12
24	4	607	CHL	CAA-CBA-CGA-O2A
29	r	2630	LHG	C25-C26-C27-C28
24	R	607	CHL	C6-C7-C8-C9
29	S	2630	LHG	C8-C7-O7-C5
29	r	2630	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
33	a	409	PHO	C8-C10-C11-C12
24	4	606	CHL	C2A-CAA-CBA-CGA
29	4	2630	LHG	C3-O3-P-O6
29	5	2630	LHG	C3-O3-P-O6
29	G	2630	LHG	C3-O3-P-O6
29	G	2630	LHG	C4-O6-P-O3
29	L	101	LHG	C3-O3-P-O6
29	S	2630	LHG	C3-O3-P-O6
29	0	2630	LHG	C3-O3-P-O6
29	p	2630	LHG	C3-O3-P-O6
29	g	2630	LHG	C3-O3-P-O6
29	g	2630	LHG	C4-O6-P-O3
29	s	2630	LHG	C3-O3-P-O6
29	R	2630	LHG	C25-C26-C27-C28
24	Y	609	CHL	C16-C17-C18-C19
35	b	623	SQD	C12-C13-C14-C15
29	0	2630	LHG	C4-C5-C6-O8
24	5	609	CHL	C4C-C3C-CAC-CBC
24	n	607	CHL	C5-C6-C7-C8
24	3	607	CHL	C6-C7-C8-C10
24	y	609	CHL	C11-C12-C13-C15
25	1	603	CLA	C11-C12-C13-C15
25	B	608	CLA	C6-C7-C8-C10
25	B	610	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	7	612	CLA	C11-C10-C8-C7
25	b	610	CLA	C11-C12-C13-C15
25	c	502	CLA	C12-C13-C15-C16
25	y	603	CLA	C11-C10-C8-C7
29	D	410	LHG	C29-C30-C31-C32
29	d	410	LHG	C29-C30-C31-C32
24	q	601	CHL	C3-C5-C6-C7
24	3	605	CHL	C11-C12-C13-C14
24	4	601	CHL	C11-C10-C8-C9
24	6	606	CHL	C11-C12-C13-C14
24	N	601	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C12-C13-C14
24	0	606	CHL	C11-C12-C13-C14
24	8	605	CHL	C14-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C9
24	n	605	CHL	C6-C7-C8-C9
24	n	609	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	y	601	CHL	C14-C13-C15-C16
25	1	603	CLA	C14-C13-C15-C16
25	1	604	CLA	C6-C7-C8-C9
25	1	613	CLA	C6-C7-C8-C9
25	3	613	CLA	C11-C10-C8-C9
25	6	612	CLA	C6-C7-C8-C9
25	6	612	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	B	608	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	N	603	CLA	C11-C12-C13-C14
25	Y	612	CLA	C6-C7-C8-C9
25	Y	613	CLA	C11-C10-C8-C9
25	0	612	CLA	C14-C13-C15-C16
25	0	613	CLA	C11-C10-C8-C9
25	7	604	CLA	C6-C7-C8-C9
25	8	613	CLA	C11-C10-C8-C9
25	p	603	CLA	C11-C10-C8-C9
25	p	603	CLA	C14-C13-C15-C16
25	p	610	CLA	C11-C10-C8-C9
25	q	603	CLA	C11-C10-C8-C9
25	q	610	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	c	505	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C9
25	y	612	CLA	C6-C7-C8-C9
25	R	602	CLA	C8-C10-C11-C12
34	C	516	BCR	C15-C16-C17-C18
34	c	516	BCR	C15-C16-C17-C18
24	r	607	CHL	C6-C7-C8-C9
29	1	2630	LHG	C32-C33-C34-C35
33	A	408	PHO	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
25	6	602	CLA	C8-C10-C11-C12
25	b	615	CLA	C13-C15-C16-C17
25	r	602	CLA	C8-C10-C11-C12
36	C	521	LMG	C32-C33-C34-C35
36	h	102	LMG	C31-C32-C33-C34
28	9	1623	NEX	C31-C32-C33-C40
25	C	511	CLA	C16-C17-C18-C20
29	0	2630	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C13-C15-C16-C17
25	0	613	CLA	C15-C16-C17-C18
25	q	613	CLA	C13-C15-C16-C17
29	7	2630	LHG	C15-C16-C17-C18
29	4	2630	LHG	C1-C2-C3-O3
29	q	2630	LHG	C1-C2-C3-O3
36	C	521	LMG	C33-C34-C35-C36
25	7	610	CLA	C4-C3-C5-C6
25	C	512	CLA	C2-C3-C5-C6
25	7	614	CLA	C6-C7-C8-C9
24	7	608	CHL	CBA-CGA-O2A-C1
36	c	521	LMG	C32-C33-C34-C35
24	n	609	CHL	O1A-CGA-O2A-C1
29	3	2630	LHG	O10-C23-O8-C6
33	a	408	PHO	O1A-CGA-O2A-C1
35	D	413	SQD	O10-C23-O48-C46
35	d	413	SQD	O10-C23-O48-C46
25	a	410	CLA	C3-C5-C6-C7
24	3	607	CHL	C4C-C3C-CAC-CBC
25	1	614	CLA	C5-C6-C7-C8
24	2	601	CHL	C5-C6-C7-C8
25	p	603	CLA	C5-C6-C7-C8
25	R	604	CLA	O2A-C1-C2-C3
33	A	408	PHO	O1A-CGA-O2A-C1
35	D	413	SQD	C24-C23-O48-C46
35	d	413	SQD	C24-C23-O48-C46
24	p	608	CHL	C4B-C3B-CAB-CBB
24	n	605	CHL	C4B-C3B-CAB-CBB
25	2	613	CLA	C4B-C3B-CAB-CBB
25	4	602	CLA	C4B-C3B-CAB-CBB
25	4	612	CLA	C4B-C3B-CAB-CBB
25	5	602	CLA	C4B-C3B-CAB-CBB
25	6	602	CLA	C4B-C3B-CAB-CBB
25	6	613	CLA	C4B-C3B-CAB-CBB
25	A	405	CLA	C4B-C3B-CAB-CBB
25	B	608	CLA	C4B-C3B-CAB-CBB
25	B	615	CLA	C4B-C3B-CAB-CBB
25	N	604	CLA	C4B-C3B-CAB-CBB
25	R	604	CLA	C4B-C3B-CAB-CBB
25	R	613	CLA	C4B-C3B-CAB-CBB
25	0	602	CLA	C4B-C3B-CAB-CBB
25	8	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	9	602	CLA	C4B-C3B-CAB-CBB
25	9	610	CLA	C4B-C3B-CAB-CBB
25	9	613	CLA	C4B-C3B-CAB-CBB
25	p	602	CLA	C4B-C3B-CAB-CBB
25	q	602	CLA	C4B-C3B-CAB-CBB
25	q	603	CLA	C4B-C3B-CAB-CBB
25	q	612	CLA	C4B-C3B-CAB-CBB
25	a	405	CLA	C4B-C3B-CAB-CBB
25	b	615	CLA	C4B-C3B-CAB-CBB
25	c	513	CLA	C4B-C3B-CAB-CBB
25	g	604	CLA	C4B-C3B-CAB-CBB
25	y	603	CLA	C4B-C3B-CAB-CBB
25	r	604	CLA	C4B-C3B-CAB-CBB
25	r	613	CLA	C4B-C3B-CAB-CBB
24	p	607	CHL	C2A-CAA-CBA-CGA
25	B	615	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
35	b	623	SQD	O5-C1-O6-C44
36	S	2631	LMG	O6-C1-O1-C7
36	s	2631	LMG	O6-C1-O1-C7
34	B	618	BCR	C19-C20-C21-C22
34	b	618	BCR	C19-C20-C21-C22
37	C	519	DGD	O1B-C1B-O2G-C2G
24	7	608	CHL	O1A-CGA-O2A-C1
29	d	410	LHG	O6-C4-C5-O7
25	6	611	CLA	C16-C17-C18-C19
25	C	511	CLA	C16-C17-C18-C19
33	A	409	PHO	C16-C17-C18-C19
33	a	409	PHO	C16-C17-C18-C19
36	c	521	LMG	C33-C34-C35-C36
25	R	610	CLA	C4-C3-C5-C6
25	7	613	CLA	C13-C15-C16-C17
29	3	2630	LHG	C29-C30-C31-C32
29	D	408	LHG	C25-C26-C27-C28
29	4	2630	LHG	O10-C23-O8-C6
25	1	613	CLA	C13-C15-C16-C17
37	c	519	DGD	O1B-C1B-O2G-C2G
29	7	2630	LHG	C32-C33-C34-C35
25	4	612	CLA	CBD-CGD-O2D-CED
24	6	609	CHL	C2-C1-O2A-CGA
24	Y	609	CHL	C2-C1-O2A-CGA
24	0	608	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	0	609	CHL	C2-C1-O2A-CGA
25	1	611	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	R	603	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
25	r	603	CLA	C2-C1-O2A-CGA
33	A	409	PHO	C16-C17-C18-C20
33	a	409	PHO	C16-C17-C18-C20
29	d	408	LHG	C25-C26-C27-C28
24	S	601	CHL	CAA-CBA-CGA-O1A
40	F	101	HEM	CAD-CBD-CGD-O1D
25	1	613	CLA	C2A-CAA-CBA-CGA
25	4	613	CLA	C2A-CAA-CBA-CGA
25	6	613	CLA	C2A-CAA-CBA-CGA
25	7	613	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
29	2	2630	LHG	O7-C5-C6-O8
29	c	2630	LHG	C34-C35-C36-C37
24	6	606	CHL	C3A-C2A-CAA-CBA
24	8	601	CHL	C3A-C2A-CAA-CBA
24	9	609	CHL	C3A-C2A-CAA-CBA
24	q	601	CHL	C3A-C2A-CAA-CBA
24	n	608	CHL	C3A-C2A-CAA-CBA
25	4	613	CLA	C3A-C2A-CAA-CBA
25	B	605	CLA	C3A-C2A-CAA-CBA
25	B	610	CLA	C3A-C2A-CAA-CBA
25	q	613	CLA	C3A-C2A-CAA-CBA
25	b	605	CLA	C3A-C2A-CAA-CBA
25	b	610	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	C16-C17-C18-C19
24	0	609	CHL	C4C-C3C-CAC-CBC
24	q	607	CHL	O2A-C1-C2-C3
26	q	1621	LUT	C9-C10-C11-C12
25	1	603	CLA	C4-C3-C5-C6
25	6	613	CLA	C4-C3-C5-C6
25	N	613	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	n	613	CLA	C4-C3-C5-C6
25	r	610	CLA	C4-C3-C5-C6
25	n	613	CLA	C2-C3-C5-C6
24	1	609	CHL	C6-C7-C8-C9
24	3	605	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	N	609	CHL	C6-C7-C8-C9
24	R	606	CHL	C6-C7-C8-C9
24	Y	606	CHL	C14-C13-C15-C16
24	Y	609	CHL	C14-C13-C15-C16
24	0	607	CHL	C6-C7-C8-C9
24	7	606	CHL	C14-C13-C15-C16
24	n	607	CHL	C11-C12-C13-C14
24	n	609	CHL	C6-C7-C8-C9
24	y	606	CHL	C14-C13-C15-C16
24	y	609	CHL	C14-C13-C15-C16
25	1	604	CLA	C11-C12-C13-C14
25	3	603	CLA	C14-C13-C15-C16
25	3	613	CLA	C6-C7-C8-C9
25	4	603	CLA	C11-C12-C13-C14
25	B	611	CLA	C11-C12-C13-C14
25	C	502	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	7	603	CLA	C14-C13-C15-C16
25	7	604	CLA	C11-C12-C13-C14
25	8	613	CLA	C6-C7-C8-C9
25	q	610	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	c	502	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C12-C13-C14
24	8	609	CHL	C16-C17-C18-C19
24	8	609	CHL	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C20
29	d	409	LHG	C28-C29-C30-C31
24	g	605	CHL	CBA-CGA-O2A-C1
35	B	621	SQD	C13-C14-C15-C16
36	b	622	LMG	C16-C17-C18-C19
35	B	623	SQD	C12-C13-C14-C15
25	B	605	CLA	C15-C16-C17-C18
28	1	1623	NEX	C39-C29-C30-C31
28	2	1623	NEX	C39-C29-C30-C31
28	3	1623	NEX	C39-C29-C30-C31
28	4	1623	NEX	C39-C29-C30-C31
28	5	1623	NEX	C39-C29-C30-C31
28	6	1623	NEX	C39-C29-C30-C31
28	G	1623	NEX	C39-C29-C30-C31
28	N	1623	NEX	C39-C29-C30-C31
28	R	623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	S	1623	NEX	C39-C29-C30-C31
28	Y	1623	NEX	C39-C29-C30-C31
28	0	1623	NEX	C39-C29-C30-C31
28	7	1623	NEX	C39-C29-C30-C31
28	8	1623	NEX	C39-C29-C30-C31
28	9	1623	NEX	C39-C29-C30-C31
28	p	1623	NEX	C39-C29-C30-C31
28	q	1623	NEX	C39-C29-C30-C31
28	g	1623	NEX	C39-C29-C30-C31
28	n	1623	NEX	C39-C29-C30-C31
28	s	1623	NEX	C39-C29-C30-C31
28	y	1623	NEX	C39-C29-C30-C31
28	r	623	NEX	C39-C29-C30-C31
29	3	2630	LHG	C1-C2-C3-O3
29	8	2630	LHG	C1-C2-C3-O3
35	b	621	SQD	C13-C14-C15-C16
24	G	607	CHL	C2A-CAA-CBA-CGA
25	y	613	CLA	C8-C10-C11-C12
25	1	614	CLA	C6-C7-C8-C9
25	7	614	CLA	C5-C6-C7-C8
36	H	102	LMG	C31-C32-C33-C34
37	C	519	DGD	O1A-C1A-O1G-C1G
36	H	102	LMG	C4-C5-C6-O5
24	q	607	CHL	CAA-CBA-CGA-O1A
24	N	605	CHL	C16-C17-C18-C20
29	l	101	LHG	C15-C16-C17-C18
24	3	606	CHL	CAA-CBA-CGA-O1A
24	s	601	CHL	CAA-CBA-CGA-O1A
25	n	612	CLA	CAA-CBA-CGA-O1A
26	4	1621	LUT	C7-C8-C9-C19
26	N	1621	LUT	C7-C8-C9-C19
26	n	1621	LUT	C7-C8-C9-C19
34	B	618	BCR	C36-C18-C19-C20
34	b	618	BCR	C36-C18-C19-C20
29	n	2630	LHG	C24-C25-C26-C27
29	5	2630	LHG	C11-C10-C9-C8
37	C	520	DGD	C4B-C5B-C6B-C7B
24	4	605	CHL	O1A-CGA-O2A-C1
24	6	606	CHL	C8-C10-C11-C12
24	8	607	CHL	C4-C3-C5-C6
25	a	410	CLA	C4-C3-C5-C6
25	g	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	3	608	CHL	C1A-C2A-CAA-CBA
24	R	608	CHL	C1A-C2A-CAA-CBA
24	S	606	CHL	C1A-C2A-CAA-CBA
24	7	606	CHL	C1A-C2A-CAA-CBA
24	8	601	CHL	C1A-C2A-CAA-CBA
24	8	608	CHL	C1A-C2A-CAA-CBA
24	s	606	CHL	C1A-C2A-CAA-CBA
24	r	608	CHL	C1A-C2A-CAA-CBA
25	B	608	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C1A-C2A-CAA-CBA
25	8	610	CLA	C1A-C2A-CAA-CBA
25	p	602	CLA	C1A-C2A-CAA-CBA
25	q	613	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
25	b	610	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C1A-C2A-CAA-CBA
25	c	504	CLA	C1A-C2A-CAA-CBA
25	c	505	CLA	C1A-C2A-CAA-CBA
29	4	2630	LHG	C34-C35-C36-C37
36	B	622	LMG	C16-C17-C18-C19
37	c	520	DGD	C4B-C5B-C6B-C7B
24	2	601	CHL	C11-C10-C8-C7
24	3	607	CHL	C11-C12-C13-C15
24	5	601	CHL	C12-C13-C15-C16
24	5	609	CHL	C11-C10-C8-C7
24	6	609	CHL	C11-C10-C8-C7
24	N	607	CHL	C11-C12-C13-C15
24	Y	609	CHL	C11-C12-C13-C15
24	8	607	CHL	C11-C12-C13-C15
24	p	607	CHL	C11-C12-C13-C15
24	y	601	CHL	C6-C7-C8-C10
25	5	604	CLA	C12-C13-C15-C16
25	6	613	CLA	C12-C13-C15-C16
25	Y	613	CLA	C6-C7-C8-C10
25	0	604	CLA	C12-C13-C15-C16
25	7	603	CLA	C11-C12-C13-C15
25	9	603	CLA	C11-C10-C8-C7
24	y	609	CHL	C2C-C3C-CAC-CBC
24	0	606	CHL	C8-C10-C11-C12
37	c	519	DGD	O1A-C1A-O1G-C1G
24	S	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	4	610	CLA	O1D-CGD-O2D-CED
24	6	606	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C3C-C2C-CMC-OMC
24	g	607	CHL	C2A-CAA-CBA-CGA
25	B	617	CLA	C2A-CAA-CBA-CGA
25	9	610	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	C2A-CAA-CBA-CGA
33	A	408	PHO	C2A-CAA-CBA-CGA
33	a	408	PHO	C2A-CAA-CBA-CGA
24	1	607	CHL	C10-C11-C12-C13
24	7	607	CHL	C10-C11-C12-C13
25	G	610	CLA	C5-C6-C7-C8
25	0	602	CLA	C8-C10-C11-C12
25	g	610	CLA	C5-C6-C7-C8
24	8	606	CHL	CAA-CBA-CGA-O1A
24	4	607	CHL	O2A-C1-C2-C3
25	S	611	CLA	O2A-C1-C2-C3
25	q	604	CLA	O2A-C1-C2-C3
24	G	605	CHL	CBA-CGA-O2A-C1
29	y	2630	LHG	C24-C23-O8-C6
35	B	621	SQD	C27-C28-C29-C30
35	b	621	SQD	C27-C28-C29-C30
25	5	610	CLA	CBD-CGD-O2D-CED
24	1	609	CHL	C13-C15-C16-C17
24	8	606	CHL	CAA-CBA-CGA-O2A
25	p	612	CLA	CAA-CBA-CGA-O2A
40	F	101	HEM	CAD-CBD-CGD-O2D
29	1	2630	LHG	C15-C16-C17-C18
25	A	410	CLA	C4-C3-C5-C6
25	G	610	CLA	C4-C3-C5-C6
35	B	621	SQD	C34-C35-C36-C37
36	s	2631	LMG	C29-C30-C31-C32
25	Y	613	CLA	C8-C10-C11-C12
25	6	613	CLA	C2-C3-C5-C6
25	B	608	CLA	C2-C3-C5-C6
25	N	613	CLA	C2-C3-C5-C6
25	R	610	CLA	C2-C3-C5-C6
24	1	601	CHL	C2B-C3B-CAB-CBB
24	2	605	CHL	C2B-C3B-CAB-CBB
24	2	607	CHL	C2B-C3B-CAB-CBB
24	2	609	CHL	C2B-C3B-CAB-CBB
24	3	607	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	4	609	CHL	C2B-C3B-CAB-CBB
24	5	605	CHL	C2B-C3B-CAB-CBB
24	6	601	CHL	C2B-C3B-CAB-CBB
24	6	608	CHL	C2B-C3B-CAB-CBB
24	N	605	CHL	C2B-C3B-CAB-CBB
24	N	607	CHL	C2B-C3B-CAB-CBB
24	R	607	CHL	C2B-C3B-CAB-CBB
24	R	608	CHL	C2B-C3B-CAB-CBB
24	Y	601	CHL	C2B-C3B-CAB-CBB
24	Y	609	CHL	C2B-C3B-CAB-CBB
24	0	601	CHL	C2B-C3B-CAB-CBB
24	0	608	CHL	C2B-C3B-CAB-CBB
24	0	609	CHL	C2B-C3B-CAB-CBB
24	7	601	CHL	C2B-C3B-CAB-CBB
24	8	607	CHL	C2B-C3B-CAB-CBB
24	9	605	CHL	C2B-C3B-CAB-CBB
24	9	609	CHL	C2B-C3B-CAB-CBB
24	p	607	CHL	C2B-C3B-CAB-CBB
24	p	608	CHL	C2B-C3B-CAB-CBB
24	p	609	CHL	C2B-C3B-CAB-CBB
24	q	607	CHL	C2B-C3B-CAB-CBB
24	n	605	CHL	C2B-C3B-CAB-CBB
24	n	607	CHL	C2B-C3B-CAB-CBB
24	y	609	CHL	C2B-C3B-CAB-CBB
24	r	607	CHL	C2B-C3B-CAB-CBB
24	r	608	CHL	C2B-C3B-CAB-CBB
25	2	610	CLA	C2B-C3B-CAB-CBB
25	2	613	CLA	C2B-C3B-CAB-CBB
25	4	612	CLA	C2B-C3B-CAB-CBB
25	5	602	CLA	C2B-C3B-CAB-CBB
25	6	613	CLA	C2B-C3B-CAB-CBB
25	A	405	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C2B-C3B-CAB-CBB
25	C	513	CLA	C2B-C3B-CAB-CBB
25	R	604	CLA	C2B-C3B-CAB-CBB
25	S	612	CLA	C2B-C3B-CAB-CBB
25	Y	603	CLA	C2B-C3B-CAB-CBB
25	8	613	CLA	C2B-C3B-CAB-CBB
25	9	602	CLA	C2B-C3B-CAB-CBB
25	9	613	CLA	C2B-C3B-CAB-CBB
25	q	603	CLA	C2B-C3B-CAB-CBB
25	a	405	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C2B-C3B-CAB-CBB
25	b	615	CLA	C2B-C3B-CAB-CBB
25	y	603	CLA	C2B-C3B-CAB-CBB
25	r	604	CLA	C2B-C3B-CAB-CBB
29	D	408	LHG	C24-C25-C26-C27
29	c	2630	LHG	C11-C10-C9-C8
29	L	101	LHG	C15-C16-C17-C18
29	8	2630	LHG	C29-C30-C31-C32
25	5	604	CLA	C5-C6-C7-C8
25	b	605	CLA	C15-C16-C17-C18
29	r	2630	LHG	C7-C8-C9-C10
36	H	102	LMG	O9-C10-O7-C8
25	B	604	CLA	C16-C17-C18-C20
28	1	1623	NEX	C28-C29-C30-C31
28	2	1623	NEX	C28-C29-C30-C31
28	3	1623	NEX	C28-C29-C30-C31
28	4	1623	NEX	C28-C29-C30-C31
28	5	1623	NEX	C28-C29-C30-C31
28	6	1623	NEX	C28-C29-C30-C31
28	G	1623	NEX	C28-C29-C30-C31
28	N	1623	NEX	C28-C29-C30-C31
28	R	623	NEX	C28-C29-C30-C31
28	S	1623	NEX	C28-C29-C30-C31
28	Y	1623	NEX	C28-C29-C30-C31
28	0	1623	NEX	C28-C29-C30-C31
28	7	1623	NEX	C28-C29-C30-C31
28	8	1623	NEX	C28-C29-C30-C31
28	9	1623	NEX	C28-C29-C30-C31
28	p	1623	NEX	C28-C29-C30-C31
28	q	1623	NEX	C28-C29-C30-C31
28	g	1623	NEX	C28-C29-C30-C31
28	n	1623	NEX	C28-C29-C30-C31
28	s	1623	NEX	C28-C29-C30-C31
28	y	1623	NEX	C28-C29-C30-C31
28	r	623	NEX	C28-C29-C30-C31
25	N	612	CLA	CAA-CBA-CGA-O1A
29	0	2630	LHG	O7-C5-C6-O8
25	2	604	CLA	CBA-CGA-O2A-C1
25	y	614	CLA	CBA-CGA-O2A-C1
35	b	621	SQD	C34-C35-C36-C37
24	p	605	CHL	O1D-CGD-O2D-CED
25	5	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	d	410	LHG	C9-C10-C11-C12
28	y	1623	NEX	C33-C34-C35-C15
25	p	612	CLA	CAA-CBA-CGA-O1A
29	S	2630	LHG	C24-C25-C26-C27
29	R	2630	LHG	C7-C8-C9-C10
24	8	601	CHL	C10-C11-C12-C13
25	4	610	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	O1A-CGA-O2A-C1
29	0	2630	LHG	C1-C2-C3-O3
29	n	2630	LHG	C1-C2-C3-O3
29	d	408	LHG	C24-C25-C26-C27
25	4	612	CLA	O1D-CGD-O2D-CED
24	Y	606	CHL	C4-C3-C5-C6
24	7	601	CHL	C4-C3-C5-C6
24	y	606	CHL	C4-C3-C5-C6
25	C	509	CLA	C4-C3-C5-C6
24	8	609	CHL	C2-C1-O2A-CGA
24	q	609	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
24	y	609	CHL	C2-C1-O2A-CGA
25	6	611	CLA	C2-C1-O2A-CGA
25	B	605	CLA	C2-C1-O2A-CGA
25	B	611	CLA	C2-C1-O2A-CGA
25	b	605	CLA	C2-C1-O2A-CGA
25	b	611	CLA	C2-C1-O2A-CGA
25	c	505	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	1	603	CLA	C2-C3-C5-C6
25	Y	604	CLA	C2-C3-C5-C6
25	7	610	CLA	C2-C3-C5-C6
25	8	603	CLA	C2-C3-C5-C6
25	y	604	CLA	C2-C3-C5-C6
25	r	610	CLA	C2-C3-C5-C6
24	G	605	CHL	C2-C1-O2A-CGA
24	g	605	CHL	O1A-CGA-O2A-C1
25	C	506	CLA	C10-C11-C12-C13
25	9	602	CLA	C13-C15-C16-C17
24	3	606	CHL	CAA-CBA-CGA-O2A
29	N	2630	LHG	C24-C25-C26-C27
24	2	609	CHL	C11-C10-C8-C9
24	p	609	CHL	C6-C7-C8-C9
25	A	405	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	502	CLA	C11-C12-C13-C14
25	0	603	CLA	C11-C10-C8-C9
25	n	602	CLA	C11-C12-C13-C14
25	y	603	CLA	C11-C10-C8-C9
37	c	519	DGD	C2A-C1A-O1G-C1G
24	Y	609	CHL	C2C-C3C-CAC-CBC
24	G	605	CHL	O1A-CGA-O2A-C1
24	g	605	CHL	C2-C1-O2A-CGA
29	0	2630	LHG	C13-C14-C15-C16
25	7	613	CLA	C3-C5-C6-C7
24	s	601	CHL	CAA-CBA-CGA-O2A
25	c	506	CLA	C10-C11-C12-C13
33	a	409	PHO	C1A-C2A-CAA-CBA
35	a	412	SQD	C29-C30-C31-C32
25	4	611	CLA	CAA-CBA-CGA-O1A
25	4	611	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
24	6	608	CHL	O2A-C1-C2-C3
24	G	606	CHL	O2A-C1-C2-C3
24	g	606	CHL	O2A-C1-C2-C3
25	s	611	CLA	O2A-C1-C2-C3
24	q	609	CHL	O1A-CGA-O2A-C1
25	y	614	CLA	O1A-CGA-O2A-C1
26	2	1621	LUT	C1-C6-C7-C8
26	2	1621	LUT	C5-C6-C7-C8
26	G	1621	LUT	C1-C6-C7-C8
26	R	620	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C5-C6-C7-C8
26	0	1621	LUT	C1-C6-C7-C8
26	9	1621	LUT	C1-C6-C7-C8
26	y	1620	LUT	C1-C6-C7-C8
26	r	620	LUT	C1-C6-C7-C8
34	C	516	BCR	C1-C6-C7-C8
29	9	2630	LHG	C24-C25-C26-C27
35	B	621	SQD	C44-C45-C46-O48
35	b	621	SQD	C44-C45-C46-O48
25	N	612	CLA	CAA-CBA-CGA-O2A
24	4	605	CHL	C2-C1-O2A-CGA
24	6	609	CHL	O1A-CGA-O2A-C1
26	q	1621	LUT	C33-C34-C35-C15
26	n	1621	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	Y	1623	NEX	C33-C34-C35-C15
37	C	519	DGD	C2A-C1A-O1G-C1G
29	s	2630	LHG	C24-C25-C26-C27
24	1	601	CHL	C4-C3-C5-C6
24	1	609	CHL	C4-C3-C5-C6
24	N	609	CHL	C4-C3-C5-C6
24	0	606	CHL	C4-C3-C5-C6
25	Y	602	CLA	C4-C3-C5-C6
25	Y	611	CLA	C4-C3-C5-C6
39	D	405	PL9	C45-C44-C46-C47
39	d	405	PL9	C45-C44-C46-C47
27	8	1622	XAT	C31-C32-C33-C34
34	C	514	BCR	C21-C22-C23-C24
34	c	514	BCR	C21-C22-C23-C24
35	A	412	SQD	C29-C30-C31-C32
25	Y	611	CLA	C2-C3-C5-C6
29	7	2630	LHG	C26-C27-C28-C29
36	D	411	LMG	C8-C7-O1-C1
36	d	411	LMG	C8-C7-O1-C1
24	6	605	CHL	CAA-CBA-CGA-O2A
24	0	605	CHL	CAA-CBA-CGA-O2A
24	5	605	CHL	O1A-CGA-O2A-C1
25	p	611	CLA	CAA-CBA-CGA-O2A
36	a	413	LMG	C39-C40-C41-C42
24	3	609	CHL	C16-C17-C18-C19
25	b	604	CLA	C16-C17-C18-C20
36	A	413	LMG	C39-C40-C41-C42
25	6	603	CLA	C13-C15-C16-C17
29	D	410	LHG	O6-C4-C5-O7
24	6	605	CHL	CAA-CBA-CGA-O1A
25	S	612	CLA	CAA-CBA-CGA-O2A
25	s	612	CLA	CAA-CBA-CGA-O2A
25	s	611	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C13-C15-C16-C17
24	8	607	CHL	CAA-CBA-CGA-O2A
36	H	102	LMG	C38-C39-C40-C41
24	p	601	CHL	C3-C5-C6-C7
24	0	605	CHL	CAA-CBA-CGA-O1A
24	4	609	CHL	C4B-C3B-CAB-CBB
24	p	609	CHL	C4B-C3B-CAB-CBB
25	2	602	CLA	C4B-C3B-CAB-CBB
25	2	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	3	602	CLA	C4B-C3B-CAB-CBB
25	3	613	CLA	C4B-C3B-CAB-CBB
25	C	513	CLA	C4B-C3B-CAB-CBB
25	G	604	CLA	C4B-C3B-CAB-CBB
25	0	614	CLA	C4B-C3B-CAB-CBB
25	g	613	CLA	C4B-C3B-CAB-CBB
25	n	604	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C16-C17-C18-C20
25	G	602	CLA	C13-C15-C16-C17
24	6	606	CHL	C4-C3-C5-C6
25	1	610	CLA	C4-C3-C5-C6
25	5	602	CLA	C4-C3-C5-C6
25	8	603	CLA	C4-C3-C5-C6
25	y	602	CLA	C4-C3-C5-C6
39	D	405	PL9	C39-C41-C42-C43
24	N	601	CHL	C12-C13-C15-C16
24	Y	606	CHL	C2-C3-C5-C6
24	0	609	CHL	C11-C10-C8-C7
24	q	601	CHL	C11-C12-C13-C15
24	n	607	CHL	C11-C12-C13-C15
24	y	606	CHL	C2-C3-C5-C6
25	3	613	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C10-C8-C7
25	Y	603	CLA	C11-C10-C8-C7
25	0	603	CLA	C11-C10-C8-C7
25	0	613	CLA	C12-C13-C15-C16
25	8	613	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C10-C8-C7
25	y	611	CLA	C2-C3-C5-C6
24	N	607	CHL	C5-C6-C7-C8
26	4	1621	LUT	C29-C30-C31-C32
25	y	610	CLA	C16-C17-C18-C20
29	6	2630	LHG	C5-C4-O6-P
25	7	603	CLA	C15-C16-C17-C18
35	A	412	SQD	O6-C44-C45-O47
35	b	623	SQD	O47-C45-C46-O48
36	h	102	LMG	O9-C10-O7-C8
24	2	601	CHL	C2C-C3C-CAC-CBC
36	D	412	LMG	C12-C13-C14-C15
25	q	602	CLA	C3-C5-C6-C7
24	p	606	CHL	CAA-CBA-CGA-O2A
24	1	608	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	2	606	CHL	O2A-C1-C2-C3
24	3	608	CHL	O2A-C1-C2-C3
24	N	608	CHL	O2A-C1-C2-C3
24	0	608	CHL	O2A-C1-C2-C3
24	7	608	CHL	O2A-C1-C2-C3
24	8	608	CHL	O2A-C1-C2-C3
24	9	606	CHL	O2A-C1-C2-C3
25	S	604	CLA	O2A-C1-C2-C3
25	s	604	CLA	O2A-C1-C2-C3
29	6	2630	LHG	O8-C23-C24-C25
29	2	2630	LHG	C28-C29-C30-C31
25	b	607	CLA	C5-C6-C7-C8
25	C	506	CLA	C16-C17-C18-C20
25	S	612	CLA	CAA-CBA-CGA-O1A
25	q	611	CLA	CAA-CBA-CGA-O2A
25	s	612	CLA	CAA-CBA-CGA-O1A
24	3	605	CHL	O1D-CGD-O2D-CED
24	4	605	CHL	CBA-CGA-O2A-C1
29	c	2630	LHG	C12-C13-C14-C15
36	d	412	LMG	C12-C13-C14-C15
24	1	606	CHL	CAA-CBA-CGA-O2A
24	9	607	CHL	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
24	3	609	CHL	C4-C3-C5-C6
24	Y	609	CHL	C4-C3-C5-C6
24	9	609	CHL	C4-C3-C5-C6
24	p	601	CHL	C4-C3-C5-C6
25	1	604	CLA	C4-C3-C5-C6
25	4	603	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
25	y	611	CLA	C4-C3-C5-C6
25	B	607	CLA	C5-C6-C7-C8
25	p	610	CLA	C10-C11-C12-C13
29	D	408	LHG	C14-C15-C16-C17
29	y	2630	LHG	C31-C32-C33-C34
36	S	2631	LMG	C29-C30-C31-C32
25	5	612	CLA	CAA-CBA-CGA-O2A
25	6	611	CLA	C16-C17-C18-C20
25	Y	614	CLA	CBA-CGA-O2A-C1
35	D	413	SQD	O48-C23-C24-C25
35	d	413	SQD	O48-C23-C24-C25
24	1	606	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	3	607	CHL	C6-C7-C8-C9
24	4	601	CHL	C11-C12-C13-C14
24	5	609	CHL	C6-C7-C8-C9
24	5	609	CHL	C11-C12-C13-C14
24	R	606	CHL	C11-C10-C8-C9
24	Y	607	CHL	C14-C13-C15-C16
24	8	607	CHL	C6-C7-C8-C9
24	q	601	CHL	C11-C12-C13-C14
24	r	606	CHL	C11-C10-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	501	CLA	C11-C10-C8-C9
25	C	502	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C10-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	Y	613	CLA	C6-C7-C8-C9
25	0	612	CLA	C6-C7-C8-C9
25	8	603	CLA	C14-C13-C15-C16
25	9	603	CLA	C11-C10-C8-C9
25	a	405	CLA	C11-C12-C13-C14
25	b	616	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	y	613	CLA	C6-C7-C8-C9
25	b	609	CLA	C13-C15-C16-C17
36	C	521	LMG	C20-C21-C22-C23
24	3	601	CHL	C3A-C2A-CAA-CBA
24	3	608	CHL	C3A-C2A-CAA-CBA
24	S	606	CHL	C3A-C2A-CAA-CBA
24	8	608	CHL	C3A-C2A-CAA-CBA
25	4	614	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	c	503	CLA	C3A-C2A-CAA-CBA
36	S	2631	LMG	C40-C41-C42-C43
24	2	607	CHL	CAA-CBA-CGA-O2A
25	q	603	CLA	CAA-CBA-CGA-O2A
29	2	2630	LHG	O7-C7-C8-C9
25	g	602	CLA	CBD-CGD-O2D-CED
29	d	408	LHG	C14-C15-C16-C17
24	2	608	CHL	CAD-CBD-CGD-O2D
24	4	605	CHL	CAD-CBD-CGD-O2D
24	6	601	CHL	CAD-CBD-CGD-O2D
24	G	606	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	R	606	CHL	CAD-CBD-CGD-O2D
24	0	607	CHL	CAD-CBD-CGD-O2D
24	9	601	CHL	CAD-CBD-CGD-O2D
24	p	608	CHL	CAD-CBD-CGD-O2D
24	q	605	CHL	CAD-CBD-CGD-O2D
24	g	606	CHL	CAD-CBD-CGD-O2D
24	g	607	CHL	CAD-CBD-CGD-O2D
24	r	606	CHL	CAD-CBD-CGD-O2D
25	1	610	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CAD-CBD-CGD-O2D
25	2	610	CLA	CAD-CBD-CGD-O2D
25	3	610	CLA	CAD-CBD-CGD-O2D
25	3	613	CLA	CAD-CBD-CGD-O2D
25	4	603	CLA	CAD-CBD-CGD-O2D
25	4	610	CLA	CAD-CBD-CGD-O2D
25	4	614	CLA	CAD-CBD-CGD-O2D
25	5	602	CLA	CAD-CBD-CGD-O2D
25	6	602	CLA	CAD-CBD-CGD-O2D
25	6	610	CLA	CAD-CBD-CGD-O2D
25	6	614	CLA	CAD-CBD-CGD-O2D
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CAD-CBD-CGD-O2D
25	C	509	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	G	604	CLA	CAD-CBD-CGD-O2D
25	N	613	CLA	CAD-CBD-CGD-O2D
25	Y	610	CLA	CAD-CBD-CGD-O2D
25	0	610	CLA	CAD-CBD-CGD-O2D
25	7	610	CLA	CAD-CBD-CGD-O2D
25	8	610	CLA	CAD-CBD-CGD-O2D
25	8	613	CLA	CAD-CBD-CGD-O2D
25	9	610	CLA	CAD-CBD-CGD-O2D
25	9	612	CLA	CAD-CBD-CGD-O2D
25	9	614	CLA	CAD-CBD-CGD-O2D
25	p	604	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
25	y	610	CLA	CAD-CBD-CGD-O2D
24	q	609	CHL	CBA-CGA-O2A-C1
24	3	609	CHL	C16-C17-C18-C20
25	y	610	CLA	C16-C17-C18-C19
24	5	608	CHL	C2A-CAA-CBA-CGA
25	3	602	CLA	C2A-CAA-CBA-CGA
29	q	2630	LHG	O9-C7-O7-C5
29	L	101	LHG	C13-C14-C15-C16
24	6	608	CHL	C2-C1-O2A-CGA
25	y	604	CLA	C2-C1-O2A-CGA
24	1	605	CHL	CAA-CBA-CGA-O2A
24	3	607	CHL	CAA-CBA-CGA-O2A
24	6	607	CHL	CAA-CBA-CGA-O2A
25	q	604	CLA	CAA-CBA-CGA-O2A
25	r	616	CLA	CAA-CBA-CGA-O2A
25	0	612	CLA	CBD-CGD-O2D-CED
24	6	609	CHL	CBA-CGA-O2A-C1
24	n	609	CHL	C4-C3-C5-C6
24	y	609	CHL	C4-C3-C5-C6
25	7	604	CLA	C4-C3-C5-C6
24	n	609	CHL	C16-C17-C18-C20
25	5	612	CLA	CAA-CBA-CGA-O1A
37	C	524	DGD	C2B-C3B-C4B-C5B
35	D	413	SQD	O5-C1-O6-C44
35	d	413	SQD	O5-C1-O6-C44
25	1	603	CLA	C15-C16-C17-C18
24	1	609	CHL	C2-C3-C5-C6
25	A	410	CLA	C2-C3-C5-C6
25	a	410	CLA	C2-C3-C5-C6
25	c	509	CLA	C2-C3-C5-C6
25	6	603	CLA	CAA-CBA-CGA-O2A
25	R	616	CLA	CAA-CBA-CGA-O2A
25	p	613	CLA	CAA-CBA-CGA-O2A
29	q	2630	LHG	O7-C7-C8-C9
26	4	1621	LUT	C7-C8-C9-C10
26	p	1620	LUT	C31-C32-C33-C34
27	3	1622	XAT	C31-C32-C33-C34
27	4	1622	XAT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	3	1623	NEX	C31-C32-C33-C34
28	0	1623	NEX	C11-C12-C13-C14
39	d	405	PL9	C39-C41-C42-C43
27	q	1622	XAT	O24-C26-C27-C28
28	3	1623	NEX	O24-C26-C27-C28
28	4	1623	NEX	O24-C26-C27-C28
28	5	1623	NEX	O24-C26-C27-C28
28	6	1623	NEX	O24-C26-C27-C28
28	G	1623	NEX	O24-C26-C27-C28
28	0	1623	NEX	O24-C26-C27-C28
28	8	1623	NEX	O24-C26-C27-C28
28	p	1623	NEX	O24-C26-C27-C28
28	q	1623	NEX	O24-C26-C27-C28
28	g	1623	NEX	O24-C26-C27-C28
29	l	101	LHG	C14-C15-C16-C17
37	c	524	DGD	C2B-C3B-C4B-C5B
25	Y	614	CLA	O1A-CGA-O2A-C1
24	0	607	CHL	CAA-CBA-CGA-O2A
25	0	603	CLA	CAA-CBA-CGA-O2A
25	7	612	CLA	CAA-CBA-CGA-O2A
35	b	623	SQD	O47-C7-C8-C9
24	q	605	CHL	C2-C1-O2A-CGA
29	N	2630	LHG	C23-C24-C25-C26
24	5	608	CHL	O2A-C1-C2-C3
24	Y	608	CHL	O2A-C1-C2-C3
24	5	607	CHL	CAA-CBA-CGA-O1A
24	1	605	CHL	CAA-CBA-CGA-O1A
25	q	611	CLA	CAA-CBA-CGA-O1A
29	6	2630	LHG	C33-C34-C35-C36
24	1	601	CHL	O2A-C1-C2-C3
24	2	601	CHL	O2A-C1-C2-C3
24	3	601	CHL	O2A-C1-C2-C3
24	6	607	CHL	O2A-C1-C2-C3
24	Y	601	CHL	O2A-C1-C2-C3
24	Y	606	CHL	O2A-C1-C2-C3
24	0	601	CHL	O2A-C1-C2-C3
24	0	607	CHL	O2A-C1-C2-C3
24	7	601	CHL	O2A-C1-C2-C3
24	8	601	CHL	O2A-C1-C2-C3
24	y	606	CHL	O2A-C1-C2-C3
25	B	603	CLA	O2A-C1-C2-C3
25	D	402	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	R	603	CLA	O2A-C1-C2-C3
25	b	603	CLA	O2A-C1-C2-C3
25	d	402	CLA	O2A-C1-C2-C3
25	r	603	CLA	O2A-C1-C2-C3
24	9	601	CHL	C2C-C3C-CAC-CBC
29	3	2630	LHG	C11-C12-C13-C14
24	9	606	CHL	CBA-CGA-O2A-C1
25	6	604	CLA	C2A-CAA-CBA-CGA
25	8	602	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C13-C15-C16-C17
25	B	609	CLA	C13-C15-C16-C17
25	y	614	CLA	C5-C6-C7-C8
24	S	608	CHL	CAA-CBA-CGA-O2A
24	s	608	CHL	CAA-CBA-CGA-O2A
25	5	613	CLA	CAA-CBA-CGA-O2A
25	S	602	CLA	CAA-CBA-CGA-O2A
24	7	605	CHL	CAA-CBA-CGA-O2A
25	R	616	CLA	C16-C17-C18-C19
25	r	616	CLA	C16-C17-C18-C19
25	2	603	CLA	O1A-CGA-O2A-C1
24	1	601	CHL	CHA-CBD-CGD-O1D
24	1	601	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	CHA-CBD-CGD-O1D
24	G	601	CHL	CHA-CBD-CGD-O2D
24	0	606	CHL	CHA-CBD-CGD-O2D
24	7	601	CHL	CHA-CBD-CGD-O1D
24	g	601	CHL	CHA-CBD-CGD-O1D
24	g	601	CHL	CHA-CBD-CGD-O2D
25	1	604	CLA	CHA-CBD-CGD-O2D
25	1	612	CLA	CHA-CBD-CGD-O1D
25	2	603	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	CHA-CBD-CGD-O1D
25	4	602	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	613	CLA	CHA-CBD-CGD-O1D
25	B	617	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O1D
25	G	602	CLA	CHA-CBD-CGD-O1D
25	G	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	G	612	CLA	CHA-CBD-CGD-O1D
25	N	604	CLA	CHA-CBD-CGD-O2D
25	N	611	CLA	CHA-CBD-CGD-O2D
25	N	612	CLA	CHA-CBD-CGD-O1D
25	N	612	CLA	CHA-CBD-CGD-O2D
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	616	CLA	CHA-CBD-CGD-O2D
25	S	602	CLA	CHA-CBD-CGD-O1D
25	S	602	CLA	CHA-CBD-CGD-O2D
25	S	604	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CHA-CBD-CGD-O2D
25	Y	604	CLA	CHA-CBD-CGD-O1D
25	Y	604	CLA	CHA-CBD-CGD-O2D
25	Y	612	CLA	CHA-CBD-CGD-O1D
25	Y	612	CLA	CHA-CBD-CGD-O2D
25	7	603	CLA	CHA-CBD-CGD-O2D
25	7	612	CLA	CHA-CBD-CGD-O1D
25	8	612	CLA	CHA-CBD-CGD-O2D
25	9	602	CLA	CHA-CBD-CGD-O2D
25	9	603	CLA	CHA-CBD-CGD-O2D
25	9	604	CLA	CHA-CBD-CGD-O1D
25	q	611	CLA	CHA-CBD-CGD-O2D
25	q	612	CLA	CHA-CBD-CGD-O1D
25	q	612	CLA	CHA-CBD-CGD-O2D
25	q	613	CLA	CHA-CBD-CGD-O1D
25	q	613	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	608	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O1D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	g	602	CLA	CHA-CBD-CGD-O1D
25	g	602	CLA	CHA-CBD-CGD-O2D
25	g	612	CLA	CHA-CBD-CGD-O1D
25	g	613	CLA	CHA-CBD-CGD-O1D
25	g	613	CLA	CHA-CBD-CGD-O2D
25	n	604	CLA	CHA-CBD-CGD-O2D
25	n	611	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	n	611	CLA	CHA-CBD-CGD-O2D
25	n	612	CLA	CHA-CBD-CGD-O1D
25	n	612	CLA	CHA-CBD-CGD-O2D
25	s	604	CLA	CHA-CBD-CGD-O1D
25	s	609	CLA	CHA-CBD-CGD-O1D
25	s	609	CLA	CHA-CBD-CGD-O2D
25	y	604	CLA	CHA-CBD-CGD-O1D
25	y	604	CLA	CHA-CBD-CGD-O2D
25	y	612	CLA	CHA-CBD-CGD-O1D
25	y	612	CLA	CHA-CBD-CGD-O2D
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	604	CLA	CHA-CBD-CGD-O2D
25	r	616	CLA	CHA-CBD-CGD-O2D
26	N	1621	LUT	C29-C30-C31-C32
24	7	605	CHL	CAA-CBA-CGA-O1A
24	2	609	CHL	C4-C3-C5-C6
24	p	608	CHL	CAA-CBA-CGA-O2A
25	C	501	CLA	CAA-CBA-CGA-O2A
25	G	602	CLA	CAA-CBA-CGA-O2A
36	c	521	LMG	C20-C21-C22-C23
24	1	601	CHL	C2-C3-C5-C6
24	Y	609	CHL	C2-C3-C5-C6
24	0	606	CHL	C2-C3-C5-C6
25	1	604	CLA	C2-C3-C5-C6
25	Y	614	CLA	C5-C6-C7-C8
29	l	101	LHG	C13-C14-C15-C16
24	Y	607	CHL	C3-C5-C6-C7
24	5	601	CHL	C10-C11-C12-C13
29	d	410	LHG	O6-C4-C5-C6
24	p	606	CHL	CAA-CBA-CGA-O1A
25	R	616	CLA	C16-C17-C18-C20
25	r	616	CLA	C16-C17-C18-C20
25	5	611	CLA	CAA-CBA-CGA-O2A
25	g	602	CLA	CAA-CBA-CGA-O2A
25	s	602	CLA	CAA-CBA-CGA-O2A
29	2	2630	LHG	O8-C23-C24-C25
35	B	623	SQD	O47-C7-C8-C9
36	C	521	LMG	O8-C28-C29-C30
36	c	521	LMG	O8-C28-C29-C30
29	3	2630	LHG	C10-C11-C12-C13
29	L	101	LHG	C14-C15-C16-C17
35	a	412	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
25	2	602	CLA	C13-C15-C16-C17
25	3	612	CLA	CAA-CBA-CGA-O1A
29	y	2630	LHG	O10-C23-O8-C6
25	1	612	CLA	CAA-CBA-CGA-O2A
25	3	602	CLA	CAA-CBA-CGA-O2A
25	6	612	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
25	8	602	CLA	CAA-CBA-CGA-O2A
25	r	603	CLA	CAA-CBA-CGA-O2A
37	C	520	DGD	O1G-C1A-C2A-C3A
37	c	520	DGD	O1G-C1A-C2A-C3A
36	h	102	LMG	C14-C15-C16-C17
25	4	610	CLA	C2A-CAA-CBA-CGA
25	6	603	CLA	C2A-CAA-CBA-CGA
25	0	603	CLA	C2A-CAA-CBA-CGA
25	0	611	CLA	C2A-CAA-CBA-CGA
25	y	604	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C16-C17-C18-C20
25	Y	610	CLA	C16-C17-C18-C20
40	f	101	HEM	CAA-CBA-CGA-O1A
25	c	504	CLA	C13-C15-C16-C17
25	6	613	CLA	CBA-CGA-O2A-C1
29	p	2630	LHG	C24-C23-O8-C6
29	5	2630	LHG	C7-C8-C9-C10
36	h	102	LMG	C38-C39-C40-C41
36	H	102	LMG	C11-C10-O7-C8
36	h	102	LMG	C11-C10-O7-C8
25	6	613	CLA	CAA-CBA-CGA-O2A
37	C	519	DGD	O1G-C1A-C2A-C3A
37	c	519	DGD	C7A-C8A-C9A-CAA
24	N	609	CHL	C12-C13-C15-C16
24	Y	607	CHL	C12-C13-C15-C16
24	7	601	CHL	C12-C13-C15-C16
24	n	609	CHL	C12-C13-C15-C16
25	4	603	CLA	C11-C12-C13-C15
25	5	602	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	501	CLA	C11-C10-C8-C7
25	C	502	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	0	603	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C12-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C10
25	n	602	CLA	C11-C12-C13-C15
25	y	613	CLA	C6-C7-C8-C10
25	C	512	CLA	C16-C17-C18-C19
25	Y	610	CLA	C16-C17-C18-C19
25	8	610	CLA	C16-C17-C18-C20
25	2	602	CLA	CAA-CBA-CGA-O2A
25	9	602	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
37	c	519	DGD	O1G-C1A-C2A-C3A
37	c	520	DGD	O2G-C1B-C2B-C3B
29	8	2630	LHG	C10-C11-C12-C13
24	2	601	CHL	C11-C10-C8-C9
24	5	609	CHL	C14-C13-C15-C16
24	6	601	CHL	C14-C13-C15-C16
24	0	601	CHL	C14-C13-C15-C16
24	7	601	CHL	C14-C13-C15-C16
24	9	601	CHL	C6-C7-C8-C9
24	9	601	CHL	C11-C12-C13-C14
25	2	602	CLA	C11-C12-C13-C14
25	5	603	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	R	609	CLA	C6-C7-C8-C9
25	Y	603	CLA	C11-C10-C8-C9
25	0	604	CLA	C14-C13-C15-C16
25	9	602	CLA	C6-C7-C8-C9
25	b	608	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	c	502	CLA	C14-C13-C15-C16
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C12-C13-C14
25	r	609	CLA	C6-C7-C8-C9
28	5	1623	NEX	C13-C14-C15-C35
29	Y	2630	LHG	C33-C34-C35-C36
24	4	606	CHL	C2B-C3B-CAB-CBB
24	8	609	CHL	C2B-C3B-CAB-CBB
25	C	508	CLA	C2B-C3B-CAB-CBB
24	p	608	CHL	O2A-C1-C2-C3
24	y	608	CHL	O2A-C1-C2-C3
25	S	610	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	n	614	CLA	O2A-C1-C2-C3
25	s	610	CLA	O2A-C1-C2-C3
25	9	603	CLA	O1A-CGA-O2A-C1
24	N	607	CHL	CAA-CBA-CGA-O2A
24	7	606	CHL	CAA-CBA-CGA-O2A
25	C	510	CLA	CAA-CBA-CGA-O2A
29	4	2630	LHG	O7-C7-C8-C9
29	9	2630	LHG	O7-C7-C8-C9
24	2	607	CHL	CAA-CBA-CGA-O1A
35	B	623	SQD	C4-C5-C6-S
35	b	623	SQD	C4-C5-C6-S
25	B	604	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
25	q	603	CLA	O1A-CGA-O2A-C1
24	4	607	CHL	C2A-CAA-CBA-CGA
24	8	606	CHL	C2A-CAA-CBA-CGA
25	5	610	CLA	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	S	611	CLA	C2A-CAA-CBA-CGA
25	Y	604	CLA	C2A-CAA-CBA-CGA
24	9	607	CHL	CAA-CBA-CGA-O1A
25	4	603	CLA	CAA-CBA-CGA-O1A
25	p	613	CLA	CAA-CBA-CGA-O1A
36	c	521	LMG	C17-C18-C19-C20
24	5	605	CHL	CAA-CBA-CGA-O2A
24	q	605	CHL	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
29	0	2630	LHG	O8-C23-C24-C25
37	C	520	DGD	O2G-C1B-C2B-C3B
25	2	603	CLA	CBA-CGA-O2A-C1
36	A	413	LMG	C29-C28-O8-C9
36	a	413	LMG	C29-C28-O8-C9
24	N	606	CHL	CAA-CBA-CGA-O1A
24	n	606	CHL	CAA-CBA-CGA-O1A
26	2	1621	LUT	C11-C12-C13-C20
29	q	2630	LHG	C23-C24-C25-C26
24	1	606	CHL	CAA-CBA-CGA-O1A
25	0	603	CLA	CAA-CBA-CGA-O1A
35	D	413	SQD	O10-C23-C24-C25
25	C	512	CLA	C10-C11-C12-C13
37	C	519	DGD	C7A-C8A-C9A-CAA
24	6	606	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	1	610	CLA	C2-C3-C5-C6
24	4	605	CHL	CAA-CBA-CGA-O2A
25	0	612	CLA	CAA-CBA-CGA-O2A
25	C	504	CLA	C13-C15-C16-C17
35	d	413	SQD	O10-C23-C24-C25
26	5	1620	LUT	C7-C8-C9-C10
26	N	1621	LUT	C7-C8-C9-C10
26	n	1621	LUT	C7-C8-C9-C10
28	9	1623	NEX	C31-C32-C33-C34
28	p	1623	NEX	C11-C12-C13-C14
24	5	605	CHL	CBA-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
29	8	2630	LHG	C24-C23-O8-C6
29	n	2630	LHG	C14-C15-C16-C17
35	B	621	SQD	C24-C25-C26-C27
35	b	621	SQD	C24-C25-C26-C27
24	3	601	CHL	C1A-C2A-CAA-CBA
24	4	606	CHL	C1A-C2A-CAA-CBA
24	5	608	CHL	C1A-C2A-CAA-CBA
24	Y	601	CHL	C1A-C2A-CAA-CBA
24	p	608	CHL	C1A-C2A-CAA-CBA
24	y	601	CHL	C1A-C2A-CAA-CBA
25	2	602	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	613	CLA	C1A-C2A-CAA-CBA
25	5	612	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C1A-C2A-CAA-CBA
25	0	613	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C1A-C2A-CAA-CBA
29	C	2630	LHG	C1-C2-C3-O3
29	N	2630	LHG	C1-C2-C3-O3
29	7	2630	LHG	C1-C2-C3-O3
29	S	2630	LHG	C32-C33-C34-C35
29	q	2630	LHG	C10-C11-C12-C13
24	0	607	CHL	CAA-CBA-CGA-O1A
24	7	606	CHL	CAA-CBA-CGA-O1A
25	R	616	CLA	CAA-CBA-CGA-O1A
25	q	604	CLA	CAA-CBA-CGA-O1A
36	a	413	LMG	C29-C30-C31-C32
25	Y	604	CLA	C2-C1-O2A-CGA
36	H	102	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	3	613	CLA	C8-C10-C11-C12
25	6	603	CLA	CBA-CGA-O2A-C1
25	C	507	CLA	CBA-CGA-O2A-C1
25	9	603	CLA	CBA-CGA-O2A-C1
25	q	603	CLA	CBA-CGA-O2A-C1
24	q	605	CHL	CAA-CBA-CGA-O1A
25	5	613	CLA	CAA-CBA-CGA-O1A
25	6	603	CLA	CAA-CBA-CGA-O1A
25	7	612	CLA	CAA-CBA-CGA-O1A
25	q	603	CLA	CAA-CBA-CGA-O1A
25	r	616	CLA	CAA-CBA-CGA-O1A
36	C	521	LMG	C17-C18-C19-C20
24	5	601	CHL	CAA-CBA-CGA-O2A
24	R	607	CHL	CAA-CBA-CGA-O2A
24	r	607	CHL	CAA-CBA-CGA-O2A
25	5	602	CLA	CAA-CBA-CGA-O2A
25	7	602	CLA	CAA-CBA-CGA-O2A
25	p	602	CLA	CAA-CBA-CGA-O2A
36	C	521	LMG	C35-C36-C37-C38
25	b	608	CLA	C2A-CAA-CBA-CGA
24	p	608	CHL	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
25	n	603	CLA	C13-C15-C16-C17
36	A	413	LMG	C29-C30-C31-C32
36	c	521	LMG	C35-C36-C37-C38
25	9	603	CLA	CAA-CBA-CGA-O2A
25	B	608	CLA	C10-C11-C12-C13
25	8	613	CLA	C8-C10-C11-C12
29	6	2630	LHG	O9-C7-O7-C5
25	9	602	CLA	C3-C5-C6-C7
25	2	602	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A
37	c	520	DGD	O1B-C1B-C2B-C3B
25	6	603	CLA	O1A-CGA-O2A-C1
35	D	413	SQD	C2-C1-O6-C44
24	8	607	CHL	C5-C6-C7-C8
25	n	603	CLA	C10-C11-C12-C13
36	H	102	LMG	C14-C15-C16-C17
24	3	607	CHL	C4B-C3B-CAB-CBB
24	4	606	CHL	C4B-C3B-CAB-CBB
24	5	609	CHL	C4B-C3B-CAB-CBB
24	G	605	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	N	607	CHL	C4B-C3B-CAB-CBB
24	R	608	CHL	C4B-C3B-CAB-CBB
24	8	609	CHL	C4B-C3B-CAB-CBB
24	p	605	CHL	C4B-C3B-CAB-CBB
24	p	607	CHL	C4B-C3B-CAB-CBB
24	r	608	CHL	C4B-C3B-CAB-CBB
25	8	602	CLA	C4B-C3B-CAB-CBB
29	1	2630	LHG	C3-O3-P-O5
29	4	2630	LHG	C3-O3-P-O5
29	5	2630	LHG	C3-O3-P-O5
29	L	101	LHG	C3-O3-P-O4
29	Y	2630	LHG	C3-O3-P-O5
29	0	2630	LHG	C3-O3-P-O5
29	7	2630	LHG	C3-O3-P-O5
24	2	601	CHL	C4C-C3C-CAC-CBC
24	6	607	CHL	CAA-CBA-CGA-O1A
24	S	608	CHL	CAA-CBA-CGA-O1A
24	p	607	CHL	CAA-CBA-CGA-O1A
24	s	608	CHL	CAA-CBA-CGA-O1A
25	3	602	CLA	CAA-CBA-CGA-O1A
25	C	501	CLA	CAA-CBA-CGA-O1A
25	G	602	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	S	602	CLA	CAA-CBA-CGA-O1A
25	s	602	CLA	CAA-CBA-CGA-O1A
29	2	2630	LHG	O9-C7-C8-C9
29	6	2630	LHG	O10-C23-C24-C25
29	0	2630	LHG	O10-C23-C24-C25
29	q	2630	LHG	O9-C7-C8-C9
36	c	521	LMG	O10-C28-C29-C30
37	C	519	DGD	O1A-C1A-C2A-C3A
37	C	520	DGD	O1B-C1B-C2B-C3B
37	c	519	DGD	O1A-C1A-C2A-C3A
25	2	604	CLA	O2A-C1-C2-C3
25	N	614	CLA	O2A-C1-C2-C3
25	9	604	CLA	O2A-C1-C2-C3
25	7	611	CLA	CAA-CBA-CGA-O2A
25	8	604	CLA	CAA-CBA-CGA-O2A
26	R	620	LUT	C5-C6-C7-C8
26	g	1621	LUT	C1-C6-C7-C8
26	y	1620	LUT	C5-C6-C7-C8
26	r	620	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	C	516	BCR	C5-C6-C7-C8
34	c	516	BCR	C5-C6-C7-C8
25	6	613	CLA	CAA-CBA-CGA-O1A
25	9	602	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
29	9	2630	LHG	O9-C7-C8-C9
35	B	623	SQD	O49-C7-C8-C9
35	b	623	SQD	O49-C7-C8-C9
36	C	521	LMG	O10-C28-C29-C30
24	3	601	CHL	CAA-CBA-CGA-O2A
25	B	608	CLA	CAA-CBA-CGA-O2A
25	S	605	CLA	CAA-CBA-CGA-O2A
24	1	607	CHL	C16-C17-C18-C20
29	q	2630	LHG	C24-C25-C26-C27
25	2	614	CLA	C2A-CAA-CBA-CGA
25	9	613	CLA	C2A-CAA-CBA-CGA
25	9	614	CLA	C2A-CAA-CBA-CGA
25	q	610	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	CAA-CBA-CGA-O1A
24	y	609	CHL	C4C-C3C-CAC-CBC
25	q	602	CLA	CAA-CBA-CGA-O2A
25	g	602	CLA	CAA-CBA-CGA-O1A
24	8	607	CHL	C2-C3-C5-C6
24	7	601	CHL	C16-C17-C18-C19
29	g	2630	LHG	C29-C30-C31-C32
24	g	609	CHL	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	S	602	CLA	CAD-CBD-CGD-O1D
25	S	604	CLA	CAD-CBD-CGD-O1D
25	9	604	CLA	CAD-CBD-CGD-O1D
25	q	602	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	g	613	CLA	CAD-CBD-CGD-O1D
35	b	623	SQD	C5-C6-S-O7
37	C	520	DGD	O1A-C1A-C2A-C3A
37	c	520	DGD	O1A-C1A-C2A-C3A
25	b	604	CLA	C13-C15-C16-C17
29	C	2630	LHG	O2-C2-C3-O3
24	6	609	CHL	C11-C10-C8-C9
24	Y	606	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	y	601	CHL	C6-C7-C8-C9
24	y	606	CHL	C11-C10-C8-C9
25	2	603	CLA	C11-C10-C8-C9
25	5	602	CLA	C11-C12-C13-C14
25	5	604	CLA	C14-C13-C15-C16
25	5	610	CLA	C11-C10-C8-C9
25	A	410	CLA	C6-C7-C8-C9
25	B	604	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	0	603	CLA	C14-C13-C15-C16
25	a	410	CLA	C6-C7-C8-C9
25	b	604	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	6	604	CLA	C8-C10-C11-C12
25	0	603	CLA	O1A-CGA-O2A-C1
25	5	611	CLA	CAA-CBA-CGA-O1A
25	4	602	CLA	C3-C5-C6-C7
24	1	601	CHL	CAA-CBA-CGA-O2A
24	9	601	CHL	CAA-CBA-CGA-O2A
24	p	601	CHL	CAA-CBA-CGA-O2A
25	4	602	CLA	CAA-CBA-CGA-O2A
25	4	604	CLA	CAA-CBA-CGA-O2A
25	B	609	CLA	CAA-CBA-CGA-O2A
25	0	610	CLA	CAA-CBA-CGA-O2A
25	0	613	CLA	CAA-CBA-CGA-O2A
25	p	604	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	CAA-CBA-CGA-O2A
29	L	101	LHG	O7-C7-C8-C9
25	N	603	CLA	C13-C15-C16-C17
25	b	608	CLA	C10-C11-C12-C13
25	3	612	CLA	CAA-CBA-CGA-O2A
40	f	101	HEM	CAA-CBA-CGA-O2A
29	G	2630	LHG	C29-C30-C31-C32
24	p	601	CHL	C2A-CAA-CBA-CGA
25	2	610	CLA	C2A-CAA-CBA-CGA
24	Y	609	CHL	C4C-C3C-CAC-CBC
29	6	2630	LHG	C13-C14-C15-C16
29	L	101	LHG	C25-C26-C27-C28
24	4	606	CHL	CAA-CBA-CGA-O2A
24	7	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	8	601	CHL	CAA-CBA-CGA-O2A
25	2	603	CLA	CAA-CBA-CGA-O2A
25	N	602	CLA	CAA-CBA-CGA-O2A
25	S	613	CLA	CAA-CBA-CGA-O2A
25	Y	602	CLA	CAA-CBA-CGA-O2A
25	b	609	CLA	CAA-CBA-CGA-O2A
25	s	613	CLA	CAA-CBA-CGA-O2A
25	y	602	CLA	CAA-CBA-CGA-O2A
29	S	2630	LHG	O7-C7-C8-C9
29	l	101	LHG	O7-C7-C8-C9
24	9	606	CHL	O1A-CGA-O2A-C1
25	4	604	CLA	O1A-CGA-O2A-C1
29	1	2630	LHG	C1-C2-C3-O3
24	8	609	CHL	C5-C6-C7-C8
25	R	609	CLA	C4C-C3C-CAC-CBC
25	y	603	CLA	C3-C5-C6-C7
25	8	602	CLA	CAA-CBA-CGA-O1A
25	p	602	CLA	CAA-CBA-CGA-O1A
29	s	2630	LHG	C32-C33-C34-C35
25	b	604	CLA	C16-C17-C18-C19
29	0	2630	LHG	C5-C4-O6-P
29	7	2630	LHG	C5-C4-O6-P
29	n	2630	LHG	C5-C4-O6-P
25	B	604	CLA	C13-C15-C16-C17
29	y	2630	LHG	C11-C12-C13-C14
25	C	508	CLA	O1A-CGA-O2A-C1
24	4	606	CHL	C3A-C2A-CAA-CBA
24	R	608	CHL	C3A-C2A-CAA-CBA
24	Y	606	CHL	C12-C13-C15-C16
24	7	601	CHL	C6-C7-C8-C10
24	7	606	CHL	C12-C13-C15-C16
24	9	601	CHL	C11-C12-C13-C15
24	p	605	CHL	C11-C12-C13-C15
24	q	601	CHL	C6-C7-C8-C10
24	n	601	CHL	C12-C13-C15-C16
24	s	606	CHL	C3A-C2A-CAA-CBA
24	y	606	CHL	C12-C13-C15-C16
24	y	609	CHL	C12-C13-C15-C16
24	r	608	CHL	C3A-C2A-CAA-CBA
25	2	603	CLA	C11-C10-C8-C7
25	5	610	CLA	C11-C10-C8-C7
25	5	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C3A-C2A-CAA-CBA
25	B	604	CLA	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	C	503	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C6-C7-C8-C10
25	R	609	CLA	C6-C7-C8-C10
25	R	616	CLA	C12-C13-C15-C16
25	9	602	CLA	C6-C7-C8-C10
25	q	614	CLA	C3A-C2A-CAA-CBA
25	b	603	CLA	C3A-C2A-CAA-CBA
25	b	604	CLA	C6-C7-C8-C10
25	b	612	CLA	C12-C13-C15-C16
25	c	501	CLA	C11-C10-C8-C7
25	c	512	CLA	C2-C3-C5-C6
25	n	610	CLA	C6-C7-C8-C10
25	r	609	CLA	C6-C7-C8-C10
25	r	616	CLA	C12-C13-C15-C16
24	R	607	CHL	CAA-CBA-CGA-O1A
24	r	607	CHL	CAA-CBA-CGA-O1A
25	5	602	CLA	CAA-CBA-CGA-O1A
25	6	612	CLA	CAA-CBA-CGA-O1A
24	5	608	CHL	CAA-CBA-CGA-O2A
24	6	606	CHL	CAA-CBA-CGA-O2A
24	n	607	CHL	CAA-CBA-CGA-O2A
24	n	608	CHL	CAA-CBA-CGA-O2A
25	6	610	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	CAA-CBA-CGA-O2A
25	b	608	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
29	D	409	LHG	O7-C7-C8-C9
29	d	409	LHG	O7-C7-C8-C9
29	g	2630	LHG	O8-C23-C24-C25
29	s	2630	LHG	O7-C7-C8-C9
24	g	601	CHL	C8-C10-C11-C12
25	r	609	CLA	C4C-C3C-CAC-CBC
26	1	1621	LUT	C11-C12-C13-C14
26	2	1621	LUT	C11-C12-C13-C14
26	3	1620	LUT	C31-C32-C33-C34
26	5	1620	LUT	C11-C12-C13-C14
26	G	1620	LUT	C27-C28-C29-C30
26	g	1620	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	B	618	BCR	C17-C18-C19-C20
34	b	618	BCR	C17-C18-C19-C20
24	5	601	CHL	CAA-CBA-CGA-O1A
25	4	604	CLA	CAA-CBA-CGA-O1A
25	B	609	CLA	CAA-CBA-CGA-O1A
25	0	612	CLA	CAA-CBA-CGA-O1A
25	7	602	CLA	CAA-CBA-CGA-O1A
25	9	603	CLA	CAA-CBA-CGA-O1A
29	S	2630	LHG	O9-C7-C8-C9
24	9	605	CHL	C2-C1-O2A-CGA
24	7	607	CHL	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	8	610	CLA	C16-C17-C18-C19
25	3	604	CLA	CAA-CBA-CGA-O2A
25	8	603	CLA	CAA-CBA-CGA-O2A
29	Y	2630	LHG	C17-C18-C19-C20
24	n	609	CHL	C15-C16-C17-C18
25	Y	612	CLA	C5-C6-C7-C8
25	c	509	CLA	C13-C15-C16-C17
29	d	410	LHG	C33-C34-C35-C36
24	7	601	CHL	CAA-CBA-CGA-O1A
25	1	612	CLA	CAA-CBA-CGA-O1A
25	6	610	CLA	CAA-CBA-CGA-O1A
25	Y	602	CLA	CAA-CBA-CGA-O1A
25	b	609	CLA	CAA-CBA-CGA-O1A
29	s	2630	LHG	O9-C7-C8-C9
40	F	101	HEM	CAA-CBA-CGA-O2A
25	C	509	CLA	C13-C15-C16-C17
25	9	610	CLA	C10-C11-C12-C13
24	2	605	CHL	C2-C1-O2A-CGA
29	D	410	LHG	C33-C34-C35-C36
29	y	2630	LHG	C33-C34-C35-C36
24	2	606	CHL	CAA-CBA-CGA-O2A
24	G	605	CHL	CAA-CBA-CGA-O2A
29	G	2630	LHG	O8-C23-C24-C25
24	8	607	CHL	C4C-C3C-CAC-CBC
36	B	622	LMG	C38-C39-C40-C41
24	7	609	CHL	C10-C11-C12-C13
25	y	612	CLA	C5-C6-C7-C8
25	s	613	CLA	CAA-CBA-CGA-O1A
25	y	602	CLA	CAA-CBA-CGA-O1A
29	4	2630	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	2	613	CLA	C2A-CAA-CBA-CGA
25	S	604	CLA	C2A-CAA-CBA-CGA
25	s	604	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
24	n	609	CHL	C16-C17-C18-C19
24	n	606	CHL	CAA-CBA-CGA-O2A
25	p	602	CLA	C15-C16-C17-C18
24	4	606	CHL	CAA-CBA-CGA-O1A
25	S	613	CLA	CAA-CBA-CGA-O1A
25	0	610	CLA	CAA-CBA-CGA-O1A
25	5	604	CLA	CAA-CBA-CGA-O2A
24	N	606	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

398 monomers are involved in 799 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	408	LHG	4	0
24	S	608	CHL	2	0
24	7	606	CHL	1	0
24	r	606	CHL	1	0
34	c	516	BCR	5	0
25	C	509	CLA	1	0
24	s	607	CHL	1	0
24	y	601	CHL	6	0
28	0	1623	NEX	1	0
26	G	1621	LUT	5	0
26	N	1620	LUT	2	0
25	Y	612	CLA	2	0
27	Y	1622	XAT	5	0
25	B	603	CLA	3	0
25	C	501	CLA	2	0
24	3	605	CHL	1	0
27	N	1622	XAT	5	0
38	D	401	BCT	2	0
35	B	621	SQD	2	0
25	S	602	CLA	2	0
29	7	2630	LHG	2	0
25	B	602	CLA	2	0
25	r	613	CLA	1	0
38	d	401	BCT	2	0
25	0	612	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	610	CLA	1	0
25	p	603	CLA	2	0
25	C	512	CLA	1	0
28	y	1623	NEX	2	0
27	3	1622	XAT	2	0
25	q	603	CLA	2	0
29	4	2630	LHG	1	0
25	G	610	CLA	2	0
25	A	406	CLA	1	0
26	6	1620	LUT	1	0
27	9	1622	XAT	2	0
24	9	601	CHL	2	0
25	Y	613	CLA	3	0
34	d	404	BCR	5	0
25	n	614	CLA	1	0
35	a	412	SQD	3	0
24	0	606	CHL	1	0
25	b	609	CLA	1	0
28	R	623	NEX	1	0
29	d	409	LHG	2	0
25	n	602	CLA	1	0
25	c	511	CLA	2	0
29	S	2630	LHG	5	0
25	6	604	CLA	1	0
26	s	1620	LUT	1	0
24	8	601	CHL	2	0
25	B	614	CLA	2	0
27	y	1622	XAT	3	0
26	g	1620	LUT	2	0
33	A	408	PHO	2	0
24	2	601	CHL	1	0
24	8	609	CHL	3	0
25	S	604	CLA	9	0
25	C	511	CLA	3	0
25	7	603	CLA	1	0
25	C	505	CLA	3	0
24	7	608	CHL	1	0
29	0	2630	LHG	2	0
25	9	613	CLA	2	0
25	c	510	CLA	1	0
24	5	609	CHL	3	0
26	n	1620	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	q	601	CHL	1	0
33	a	408	PHO	2	0
24	1	601	CHL	3	0
25	c	513	CLA	3	0
24	n	609	CHL	2	0
24	q	609	CHL	2	0
39	d	405	PL9	3	0
25	B	605	CLA	3	0
28	1	1623	NEX	3	0
24	N	601	CHL	2	0
36	h	102	LMG	2	0
27	G	1622	XAT	6	0
24	y	608	CHL	1	0
24	G	601	CHL	4	0
24	p	606	CHL	1	0
26	g	1621	LUT	3	0
37	c	523	DGD	3	0
25	5	602	CLA	1	0
24	s	601	CHL	3	0
29	r	2630	LHG	1	0
24	S	606	CHL	2	0
25	B	604	CLA	1	0
35	A	412	SQD	4	0
24	Y	608	CHL	1	0
25	B	617	CLA	1	0
24	R	606	CHL	1	0
25	0	602	CLA	2	0
25	9	610	CLA	1	0
25	p	602	CLA	1	0
25	1	614	CLA	1	0
24	8	606	CHL	1	0
24	R	607	CHL	2	0
24	R	608	CHL	3	0
24	s	608	CHL	2	0
24	s	606	CHL	2	0
25	c	505	CLA	3	0
35	b	621	SQD	2	0
25	G	613	CLA	2	0
25	q	604	CLA	1	0
25	a	406	CLA	1	0
25	b	610	CLA	2	0
25	b	614	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	6	1623	NEX	3	0
34	b	619	BCR	2	0
25	R	613	CLA	2	0
25	d	402	CLA	4	0
26	8	1621	LUT	7	0
24	0	605	CHL	1	0
24	6	607	CHL	3	0
25	B	616	CLA	1	0
25	9	603	CLA	3	0
25	n	603	CLA	1	0
24	n	607	CHL	2	0
25	r	609	CLA	2	0
24	5	601	CHL	1	0
25	s	602	CLA	2	0
37	c	524	DGD	5	0
25	N	613	CLA	1	0
25	5	604	CLA	2	0
24	N	608	CHL	1	0
25	6	612	CLA	2	0
25	b	608	CLA	2	0
26	q	1621	LUT	1	0
24	1	609	CHL	3	0
26	1	1621	LUT	2	0
25	5	603	CLA	2	0
25	1	604	CLA	3	0
25	q	613	CLA	3	0
34	a	411	BCR	2	0
25	7	602	CLA	3	0
28	n	1623	NEX	3	0
25	b	616	CLA	1	0
34	b	620	BCR	1	0
24	S	607	CHL	1	0
24	y	609	CHL	9	0
36	H	102	LMG	3	0
25	6	613	CLA	1	0
26	7	1621	LUT	1	0
25	7	613	CLA	1	0
26	R	620	LUT	4	0
25	C	504	CLA	1	0
24	7	601	CHL	3	0
25	4	612	CLA	1	0
24	G	609	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	614	CLA	1	0
33	a	409	PHO	1	0
25	g	613	CLA	3	0
25	B	610	CLA	2	0
25	y	612	CLA	2	0
24	9	607	CHL	1	0
24	9	608	CHL	2	0
29	c	2630	LHG	2	0
34	D	404	BCR	4	0
24	N	607	CHL	4	0
24	2	606	CHL	2	0
26	0	1621	LUT	4	0
34	c	517	BCR	4	0
25	3	602	CLA	3	0
27	1	1622	XAT	5	0
25	c	507	CLA	2	0
27	r	622	XAT	4	0
25	Y	603	CLA	6	0
24	3	608	CHL	2	0
27	n	1622	XAT	5	0
25	9	602	CLA	4	0
25	B	613	CLA	5	0
29	C	2630	LHG	5	0
33	A	409	PHO	2	0
24	7	607	CHL	4	0
24	N	609	CHL	4	0
29	n	2630	LHG	3	0
25	p	610	CLA	2	0
28	N	1623	NEX	4	0
25	y	610	CLA	2	0
34	C	515	BCR	1	0
24	n	606	CHL	2	0
25	3	611	CLA	1	0
25	R	601	CLA	1	0
26	6	1621	LUT	4	0
25	b	606	CLA	2	0
25	N	603	CLA	3	0
25	0	604	CLA	1	0
25	n	613	CLA	1	0
37	C	523	DGD	3	0
25	c	512	CLA	1	0
24	2	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	507	CLA	1	0
25	S	605	CLA	8	0
25	y	603	CLA	4	0
27	7	1622	XAT	4	0
25	Y	604	CLA	1	0
25	A	407	CLA	1	0
35	D	413	SQD	2	0
25	4	611	CLA	1	0
24	3	609	CHL	3	0
26	3	1620	LUT	2	0
37	c	518	DGD	2	0
34	c	515	BCR	3	0
25	y	604	CLA	1	0
25	y	611	CLA	7	0
36	B	622	LMG	4	0
36	s	2631	LMG	1	0
25	B	607	CLA	2	0
28	s	1623	NEX	3	0
25	n	610	CLA	1	0
24	8	608	CHL	2	0
25	b	612	CLA	3	0
24	2	608	CHL	2	0
26	N	1621	LUT	3	0
25	3	603	CLA	2	0
25	c	508	CLA	1	0
25	C	506	CLA	1	0
25	9	604	CLA	1	0
24	6	601	CHL	1	0
25	7	614	CLA	1	0
25	2	603	CLA	2	0
29	Y	2630	LHG	3	0
25	Y	602	CLA	2	0
25	A	405	CLA	3	0
26	s	1621	LUT	5	0
37	c	519	DGD	3	0
34	C	516	BCR	4	0
24	1	608	CHL	4	0
24	g	601	CHL	6	0
29	s	2630	LHG	10	0
25	4	613	CLA	2	0
36	b	622	LMG	3	0
29	l	101	LHG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S	1623	NEX	3	0
25	c	501	CLA	1	0
25	5	613	CLA	2	0
34	h	101	BCR	2	0
26	3	1621	LUT	5	0
25	g	610	CLA	2	0
25	0	610	CLA	3	0
26	G	1620	LUT	4	0
25	2	604	CLA	2	0
29	1	2630	LHG	2	0
26	9	1621	LUT	4	0
28	3	1623	NEX	1	0
29	D	408	LHG	3	0
24	n	605	CHL	2	0
25	a	405	CLA	3	0
29	L	101	LHG	5	0
25	C	502	CLA	1	0
24	9	606	CHL	1	0
25	C	513	CLA	6	0
25	b	603	CLA	3	0
25	1	602	CLA	2	0
25	Y	611	CLA	5	0
25	b	605	CLA	3	0
25	B	612	CLA	3	0
24	7	609	CHL	2	0
34	B	619	BCR	3	0
25	N	602	CLA	1	0
25	4	603	CLA	1	0
24	5	608	CHL	1	0
24	Y	607	CHL	1	0
35	d	413	SQD	2	0
26	y	1621	LUT	5	0
24	S	601	CHL	5	0
27	g	1622	XAT	6	0
34	b	618	BCR	3	0
25	R	611	CLA	1	0
25	y	602	CLA	3	0
26	8	1620	LUT	2	0
25	G	603	CLA	2	0
36	S	2631	LMG	2	0
25	R	609	CLA	1	0
26	2	1620	LUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	617	CLA	1	0
27	R	622	XAT	4	0
24	4	601	CHL	1	0
24	r	608	CHL	3	0
24	Y	605	CHL	1	0
25	a	407	CLA	1	0
34	C	514	BCR	1	0
25	R	603	CLA	2	0
34	H	101	BCR	1	0
26	1	1620	LUT	2	0
24	3	607	CHL	1	0
24	5	607	CHL	1	0
24	p	609	CHL	3	0
25	8	603	CLA	1	0
25	Y	610	CLA	1	0
28	r	623	NEX	2	0
34	C	517	BCR	4	0
25	8	613	CLA	1	0
26	2	1621	LUT	3	0
37	C	524	DGD	5	0
39	D	405	PL9	3	0
25	s	605	CLA	10	0
26	r	620	LUT	2	0
24	4	608	CHL	1	0
24	1	607	CHL	3	0
26	5	1621	LUT	1	0
29	G	2630	LHG	6	0
25	b	615	CLA	2	0
25	1	603	CLA	1	0
25	2	602	CLA	2	0
24	g	609	CHL	2	0
28	8	1623	NEX	1	0
26	7	1620	LUT	5	0
26	p	1621	LUT	2	0
26	Y	1620	LUT	6	0
25	6	610	CLA	3	0
24	6	609	CHL	3	0
25	s	604	CLA	11	0
25	3	613	CLA	2	0
25	b	602	CLA	1	0
24	y	605	CHL	1	0
25	0	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	607	CHL	1	0
24	G	608	CHL	2	0
25	D	402	CLA	4	0
25	0	613	CLA	1	0
25	p	612	CLA	1	0
26	n	1621	LUT	2	0
25	d	403	CLA	1	0
25	G	602	CLA	3	0
25	r	603	CLA	2	0
24	G	605	CHL	1	0
24	8	605	CHL	1	0
24	n	601	CHL	3	0
25	p	614	CLA	1	0
28	7	1623	NEX	2	0
24	Y	609	CHL	8	0
25	5	612	CLA	2	0
29	R	2630	LHG	1	0
25	R	602	CLA	1	0
25	b	613	CLA	5	0
25	r	601	CLA	2	0
24	p	608	CHL	1	0
25	y	613	CLA	2	0
26	0	1620	LUT	2	0
25	8	602	CLA	3	0
27	2	1622	XAT	1	0
37	C	518	DGD	2	0
29	g	2630	LHG	6	0
25	g	602	CLA	3	0
24	3	606	CHL	1	0
25	9	611	CLA	1	0
25	r	616	CLA	4	0
29	y	2630	LHG	4	0
26	9	1620	LUT	1	0
34	B	620	BCR	4	0
25	D	403	CLA	3	0
26	Y	1621	LUT	2	0
25	N	610	CLA	2	0
29	6	2630	LHG	1	0
24	0	607	CHL	2	0
24	0	608	CHL	1	0
24	1	606	CHL	2	0
34	B	618	BCR	3	0

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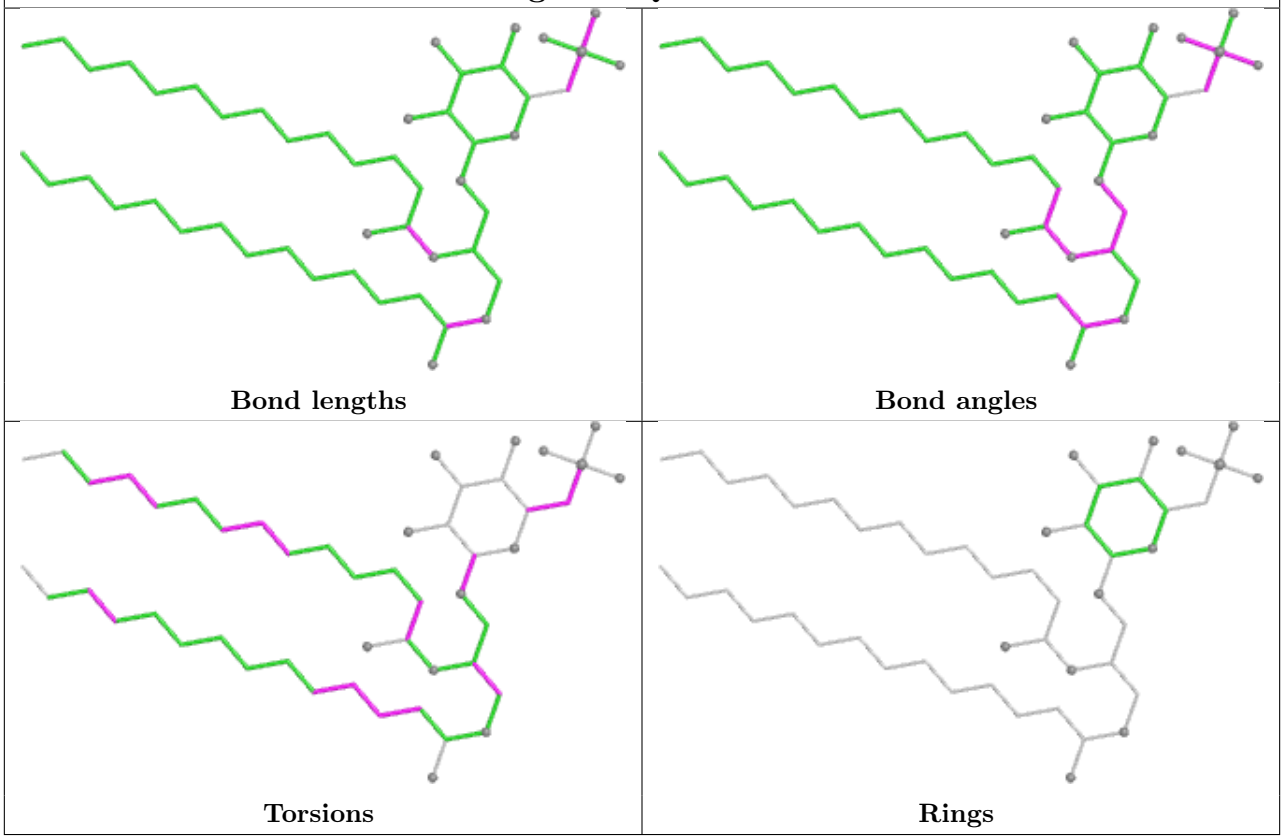
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	y	1620	LUT	3	0
24	N	606	CHL	2	0
25	C	510	CLA	1	0
24	6	608	CHL	3	0
25	C	508	CLA	2	0
25	2	613	CLA	1	0
24	q	608	CHL	1	0
25	c	504	CLA	3	0
25	R	616	CLA	3	0
25	B	608	CLA	2	0
37	C	519	DGD	1	0
34	A	411	BCR	3	0
36	A	413	LMG	2	0
24	4	609	CHL	2	0
26	S	1620	LUT	1	0
24	Y	601	CHL	4	0
24	y	607	CHL	2	0
25	p	604	CLA	1	0
29	N	2630	LHG	3	0
24	r	607	CHL	2	0
25	b	607	CLA	2	0
24	g	607	CHL	1	0
24	g	608	CHL	1	0
26	S	1621	LUT	5	0
24	N	605	CHL	1	0
25	6	602	CLA	2	0
29	D	409	LHG	2	0
28	Y	1623	NEX	3	0
27	8	1622	XAT	1	0
25	q	602	CLA	1	0
25	g	603	CLA	2	0
25	q	611	CLA	2	0
24	6	606	CHL	3	0
25	B	615	CLA	2	0
36	a	413	LMG	2	0
25	B	609	CLA	2	0
25	r	602	CLA	1	0

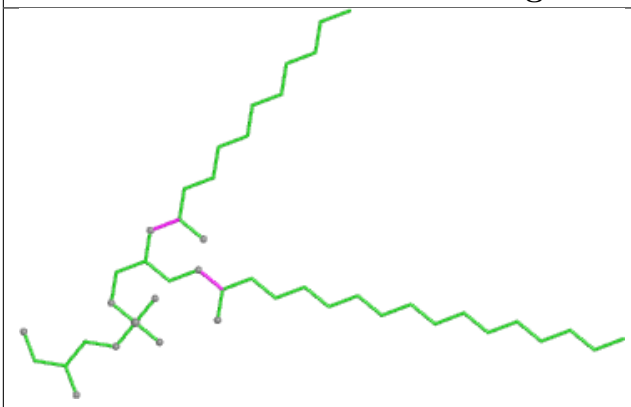
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

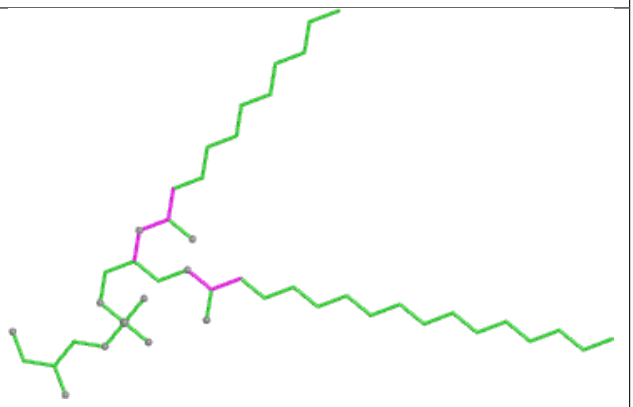
Ligand SQD b 623



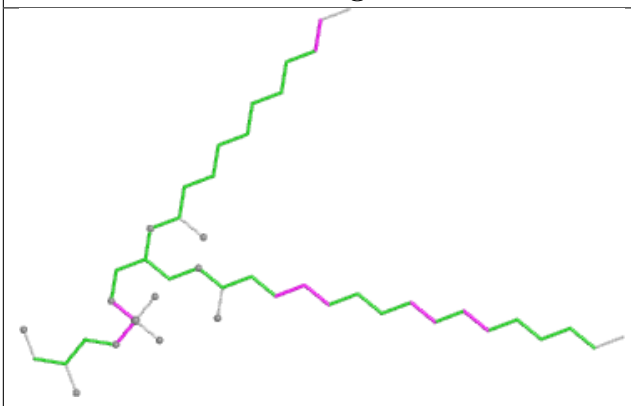
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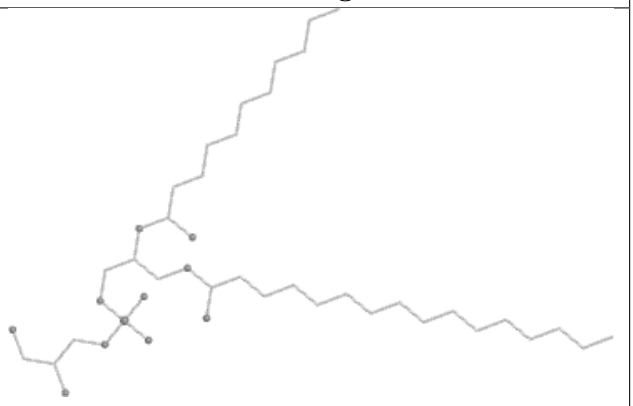
Bond lengths



Bond angles

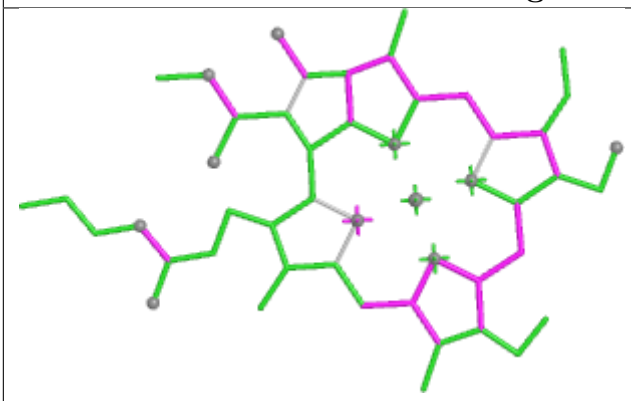


Torsions

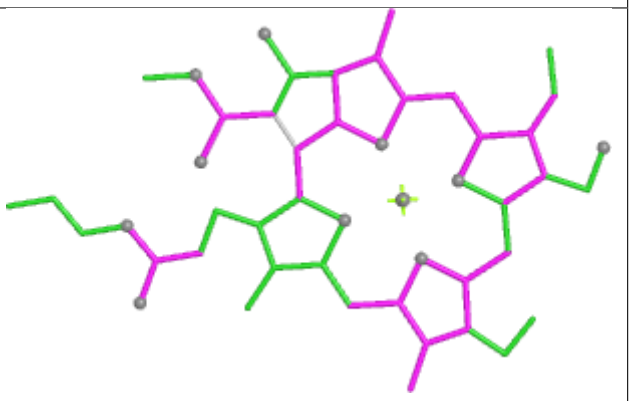


Rings

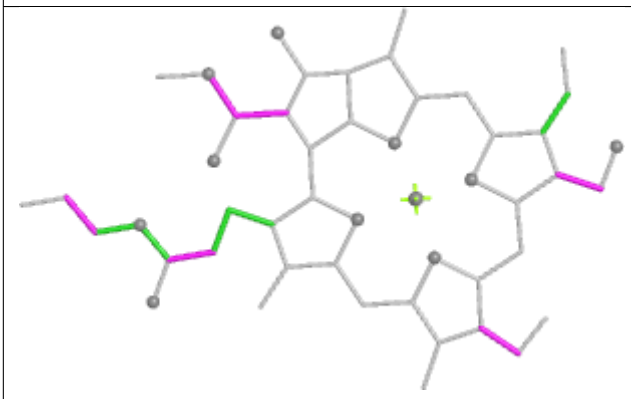
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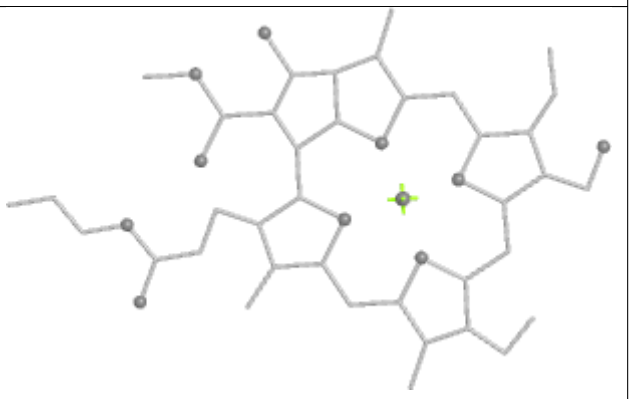
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Bond angles

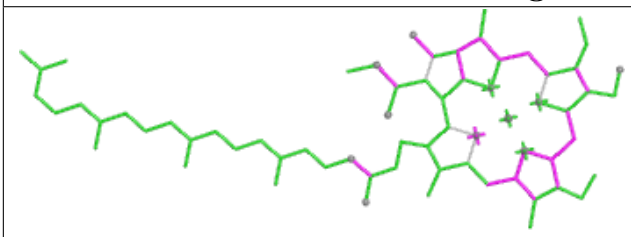


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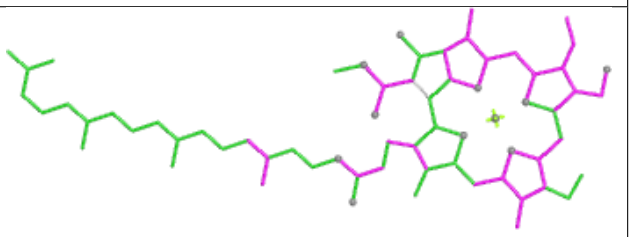


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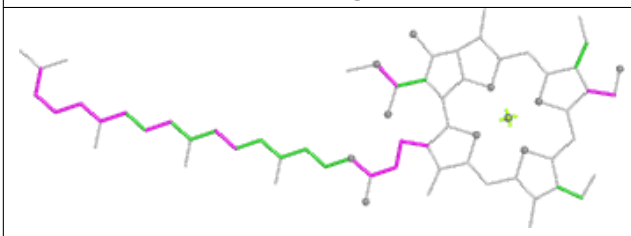
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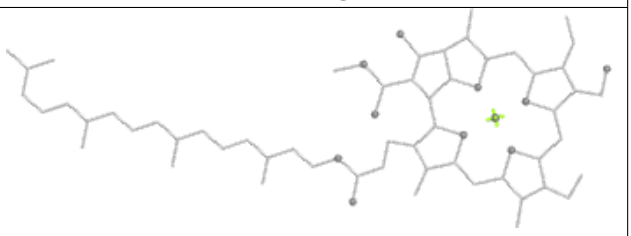
Bond lengths



Bond angles

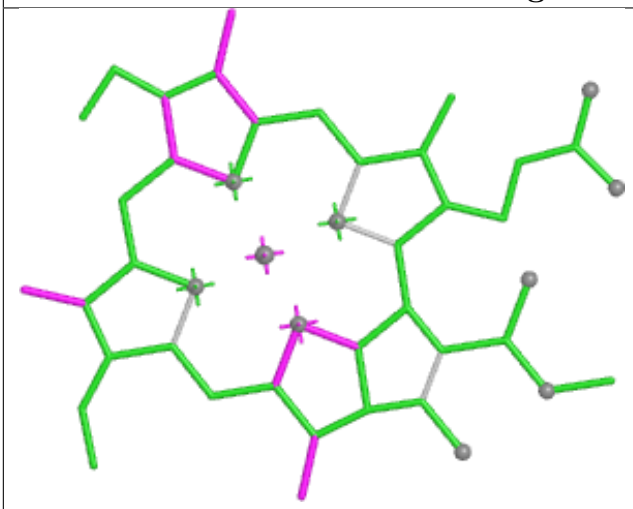


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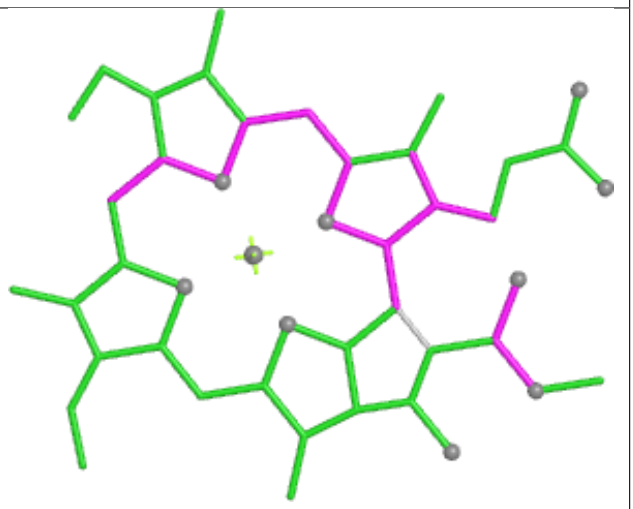


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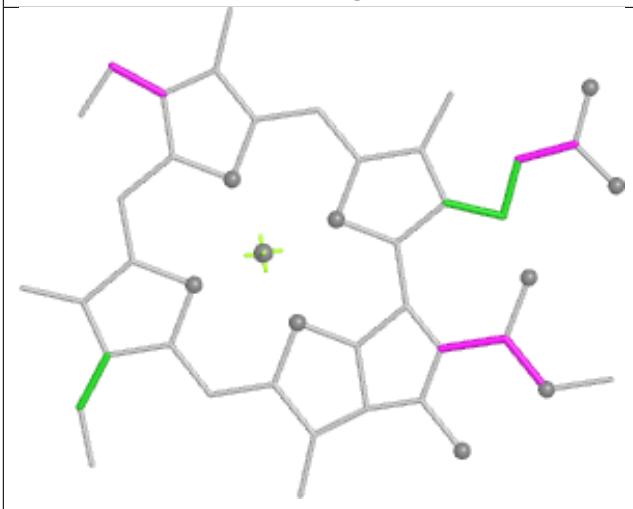
Ligand CLA n 612



Bond lengths



Bond angles

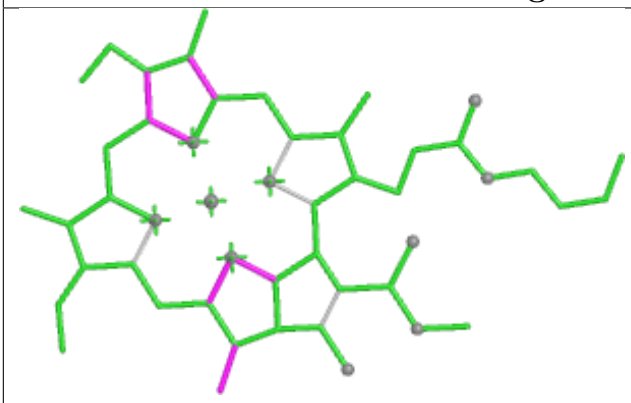


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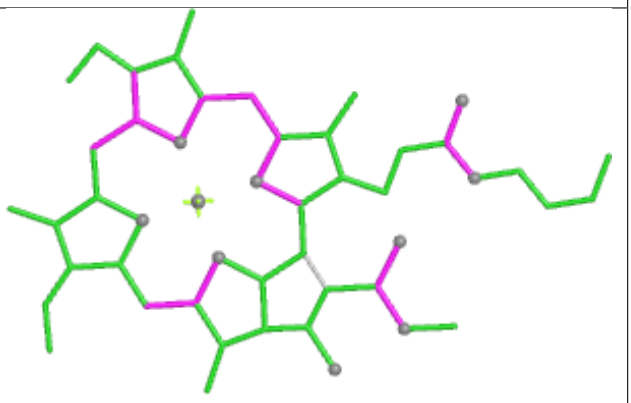


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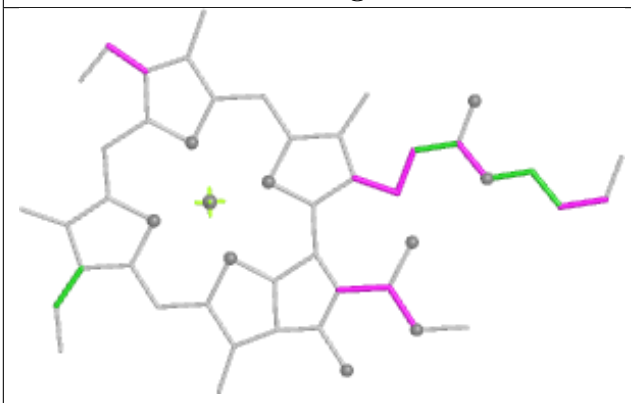
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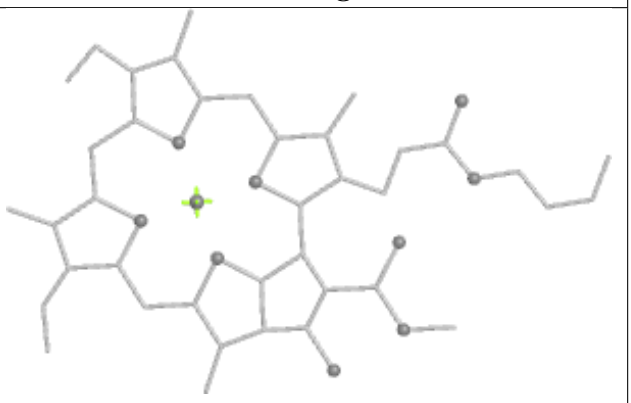
Bond lengths



Bond angles

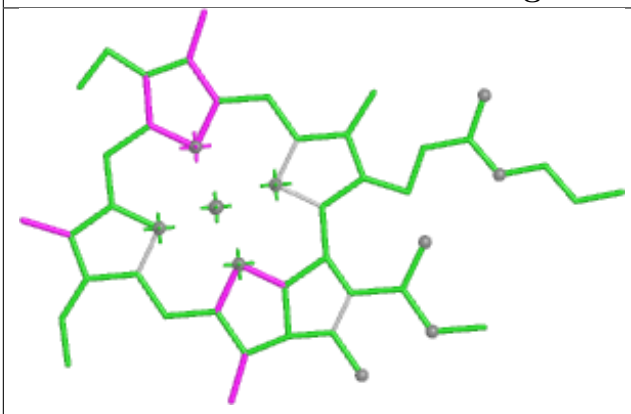


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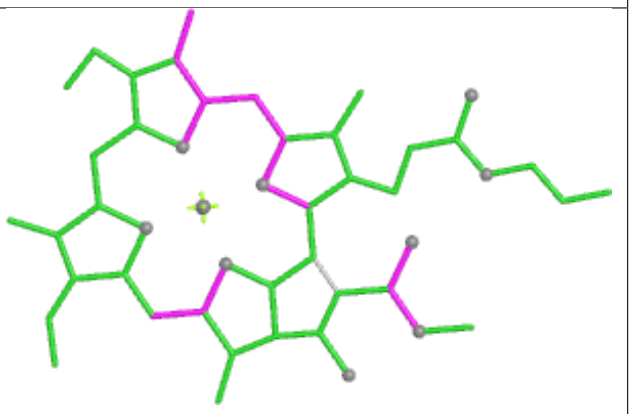


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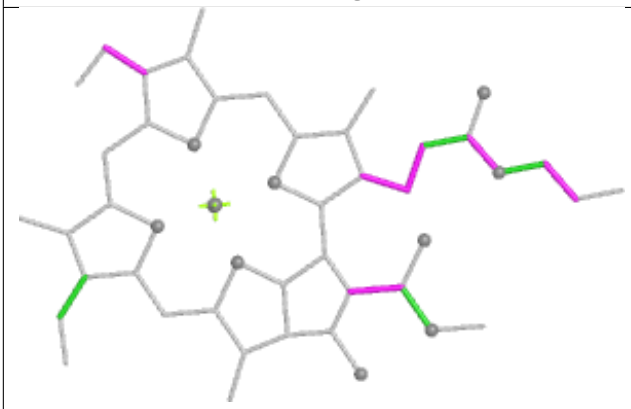
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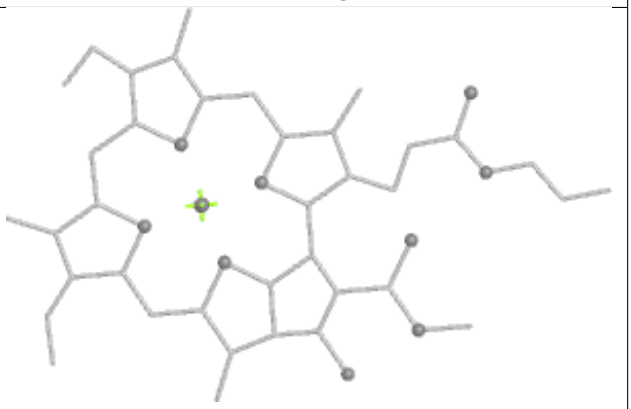
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Bond angles

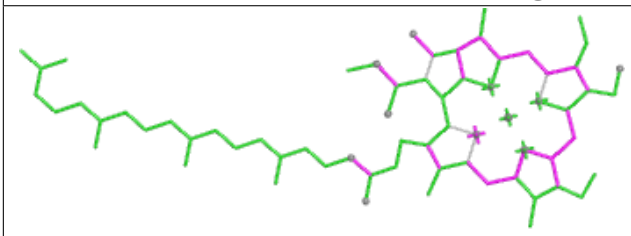


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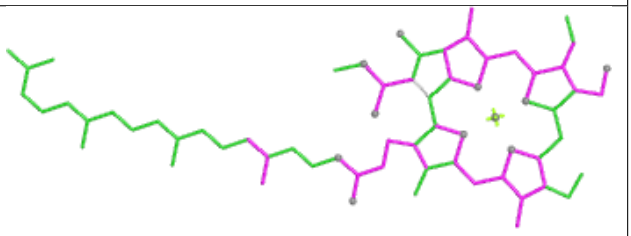


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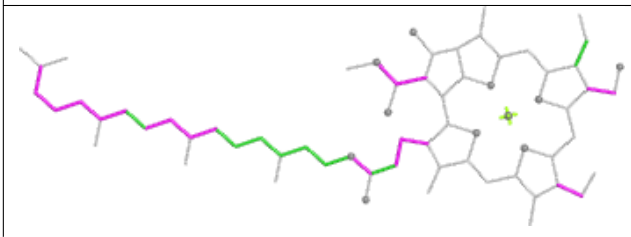
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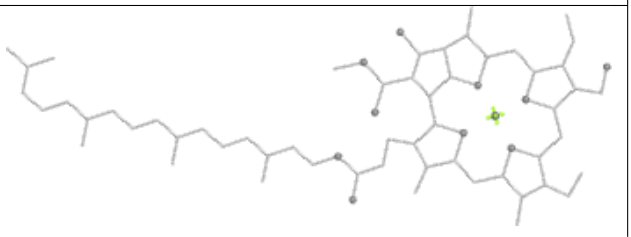
Bond lengths



Bond angles

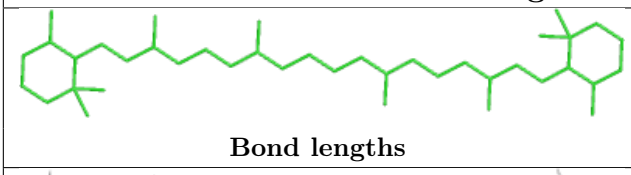


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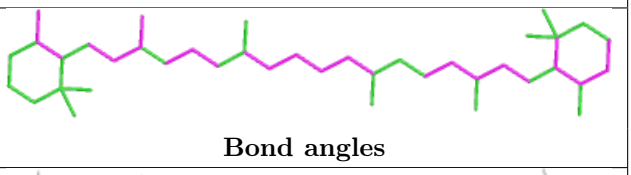


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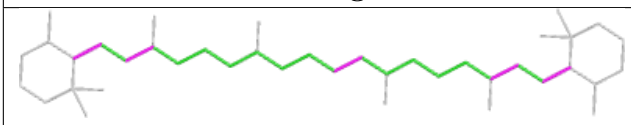
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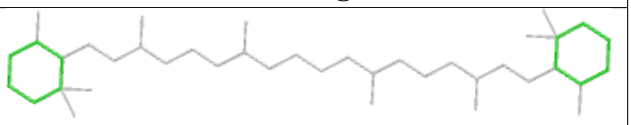
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Bond angles

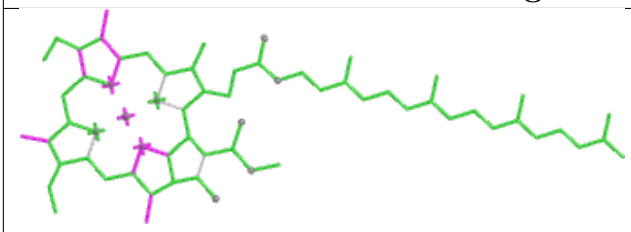


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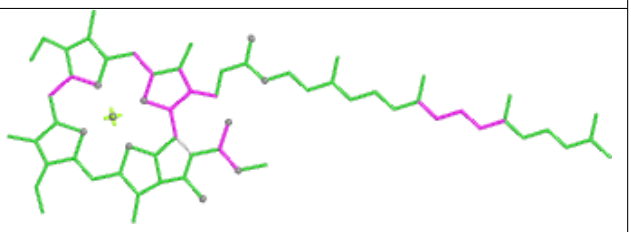


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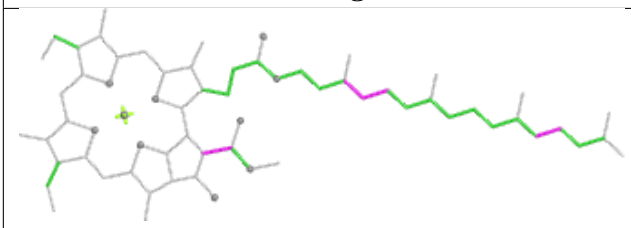
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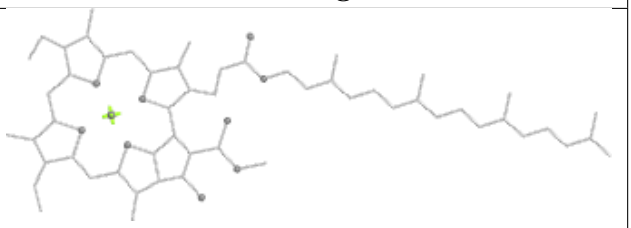
Bond lengths



Bond angles

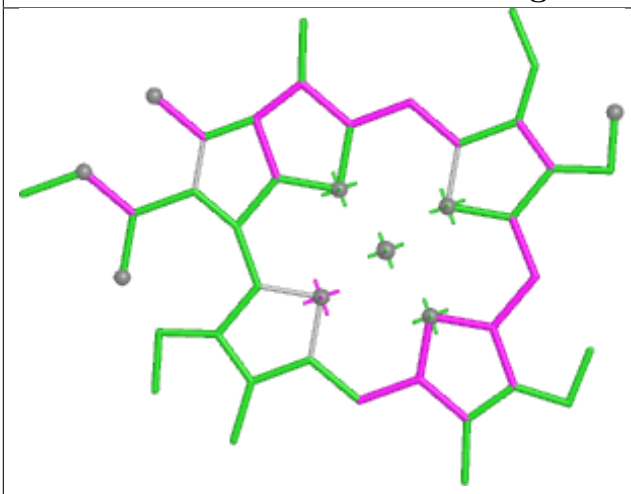


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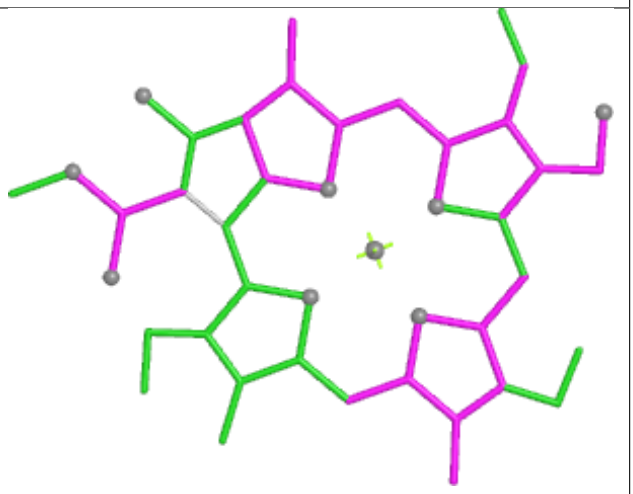


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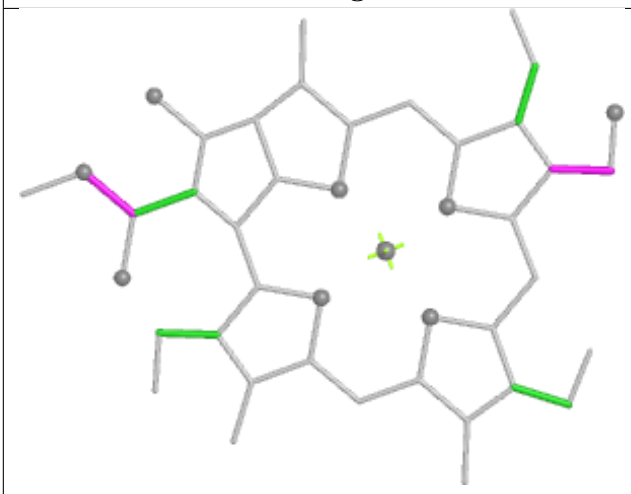
Ligand CHL s 607



Bond lengths



Bond angles

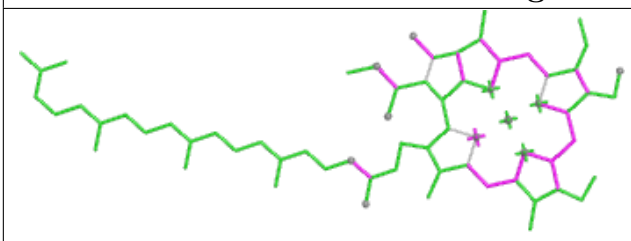


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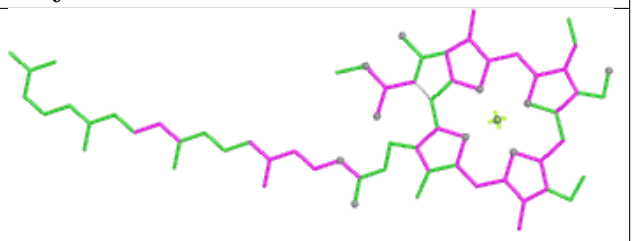


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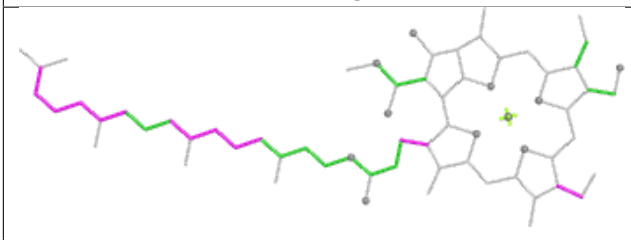
Ligand CHL y 601



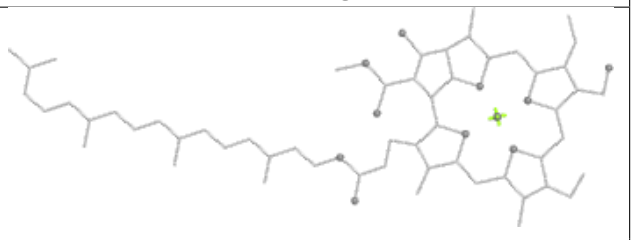
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Bond angles

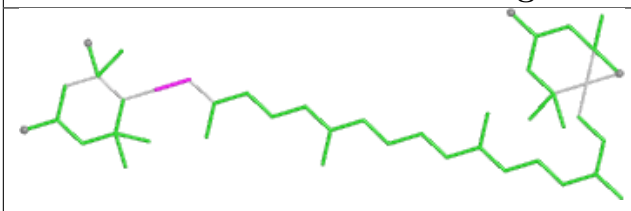


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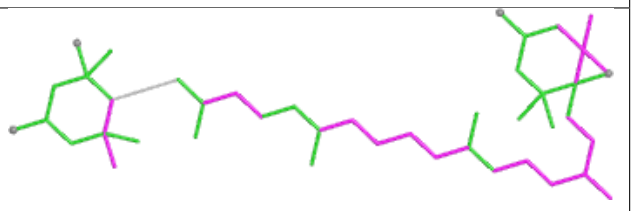


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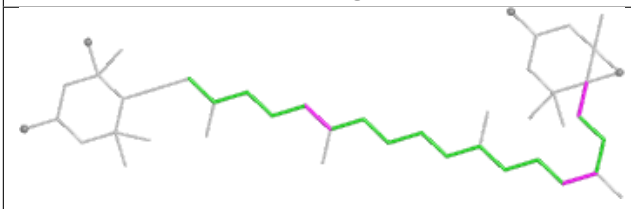
Ligand NEX 0 1623



Bond lengths



Bond angles



Torsions

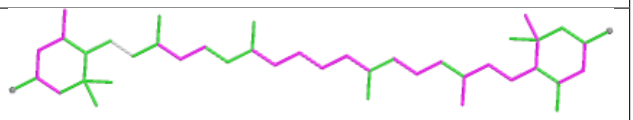


Rings

Ligand LUT G 1621



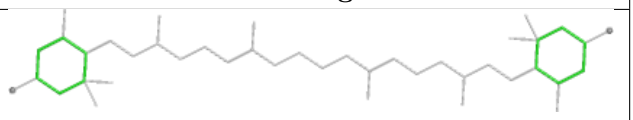
Bond lengths



Bond angles



Torsions

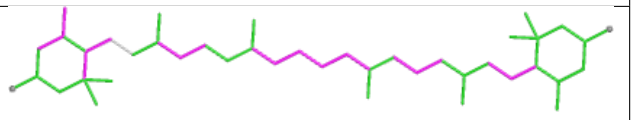


Rings

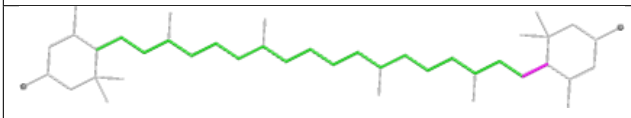
Ligand LUT N 1620



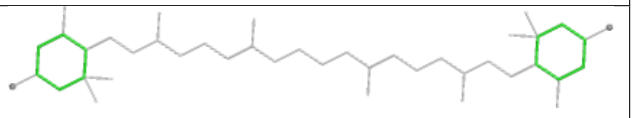
Bond lengths



Bond angles

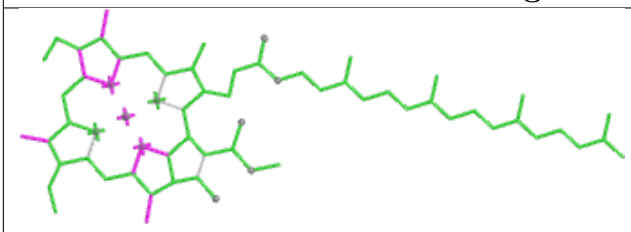


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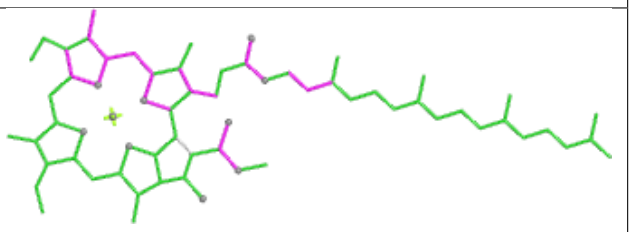


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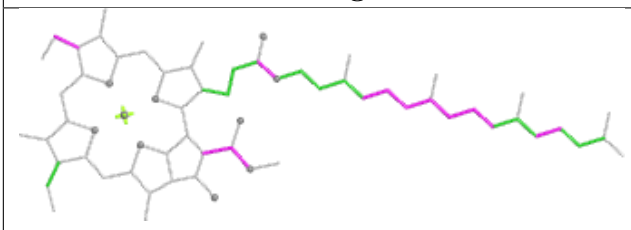
Ligand CLA Y 612



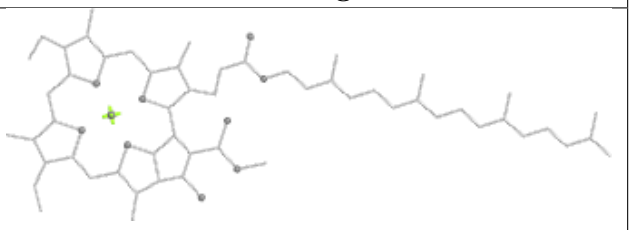
Bond lengths



Bond angles



Torsions

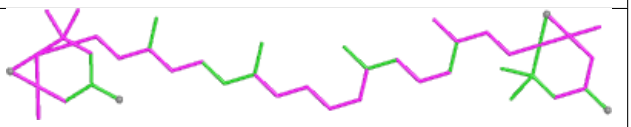


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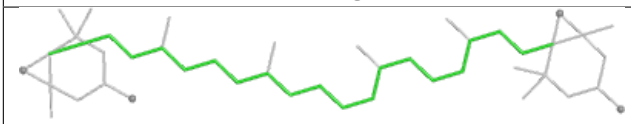
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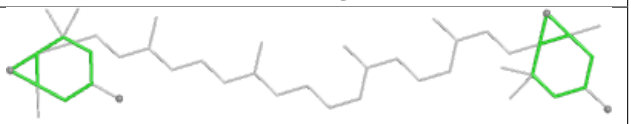
Bond lengths



Bond angles

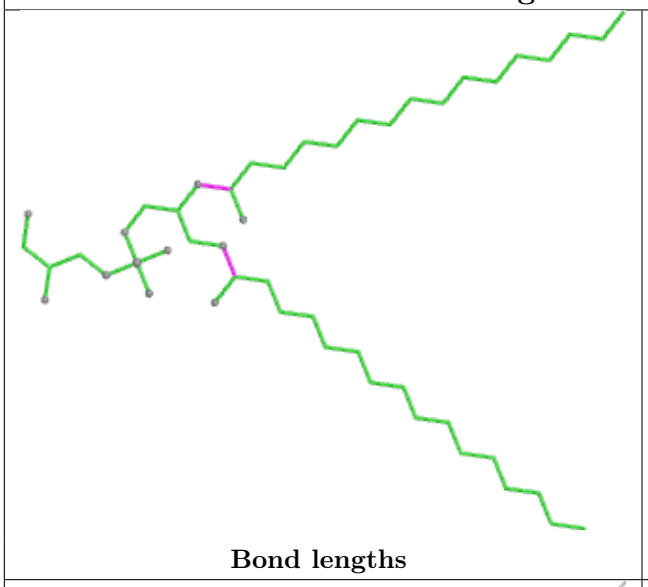


Torsions

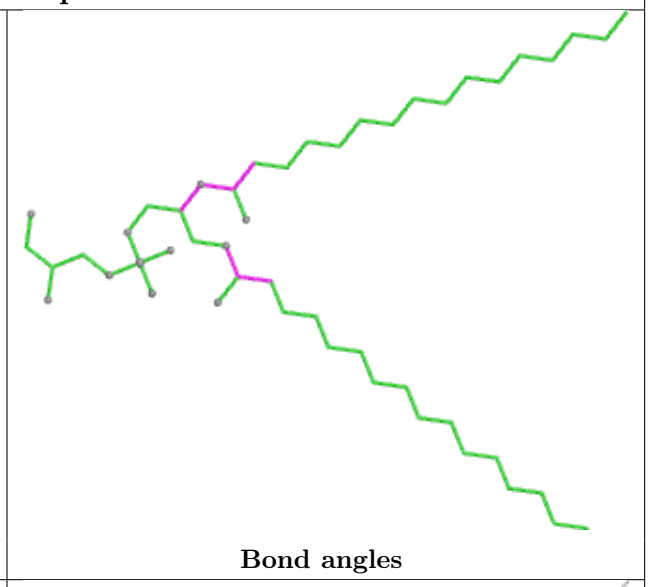


Rings

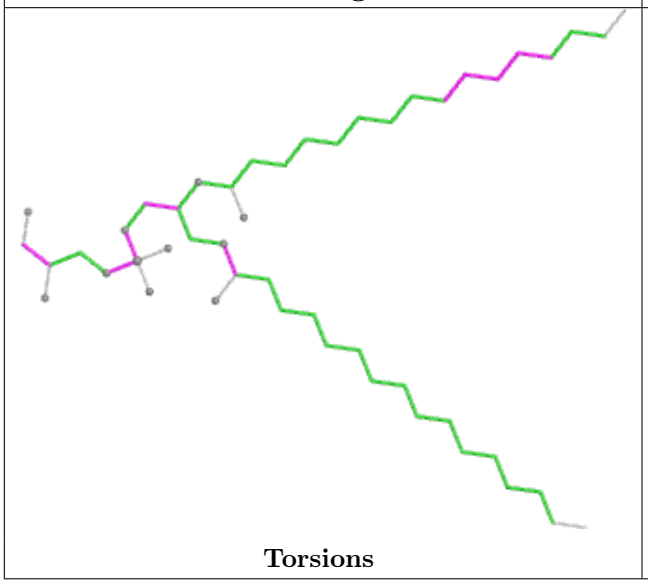
Ligand LHG p 2630



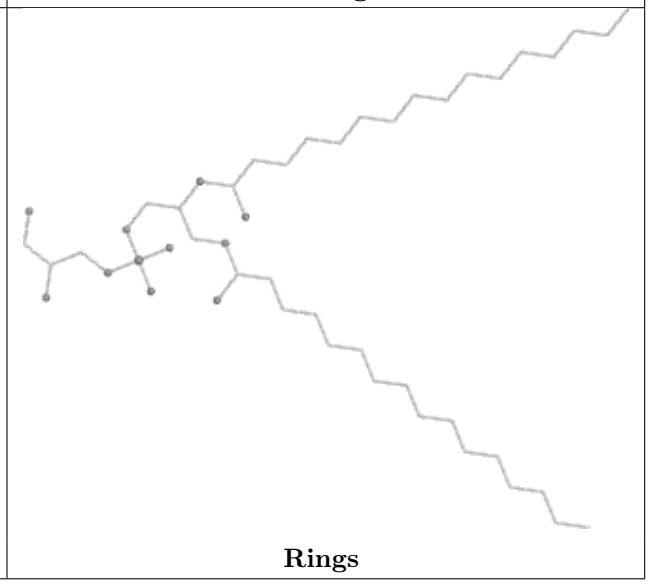
Bond lengths



Bond angles

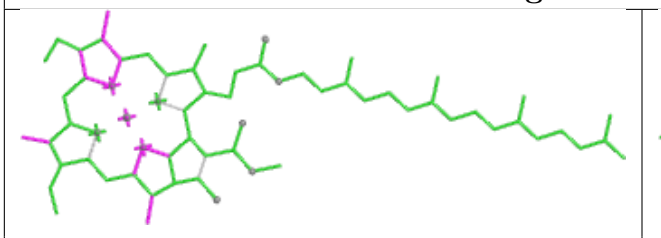


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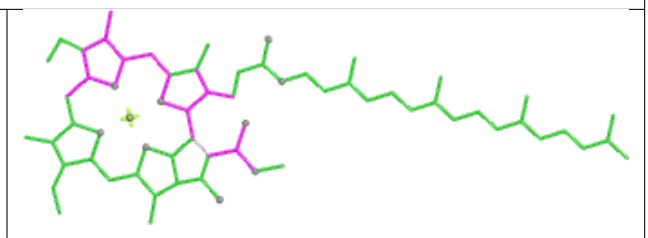


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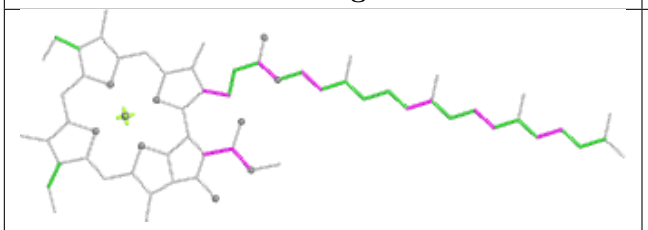
Ligand CLA B 603



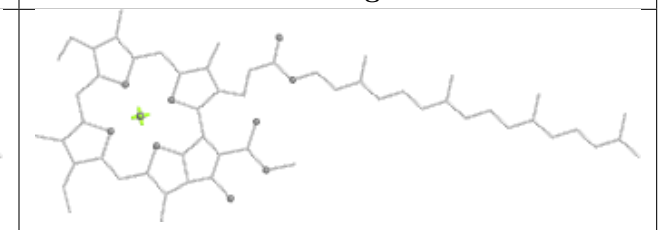
Bond lengths



Bond angles

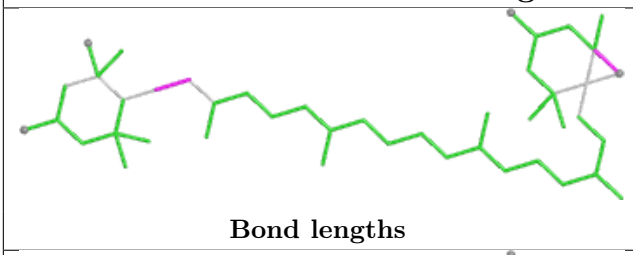


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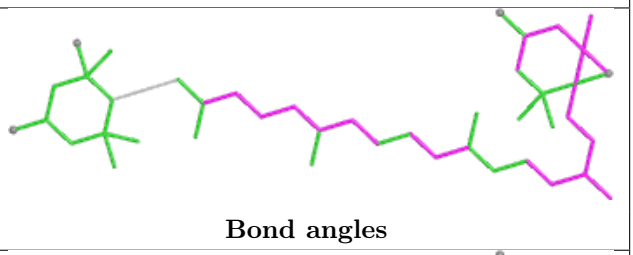


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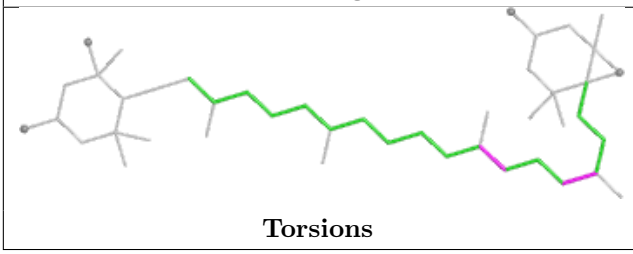
Ligand NEX 9 1623



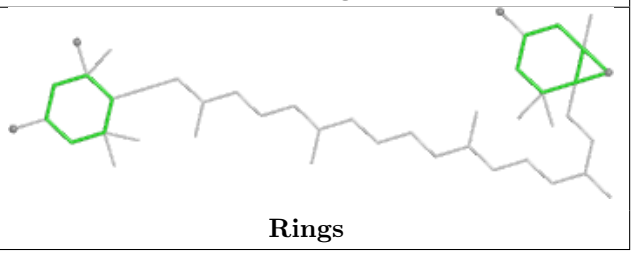
Bond lengths



Bond angles

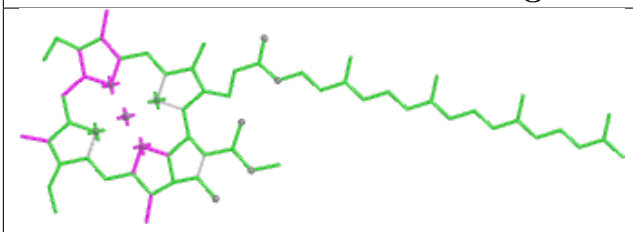


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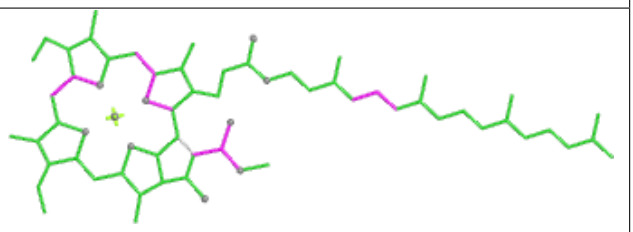


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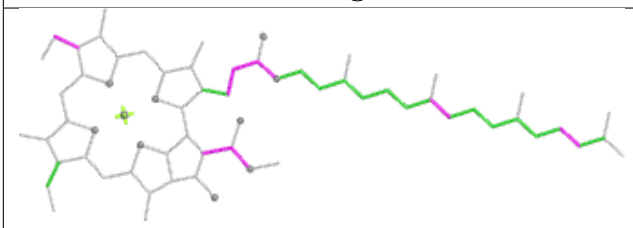
Ligand CLA C 501



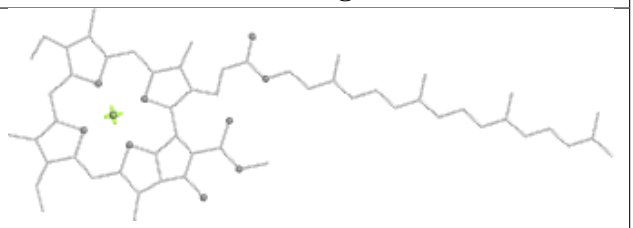
Bond lengths



Bond angles

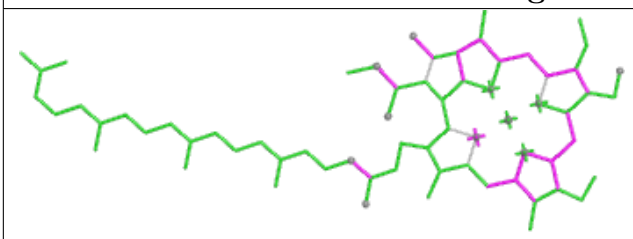


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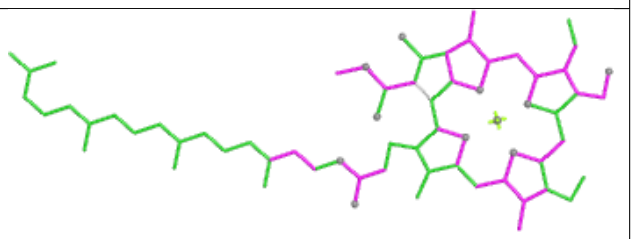


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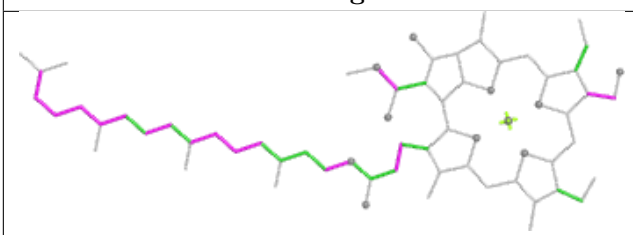
Ligand CHL 3 605



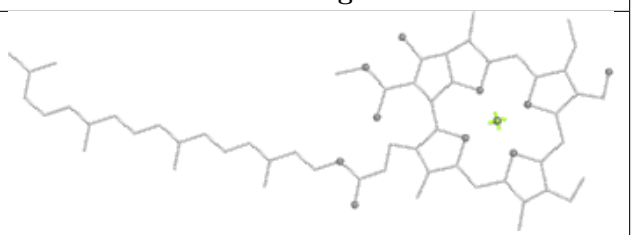
Bond lengths



Bond angles

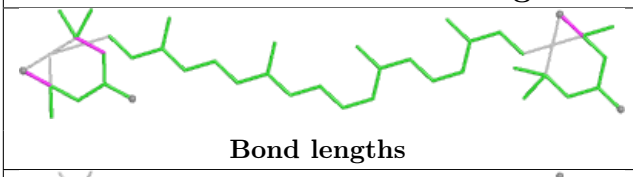


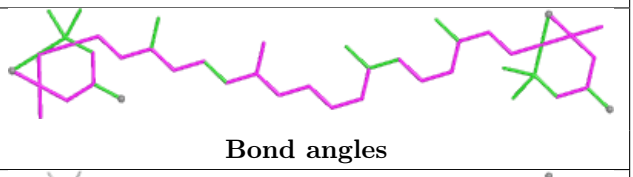
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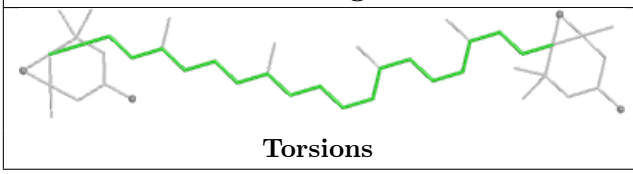


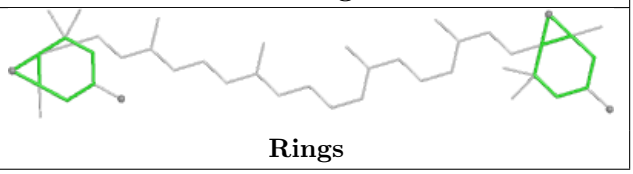
Rings

Ligand XAT N 1622

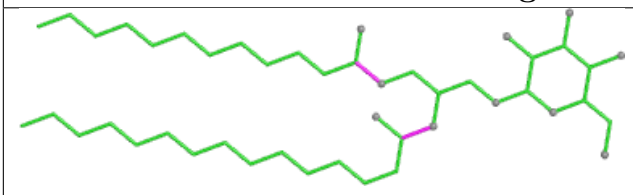

Bond lengths

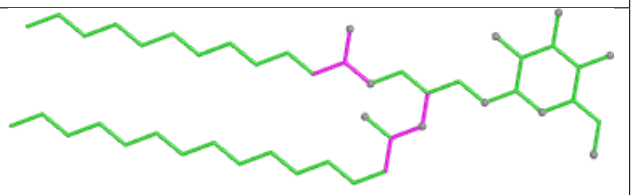

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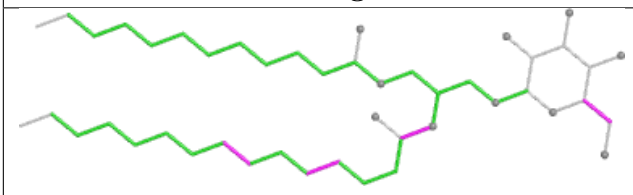

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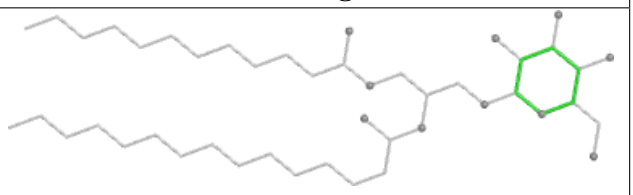

Rings

Ligand LMG D 412

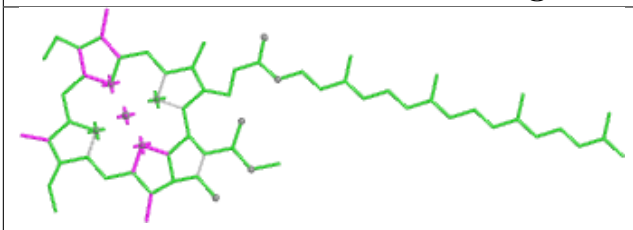

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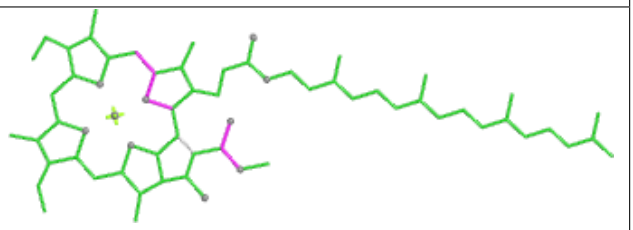

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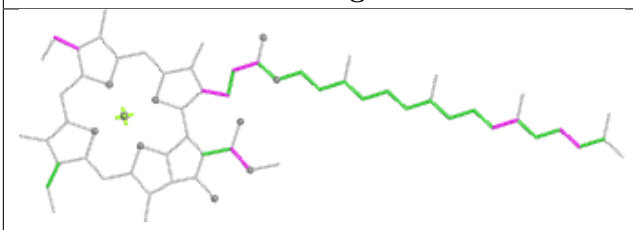

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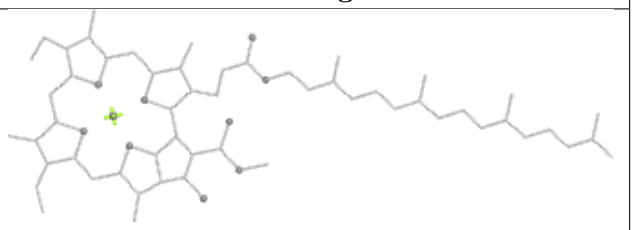

Rings

Ligand CLA 7 611

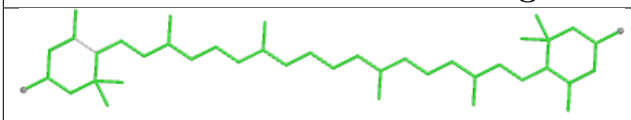

Bond lengths


Bond angles

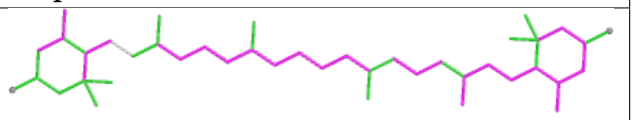

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Rings

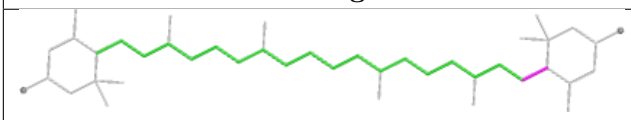
Ligand LUT q 1620



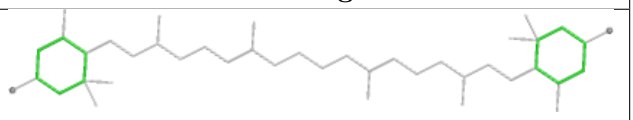
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Bond angles

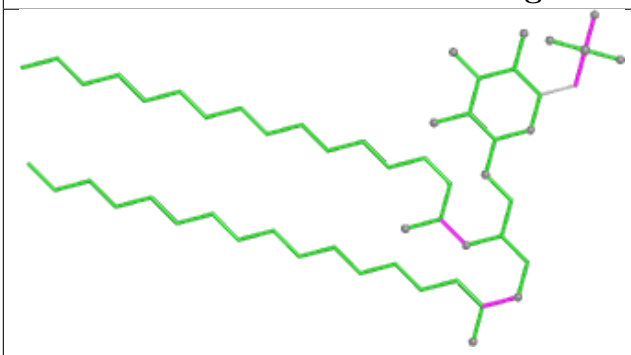


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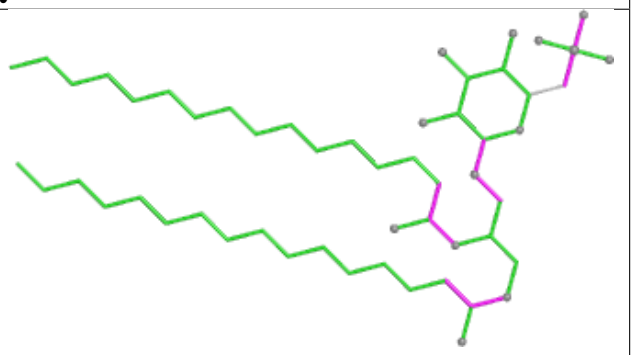


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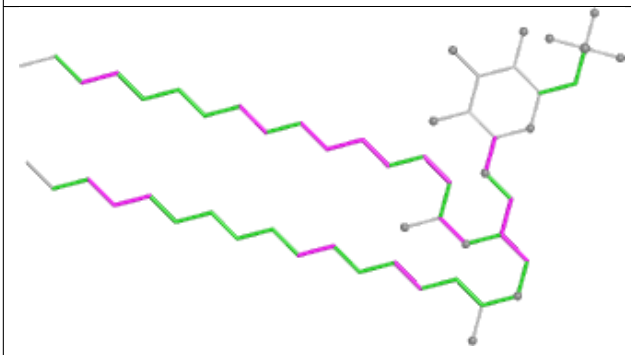
Ligand SQD B 621



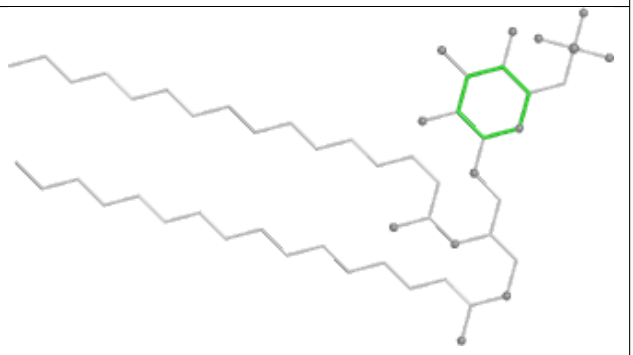
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Bond angles

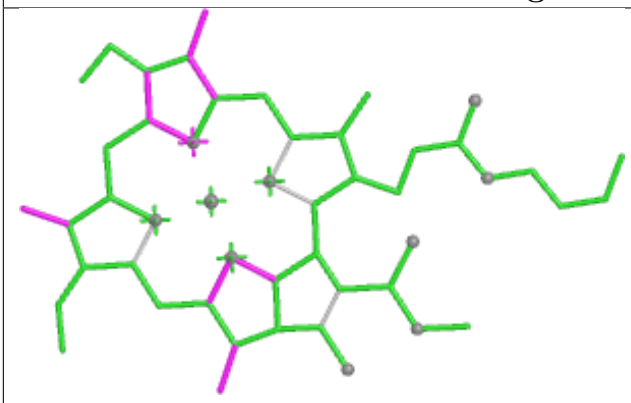


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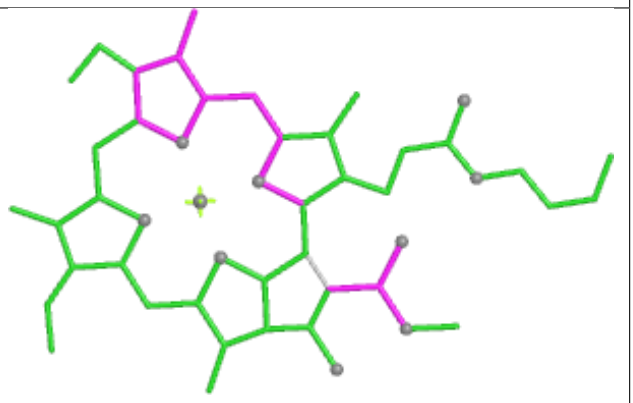


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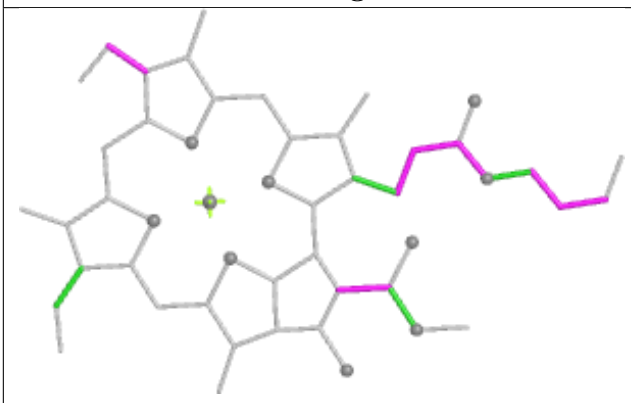
Ligand CLA S 602



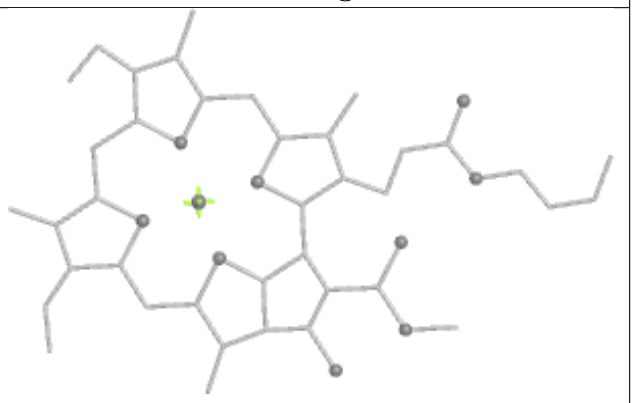
Bond lengths



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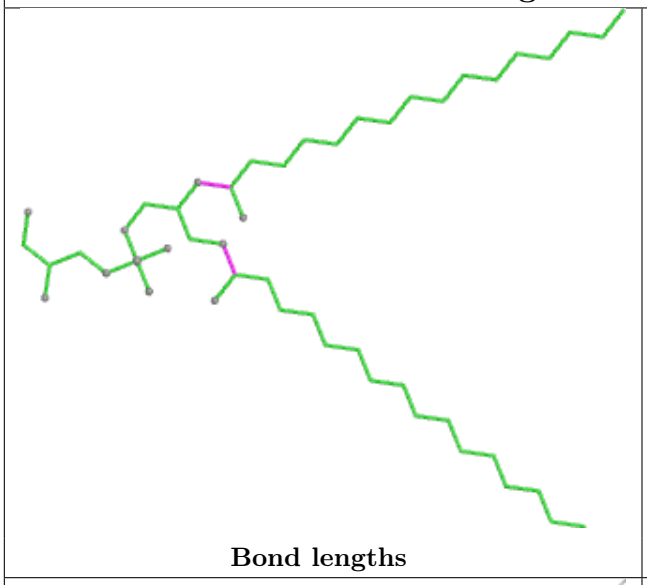


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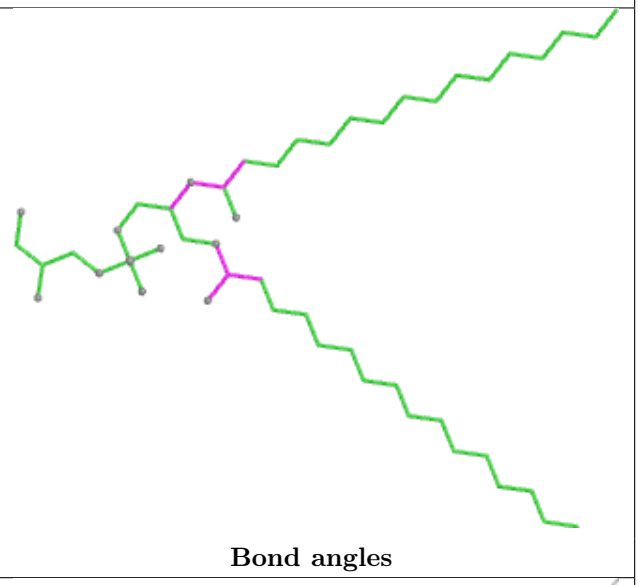


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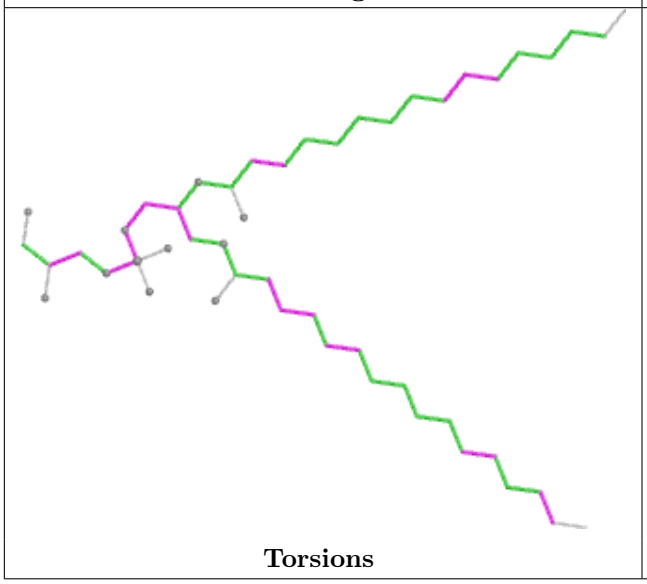
Ligand LHG 7 2630



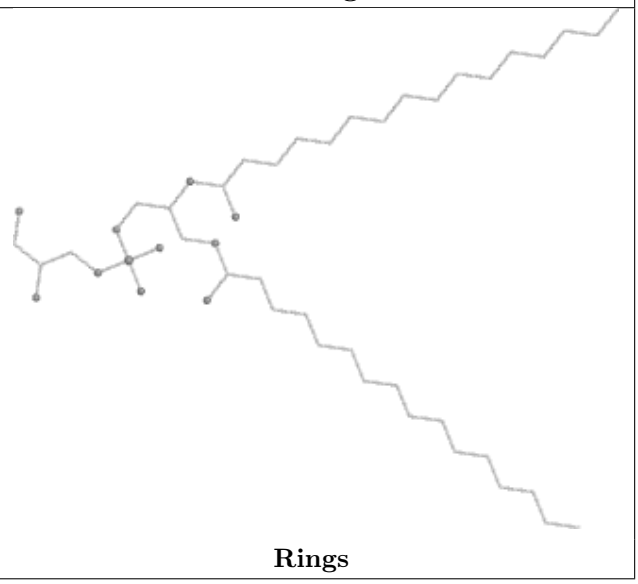
Bond lengths



Bond angles

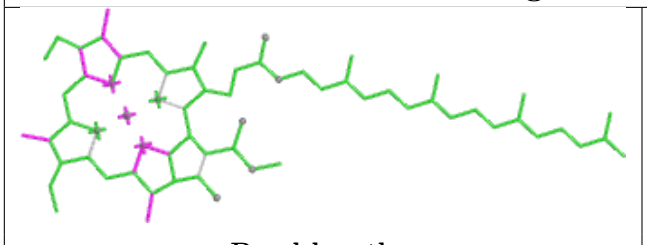


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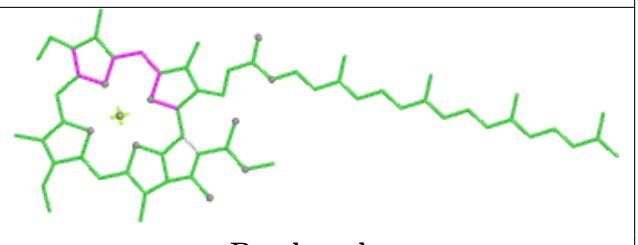


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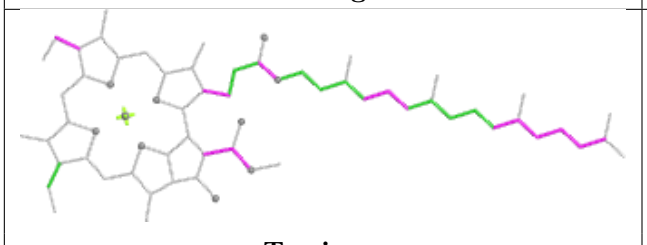
Ligand CLA B 602



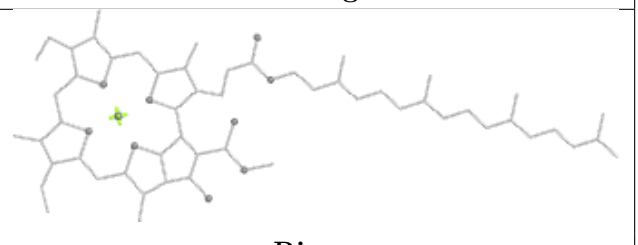
Bond lengths



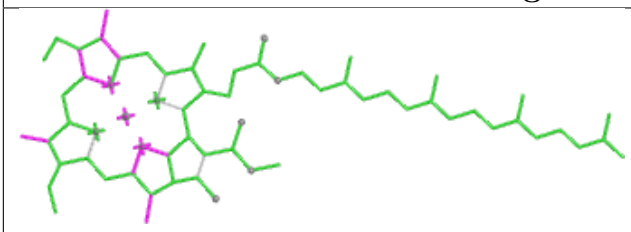
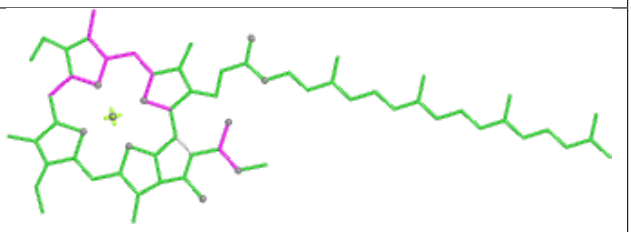
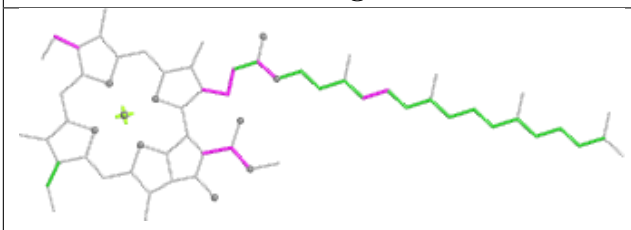
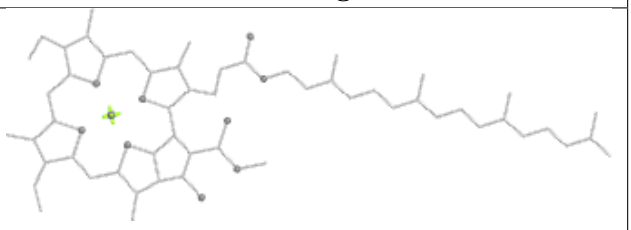
Bond angles

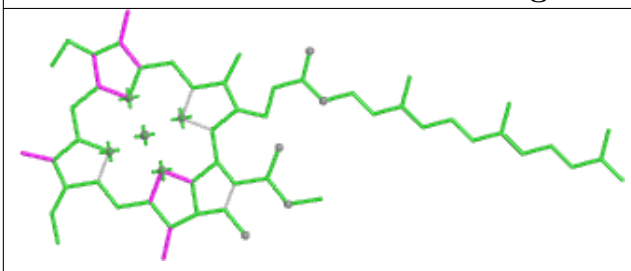
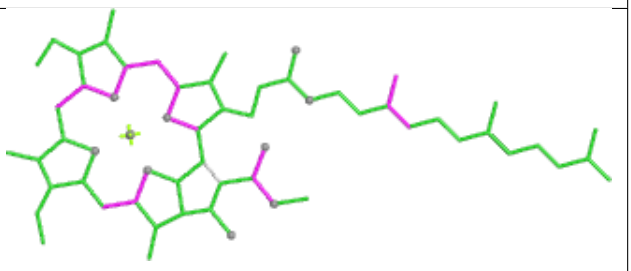
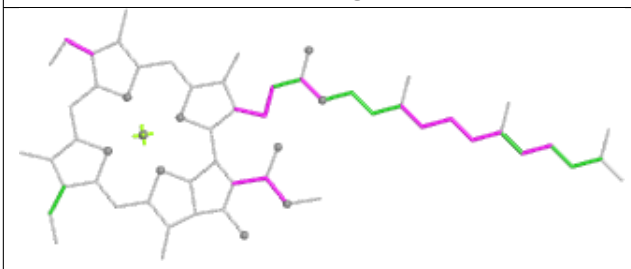
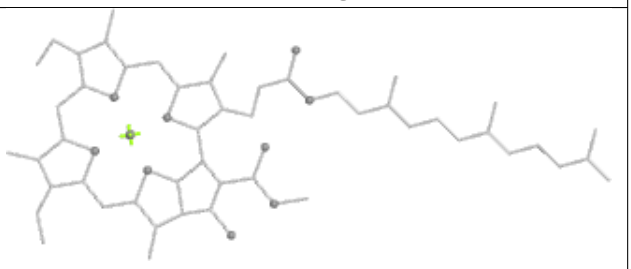


Torsions

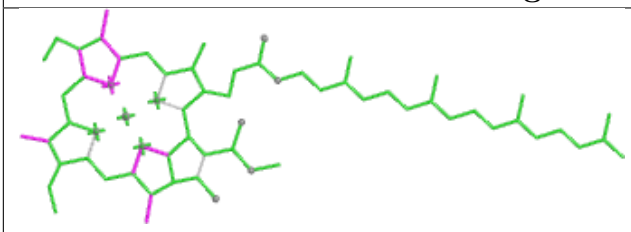


Rings

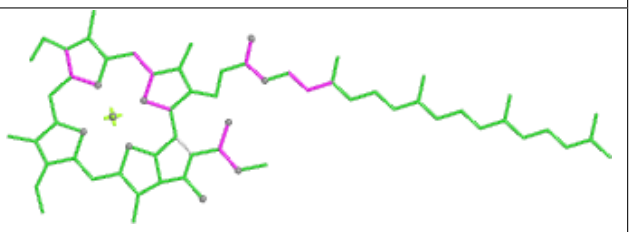
Ligand CLA N 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

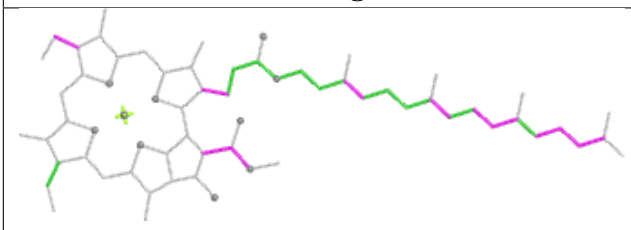
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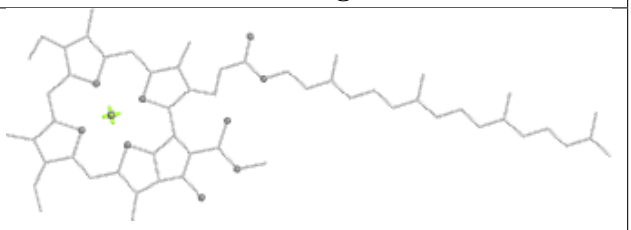
Bond lengths



Bond angles

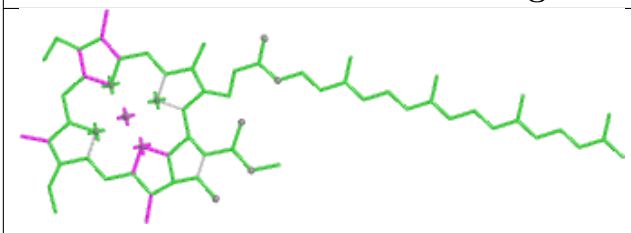


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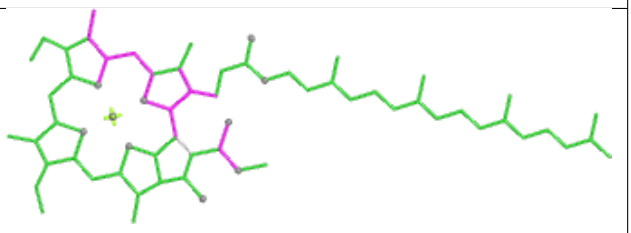


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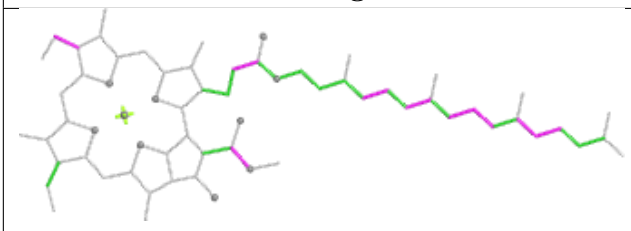
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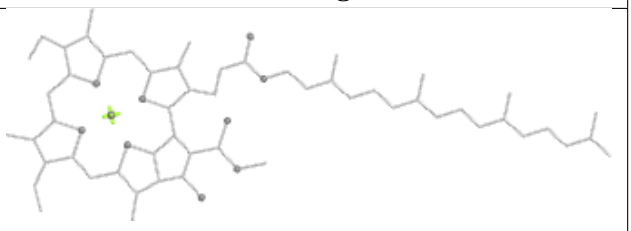
Bond lengths



Bond angles

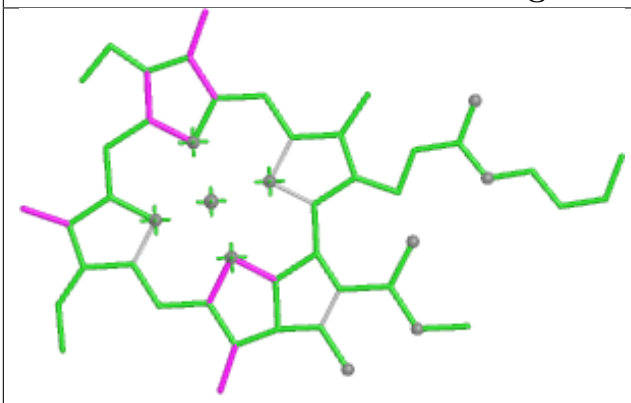


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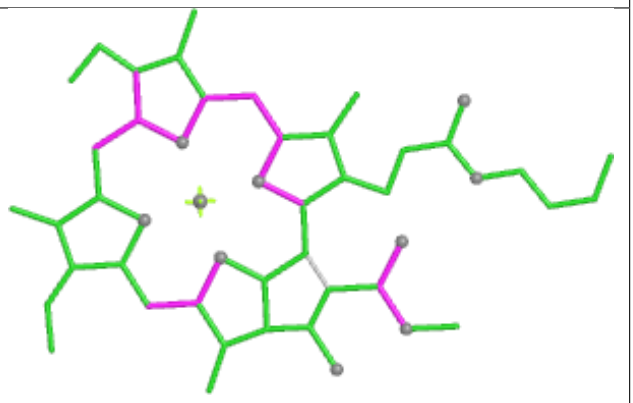


Rings

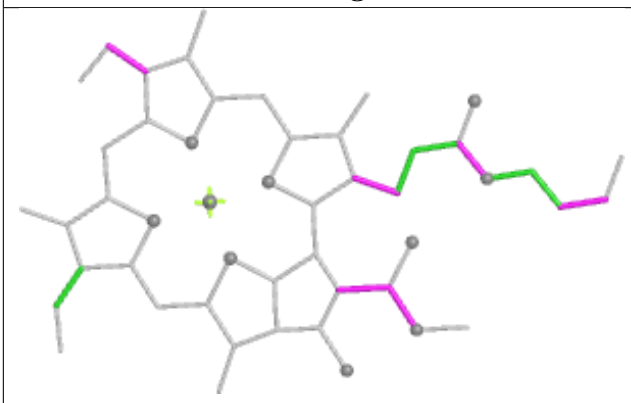
Ligand CLA 4 614



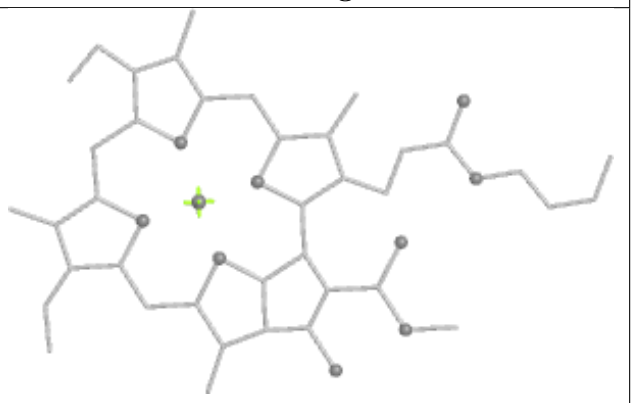
Bond lengths



Bond angles

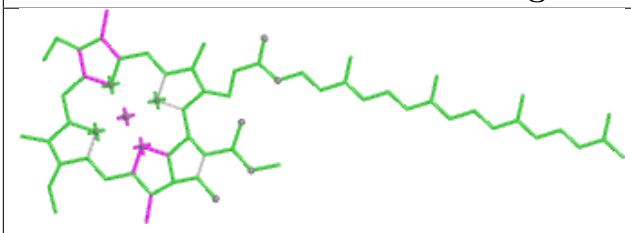


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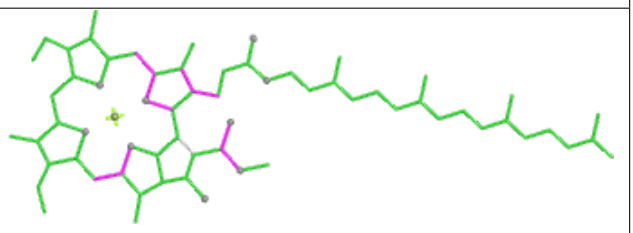


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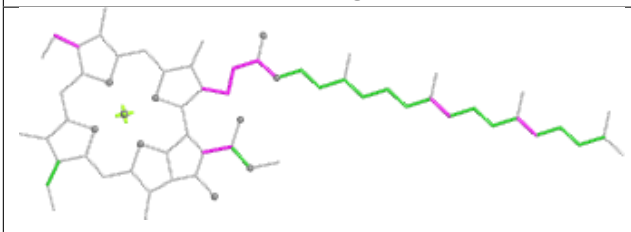
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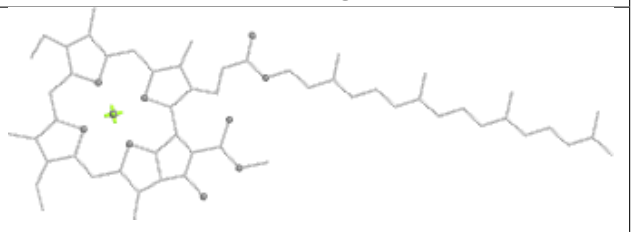
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Bond angles

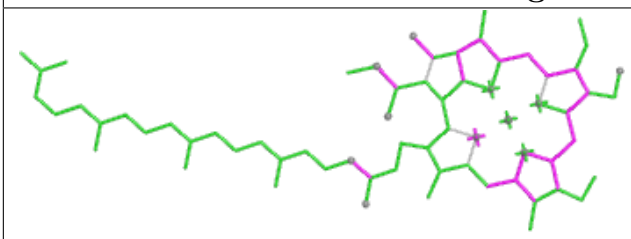


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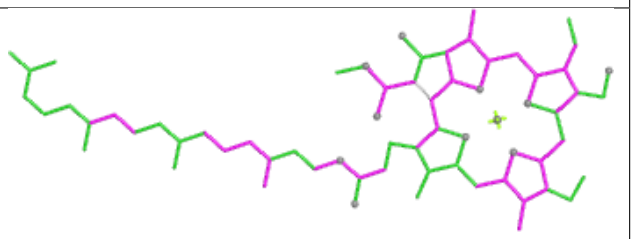


Rings

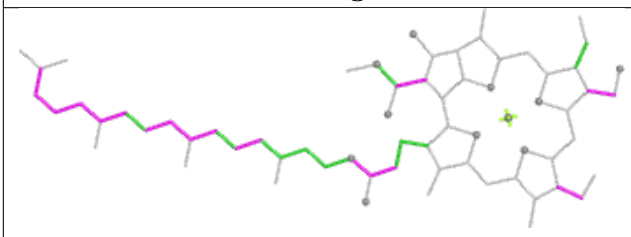
Ligand CHL 5 605



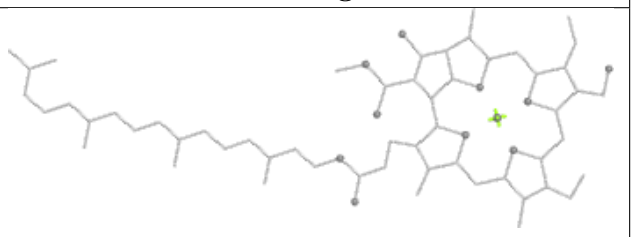
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Bond angles

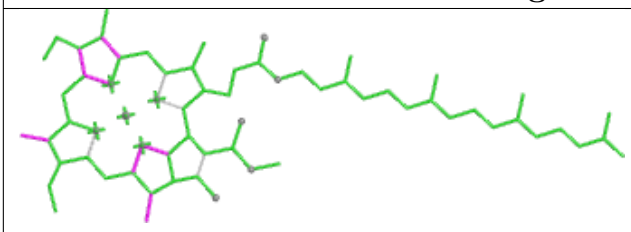


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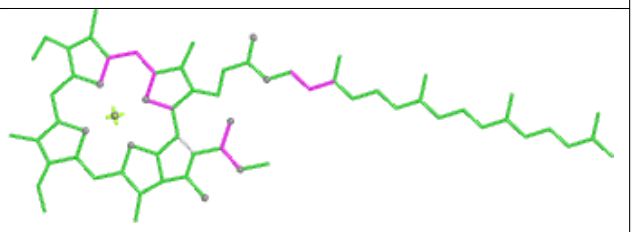


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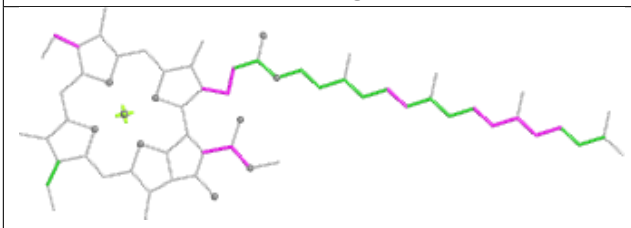
Ligand CLA 4 610



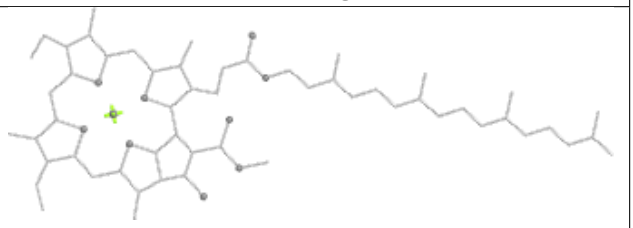
Bond lengths



Bond angles

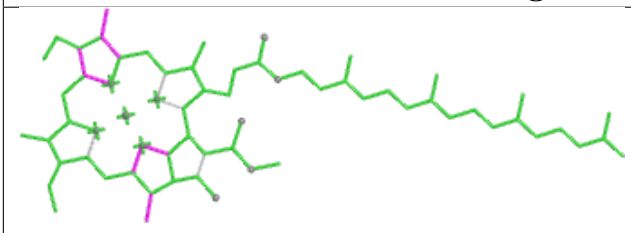


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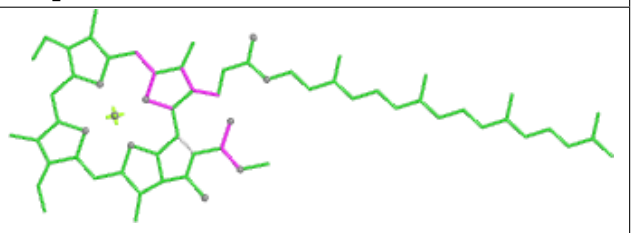


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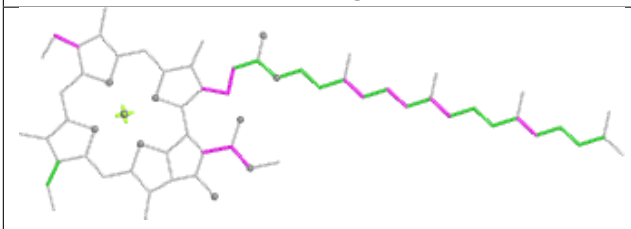
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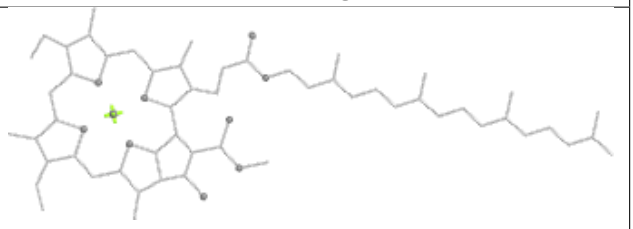
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Bond angles

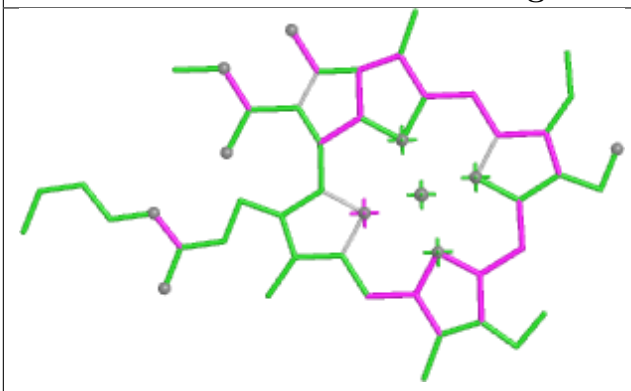


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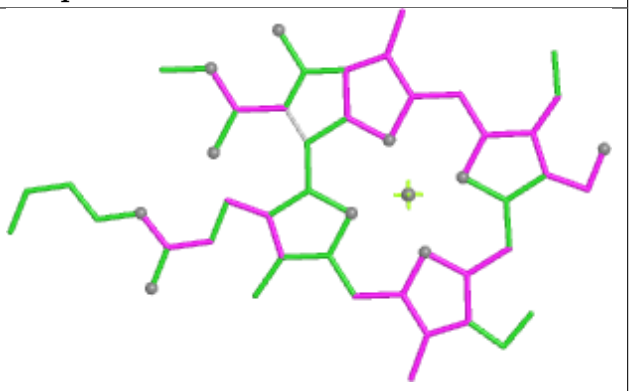


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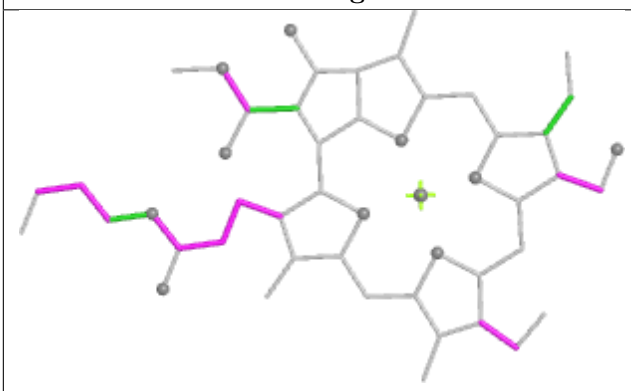
Ligand CHL q 607



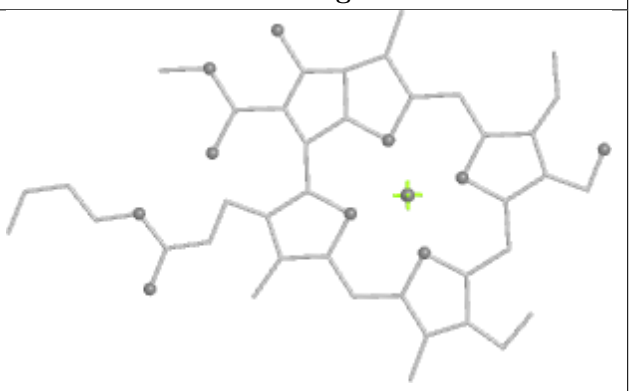
Bond lengths



Bond angles

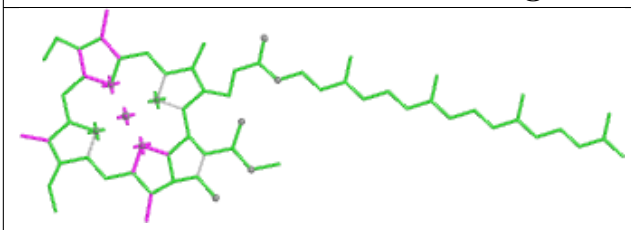


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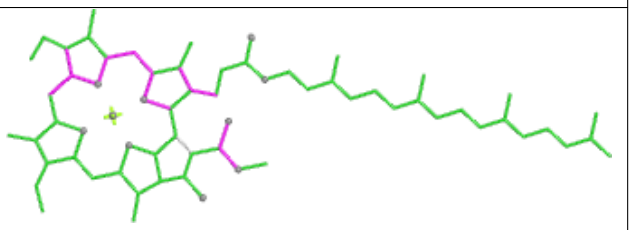


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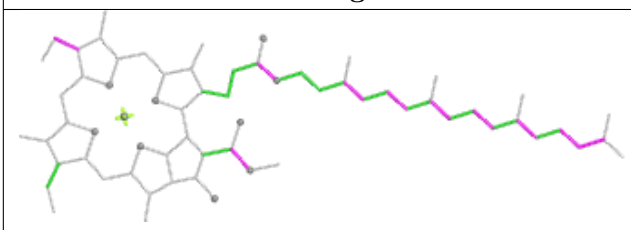
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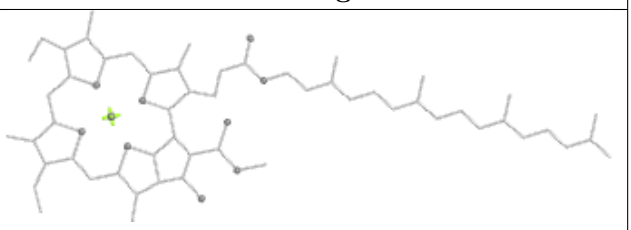
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Bond angles

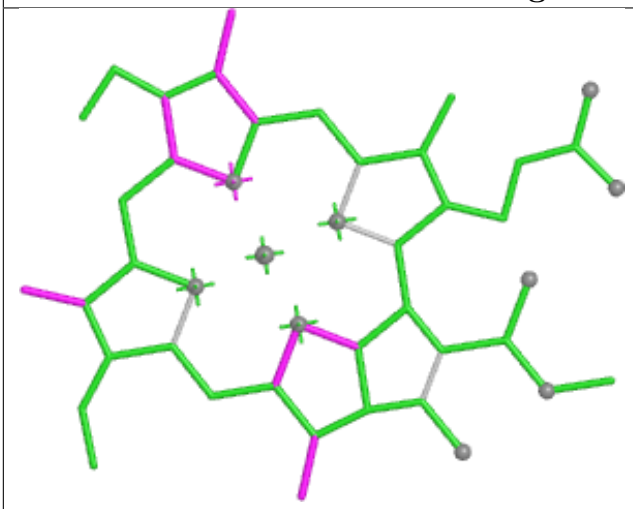


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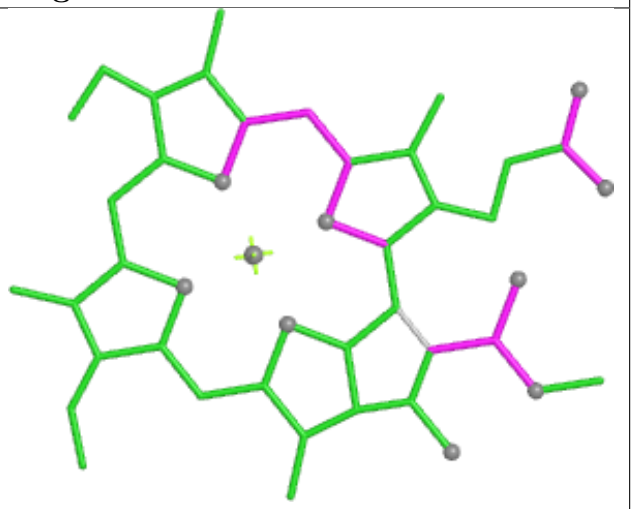


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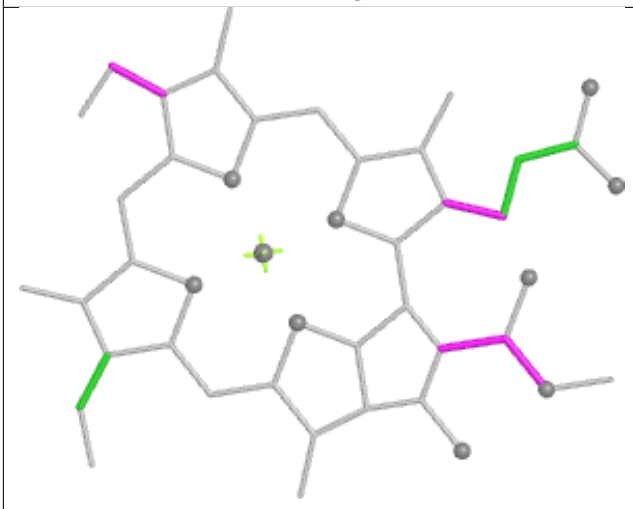
Ligand CLA g 611



Bond lengths



Bond angles

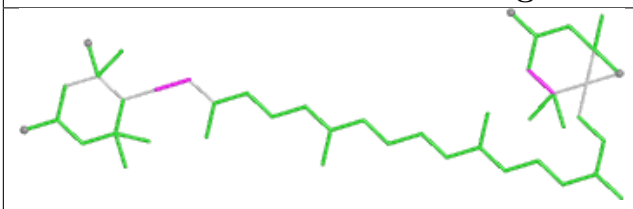


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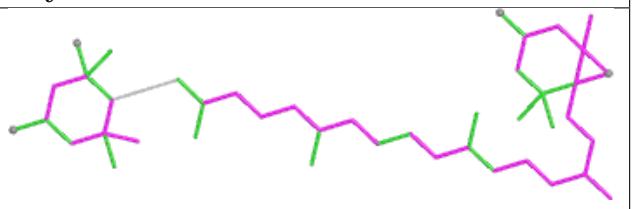


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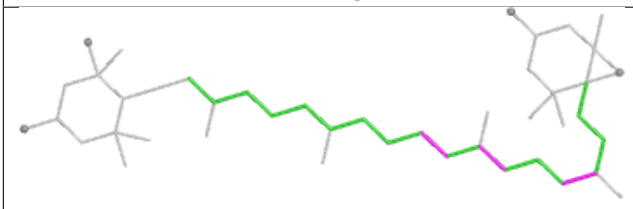
Ligand NEX y 1623



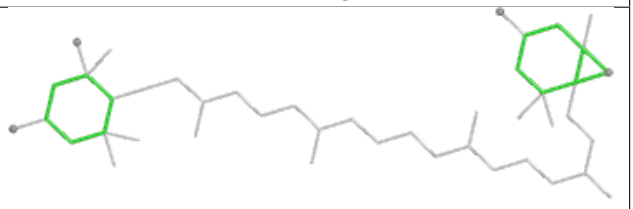
Bond lengths



Bond angles

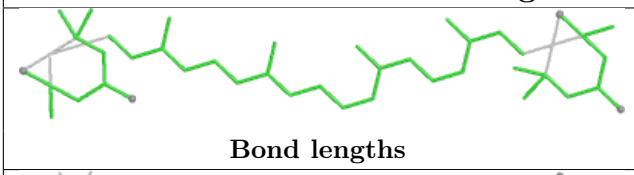


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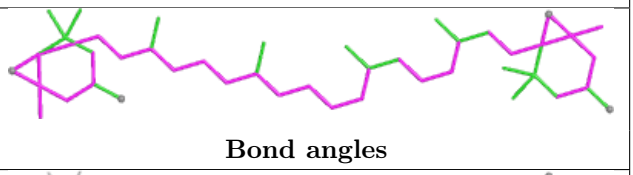


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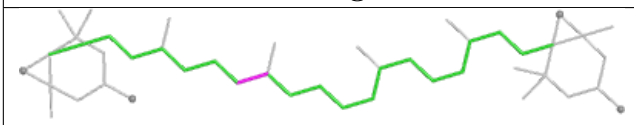
Ligand XAT 3 1622



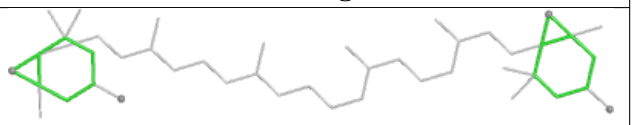
Bond lengths



Bond angles

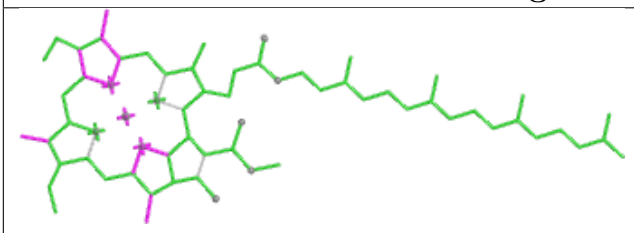


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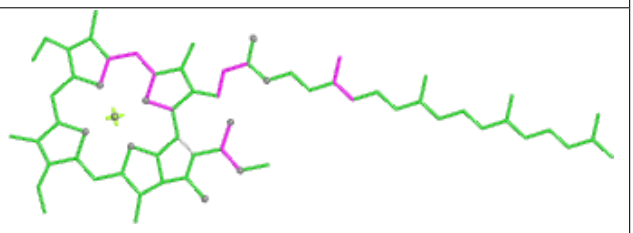


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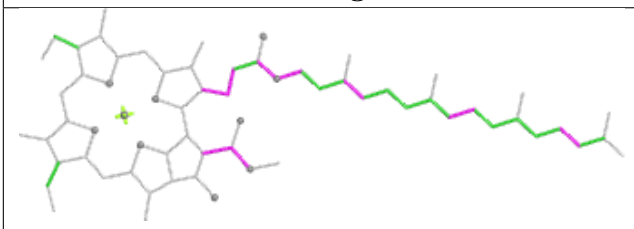
Ligand CLA c 503



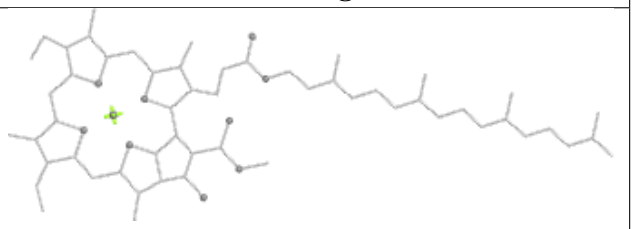
Bond lengths



Bond angles

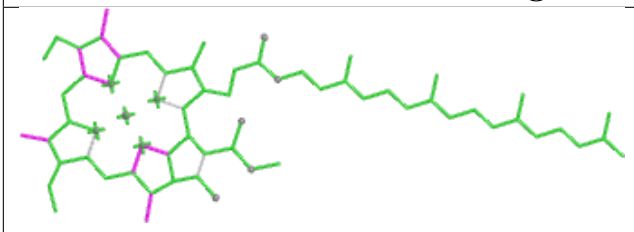


Torsions

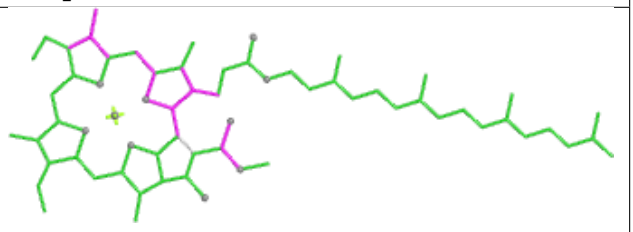


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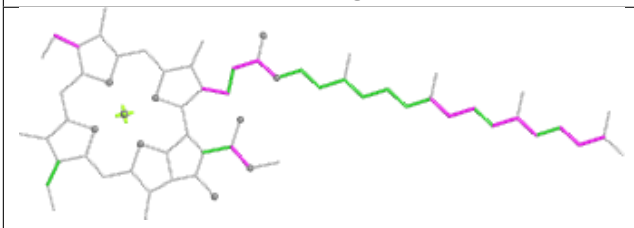
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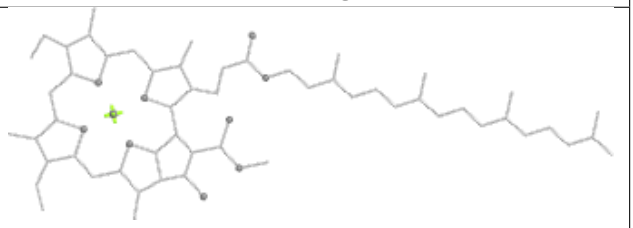
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Bond angles

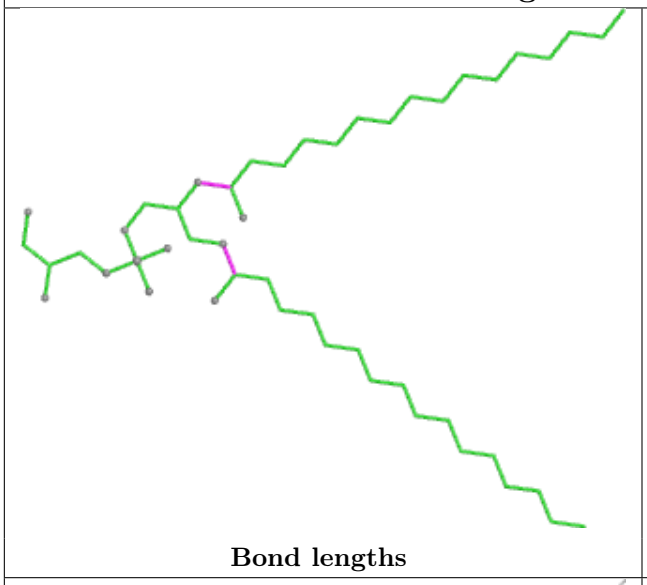


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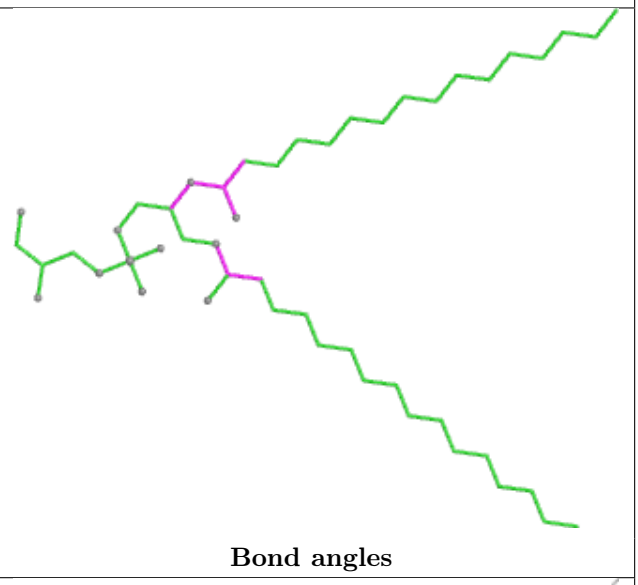


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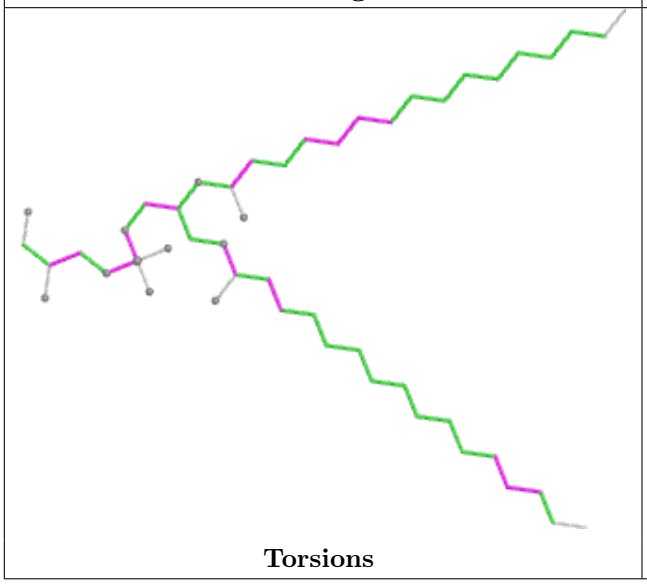
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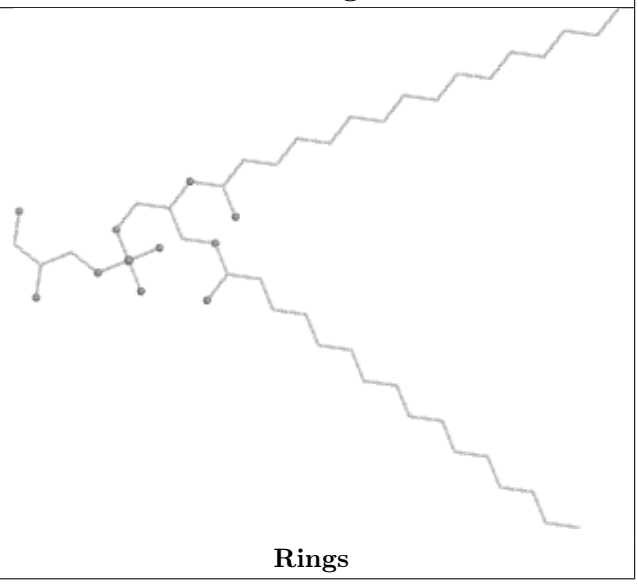
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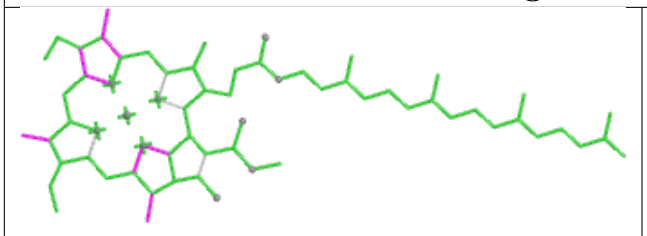


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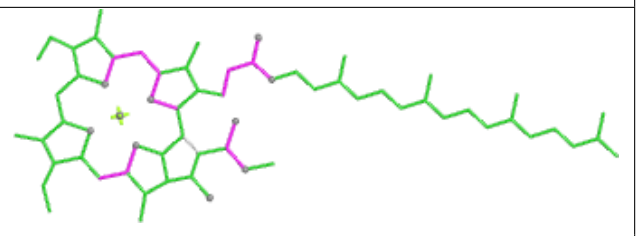


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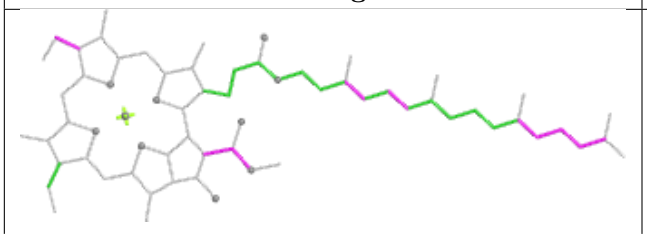
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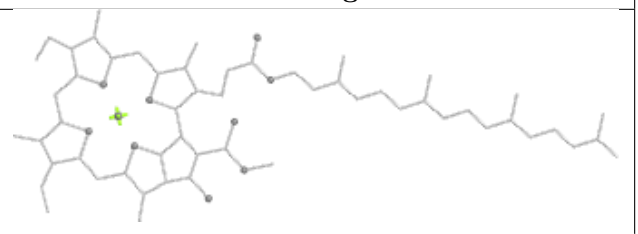
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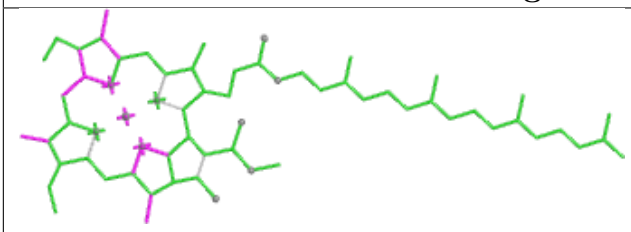


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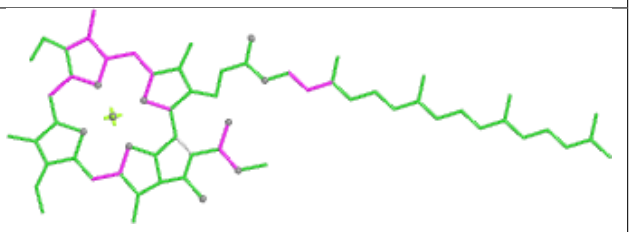


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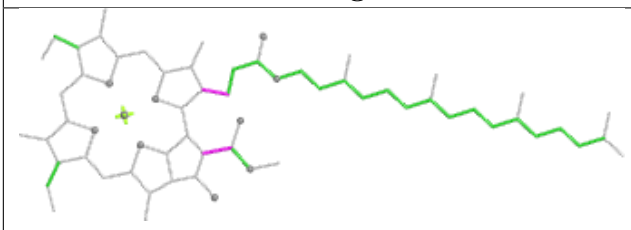
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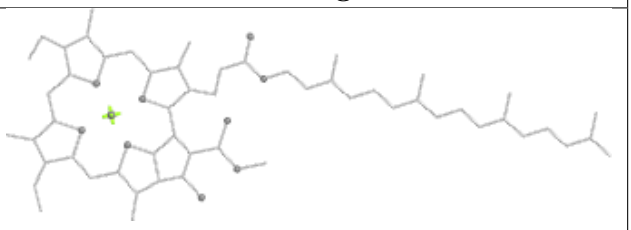
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Bond angles



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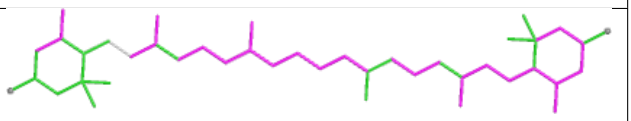


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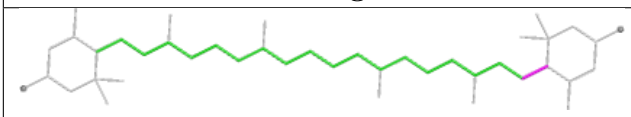
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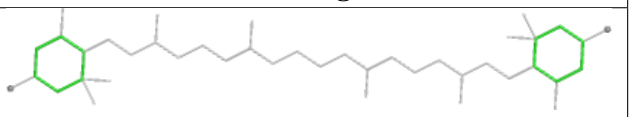
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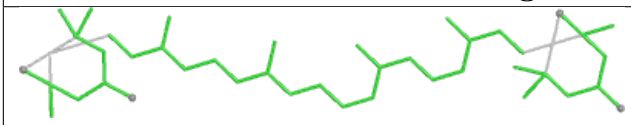


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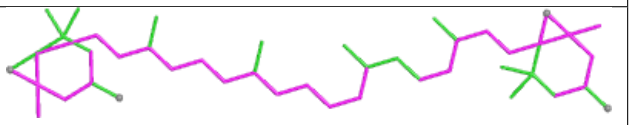


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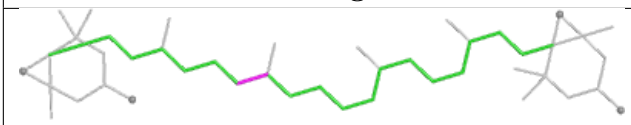
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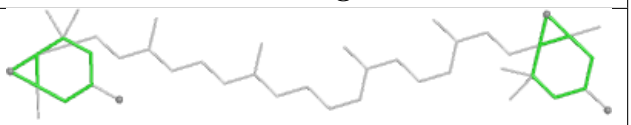
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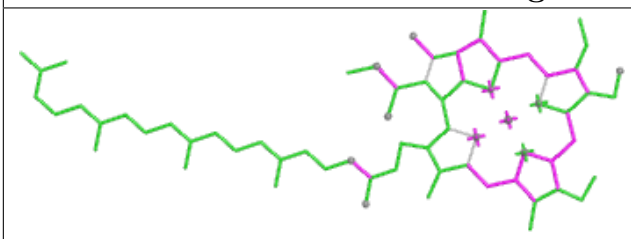


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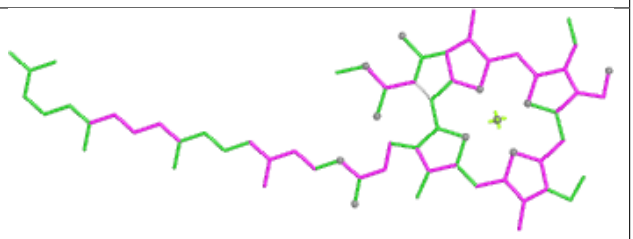


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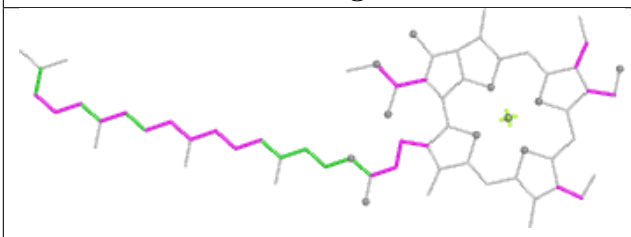
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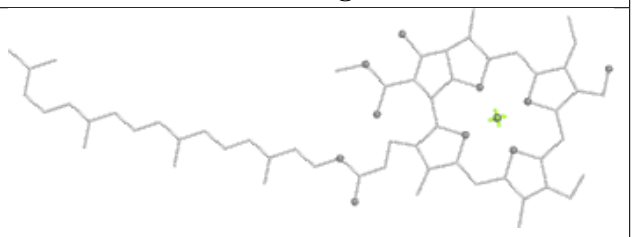
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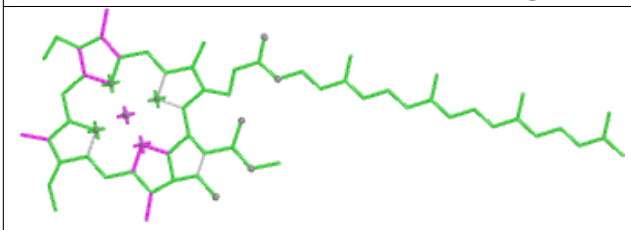


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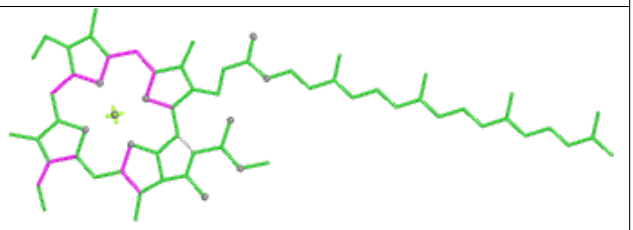


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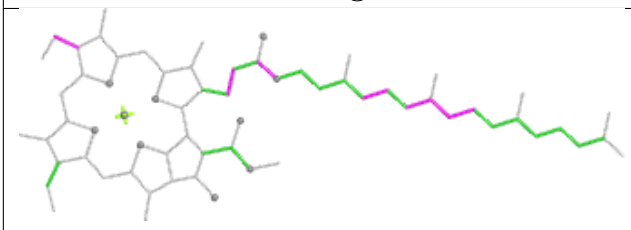
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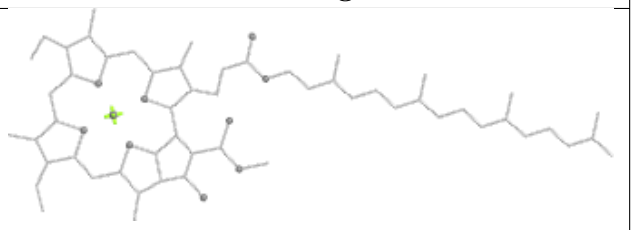
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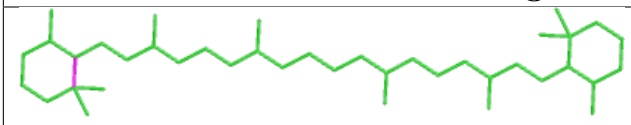


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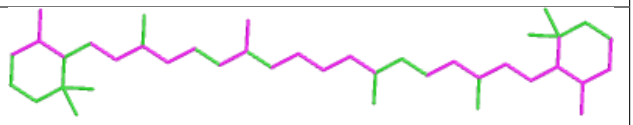


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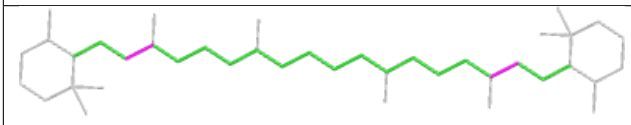
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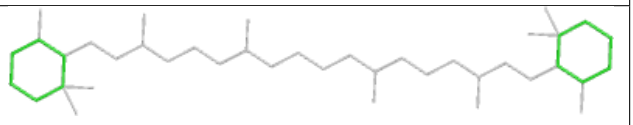
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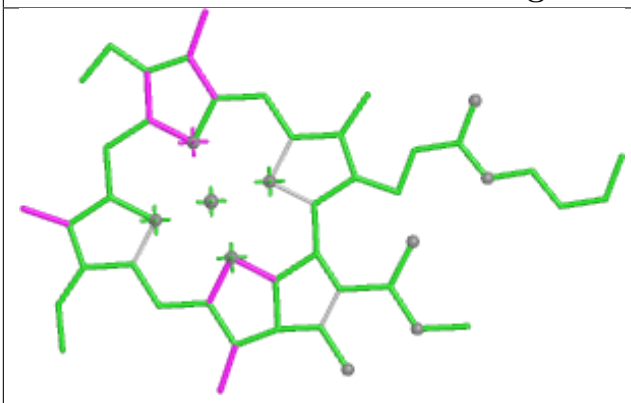


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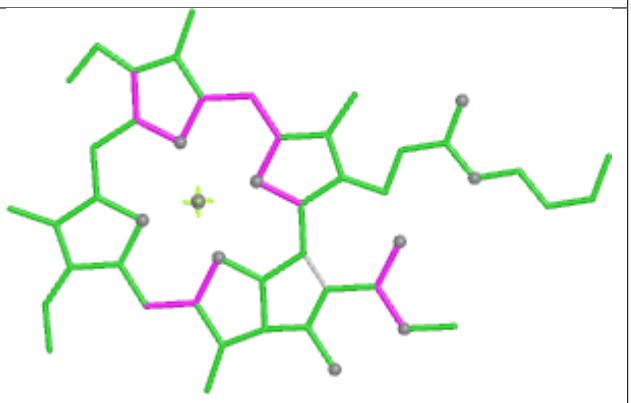


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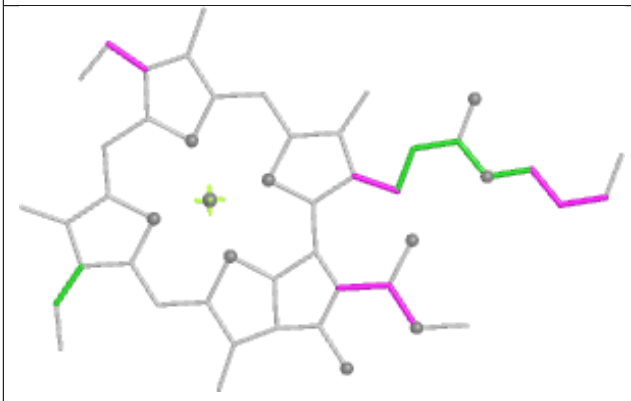
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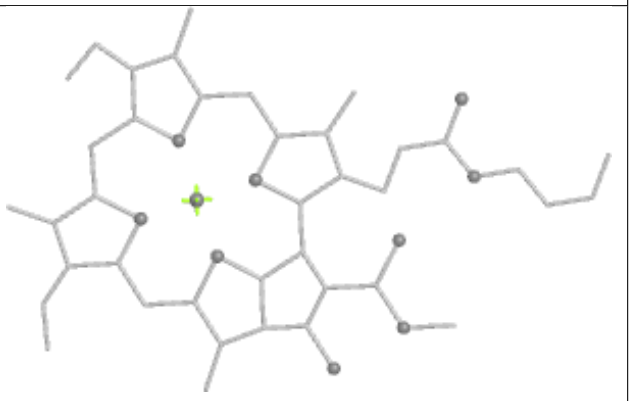
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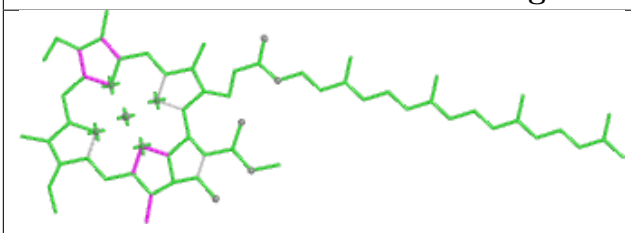


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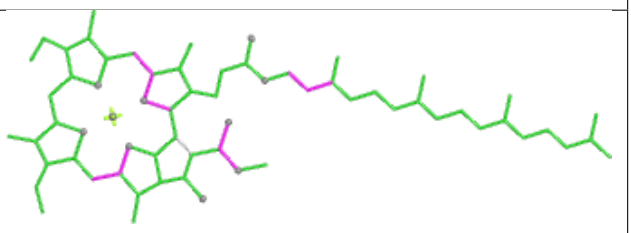


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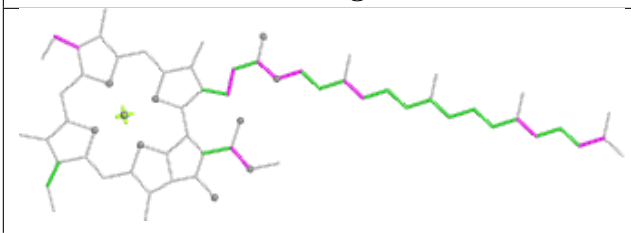
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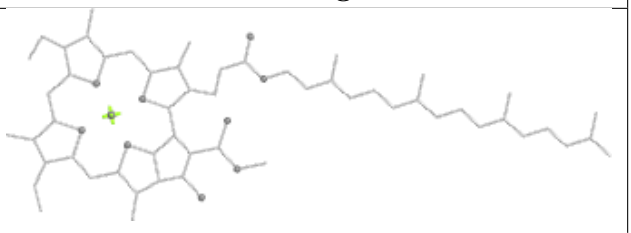
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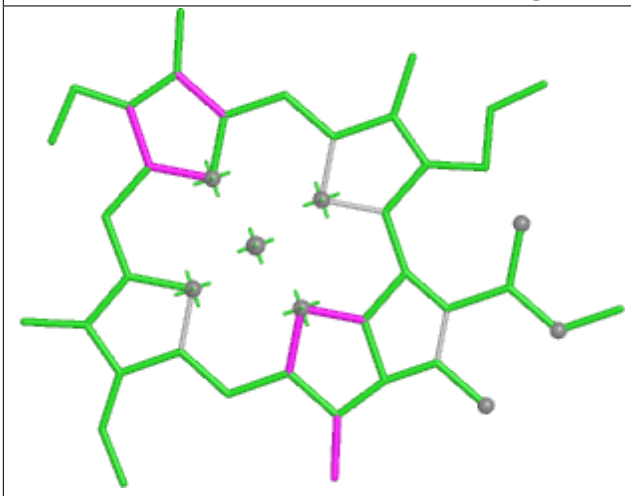


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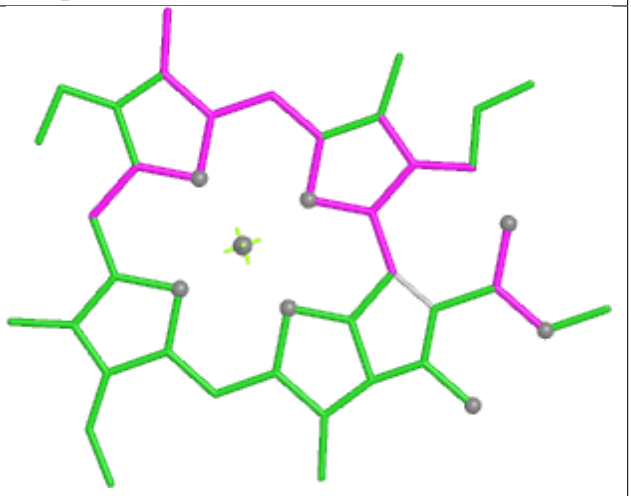


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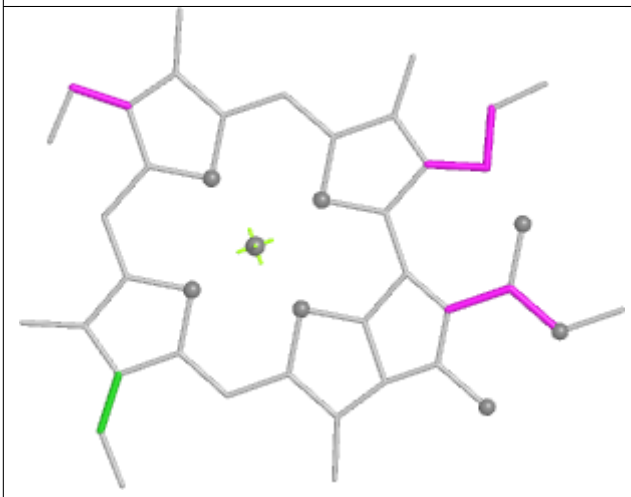
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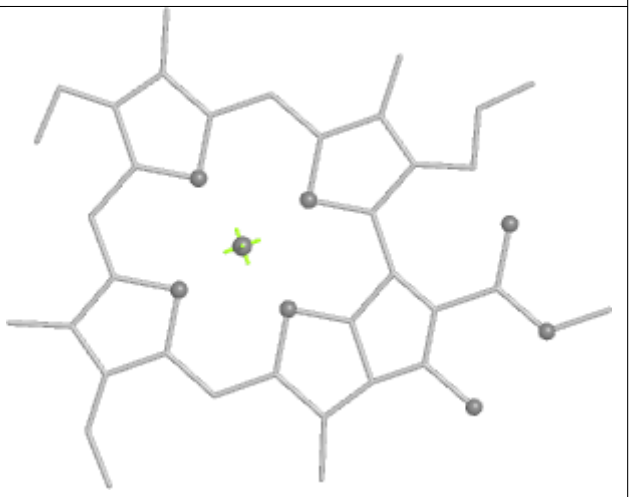
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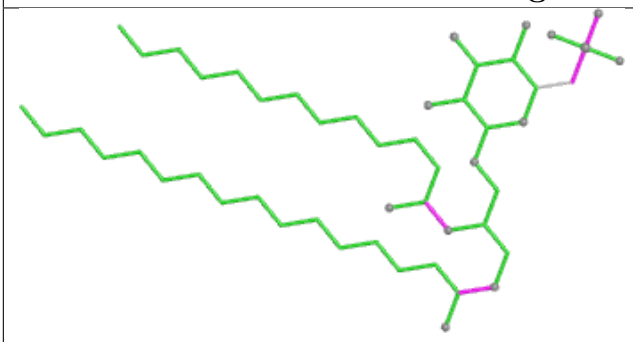


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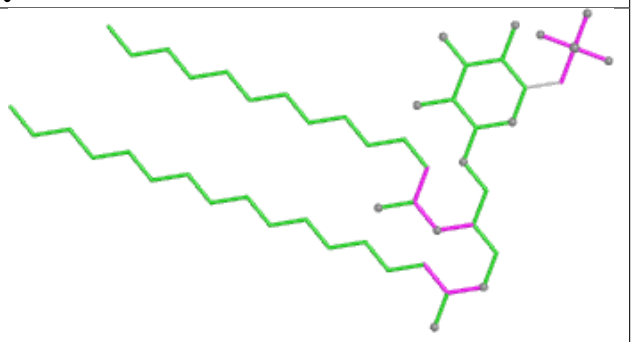


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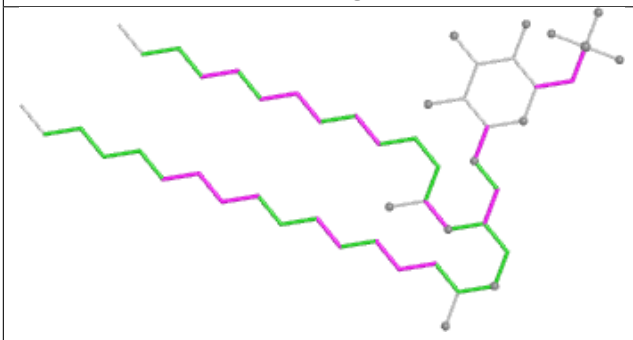
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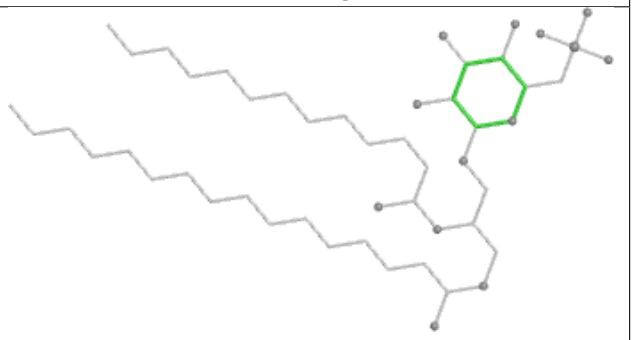
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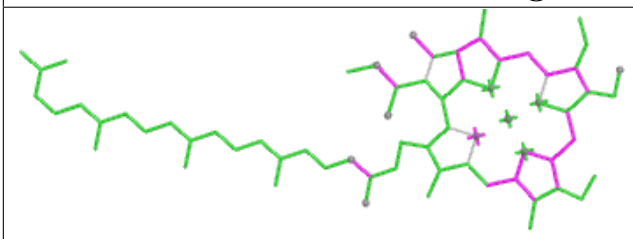


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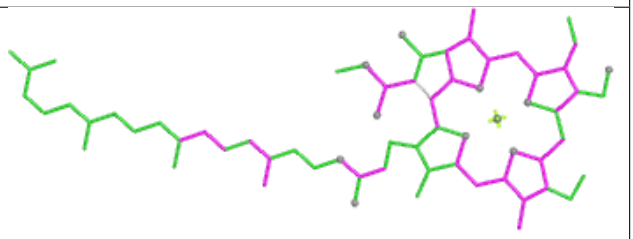


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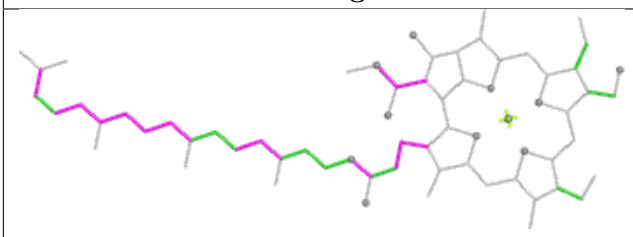
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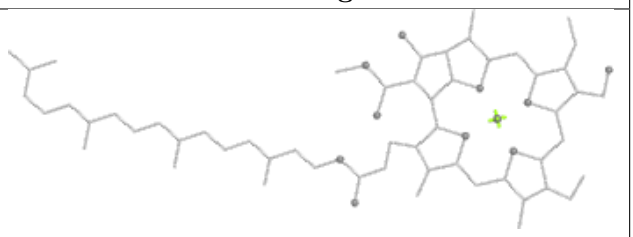
Bond lengths



Bond angles

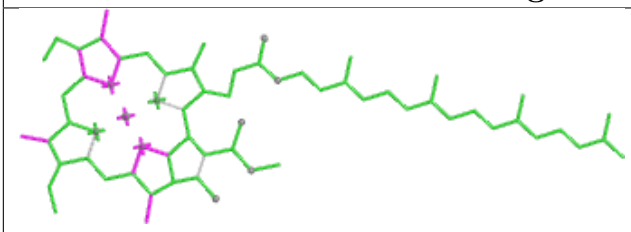


Torsions

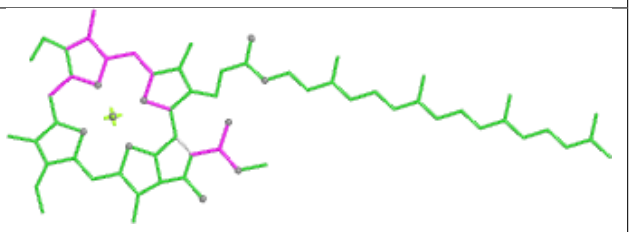


Rings

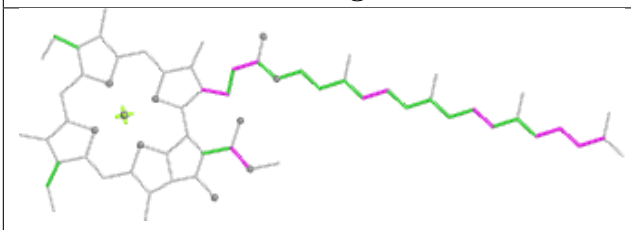
Ligand CLA b 609



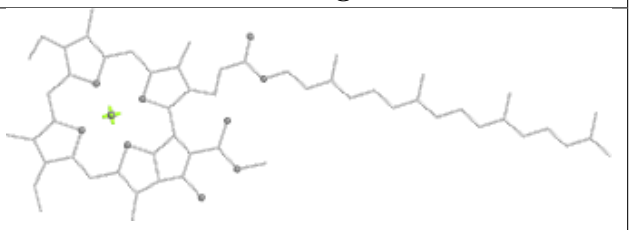
Bond lengths



Bond angles



Torsions



Rings

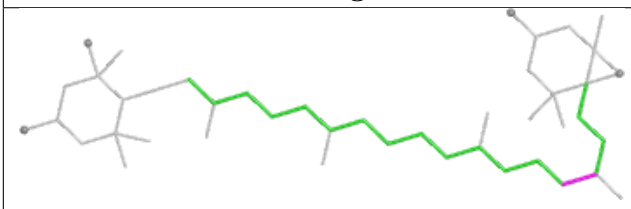
Ligand NEX R 623



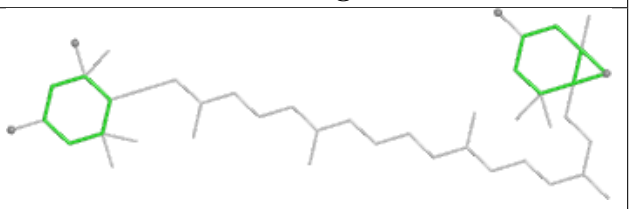
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Bond angles

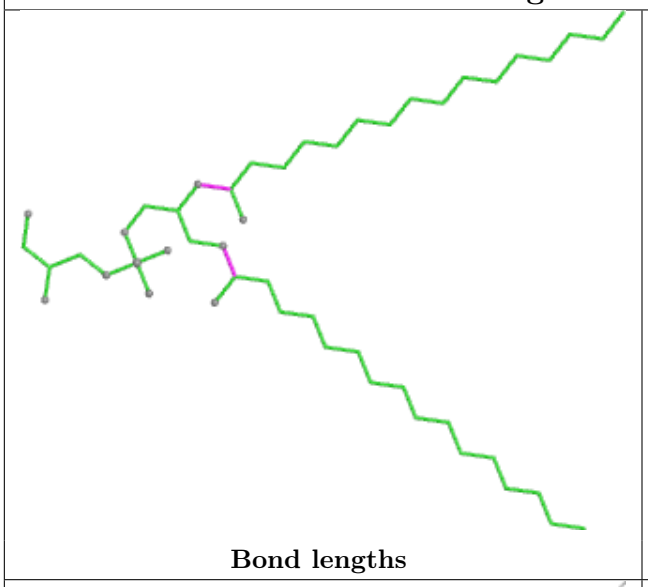


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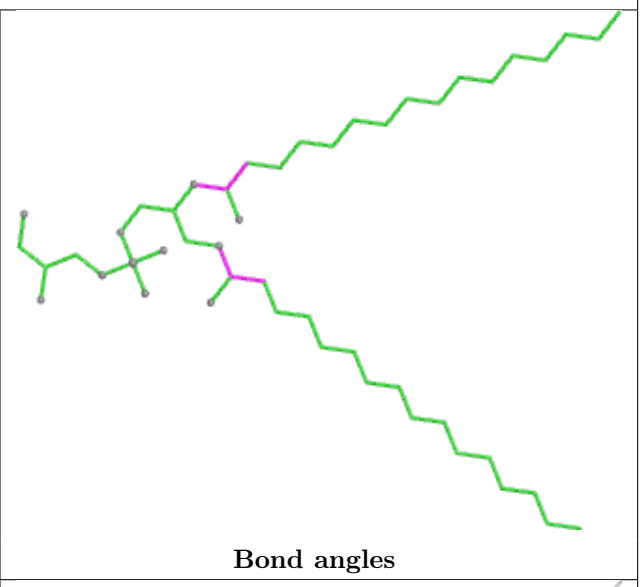


Rings

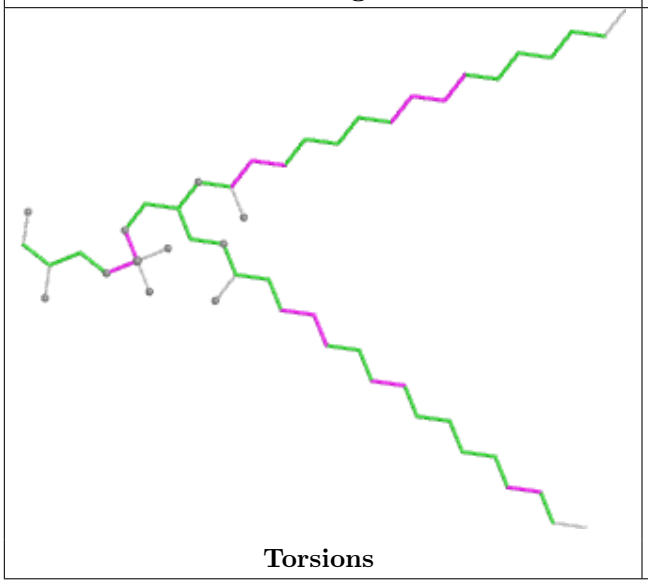
Ligand LHG d 409



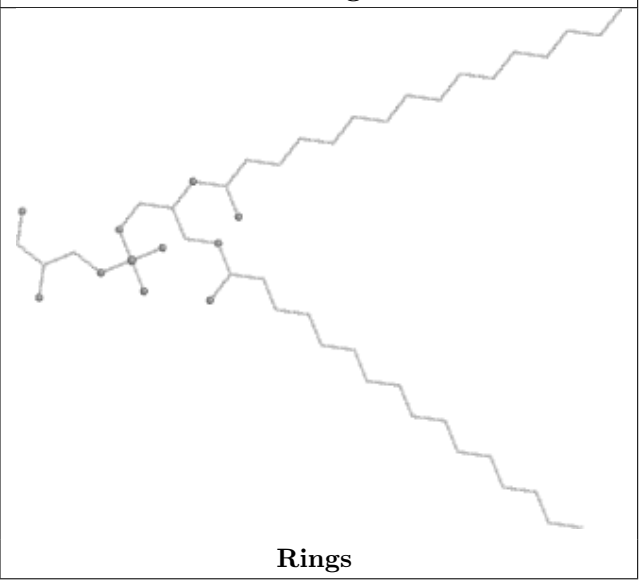
Bond lengths



Bond angles

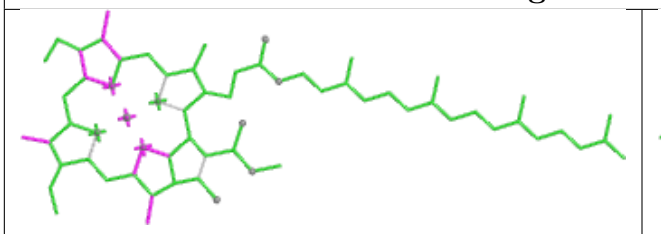


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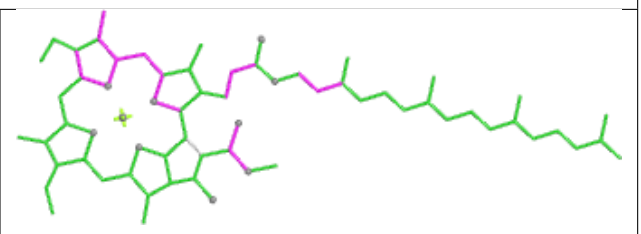


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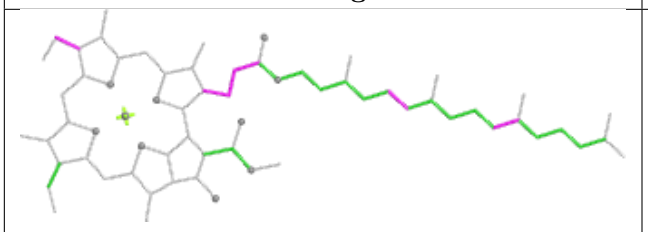
Ligand CLA n 602



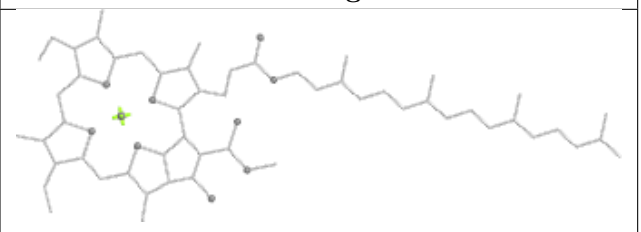
Bond lengths



Bond angles

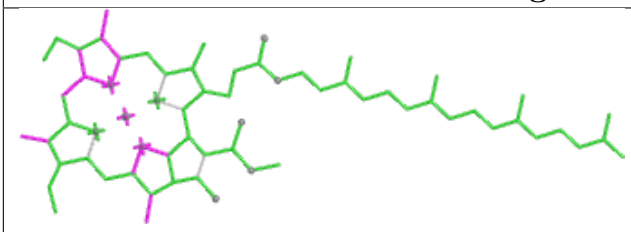


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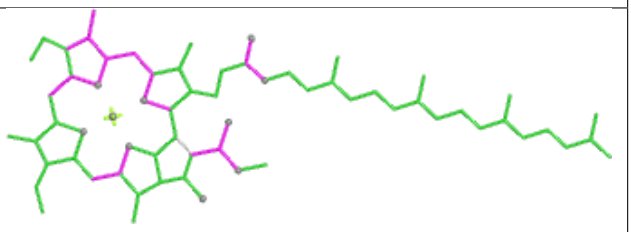


Rings

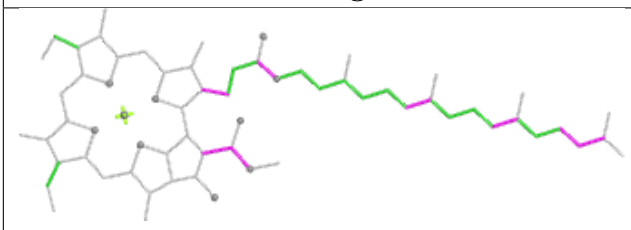
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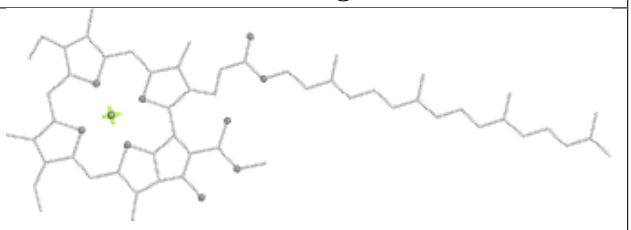
Bond lengths



Bond angles

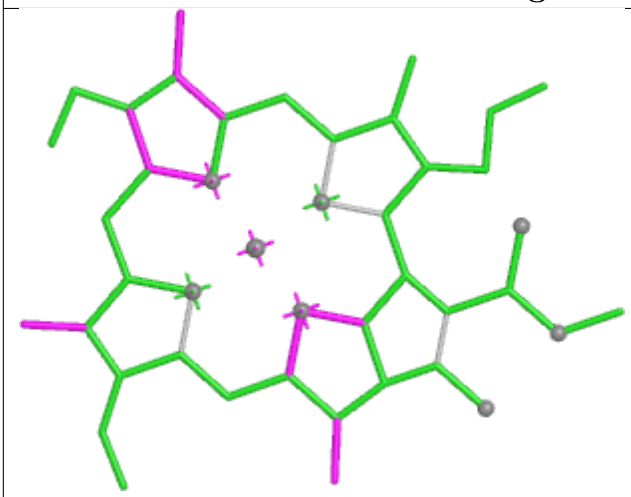


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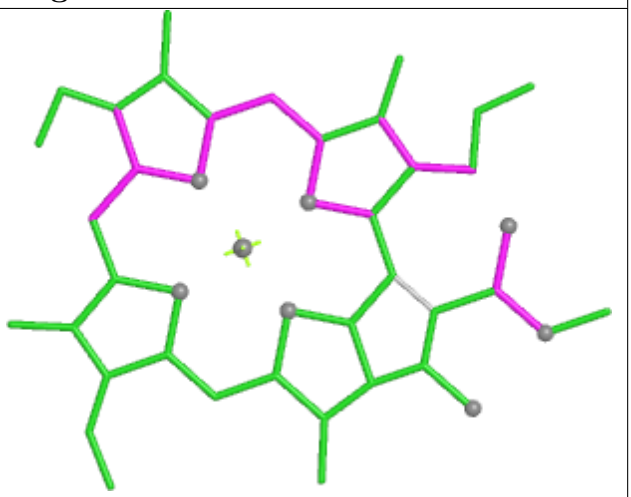


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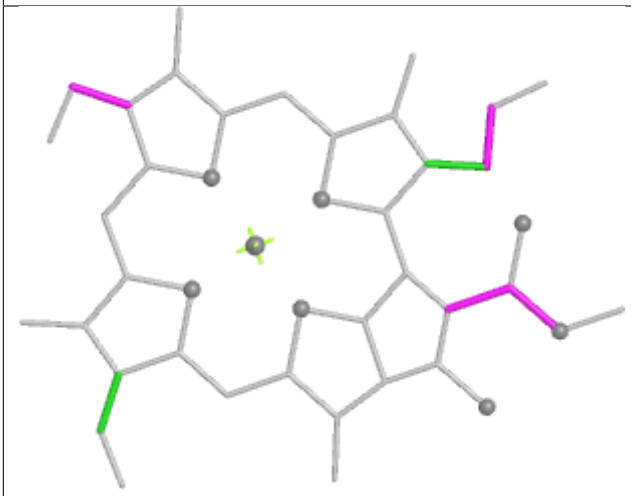
Ligand CLA g 612



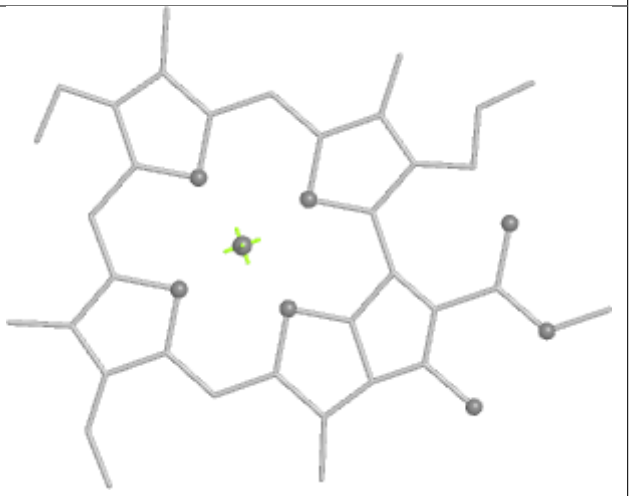
Bond lengths



Bond angles

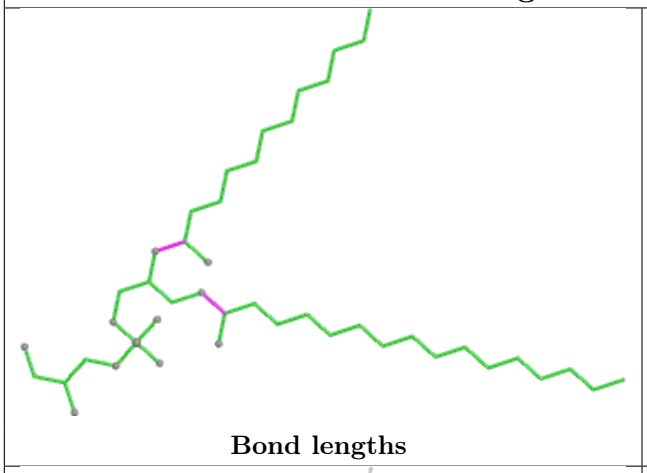


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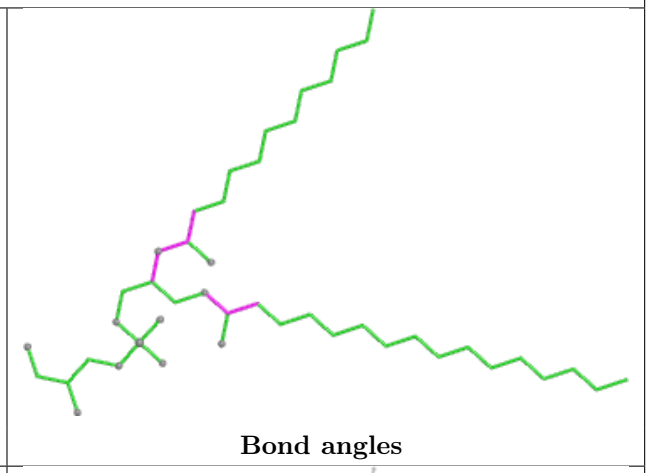


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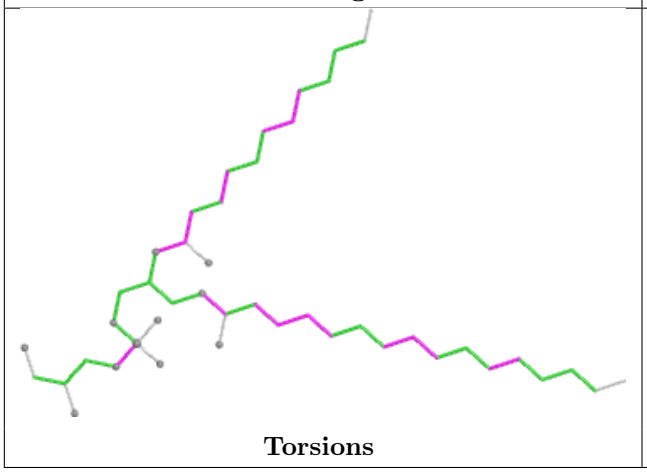
Ligand LHG S 2630



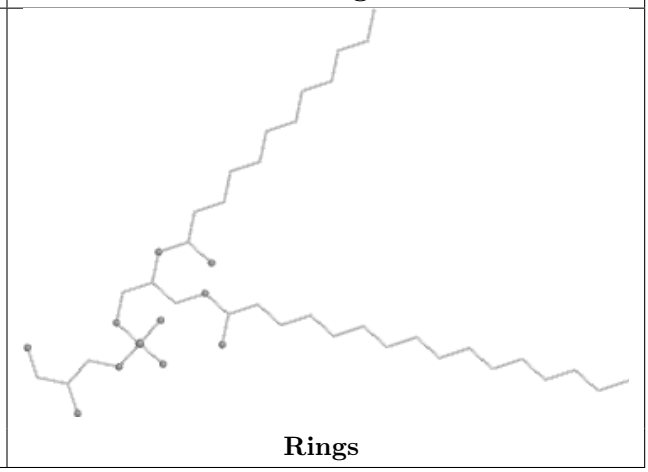
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Bond angles

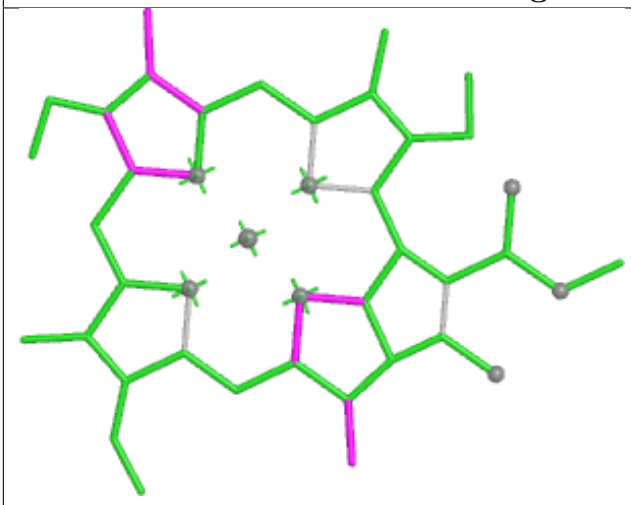


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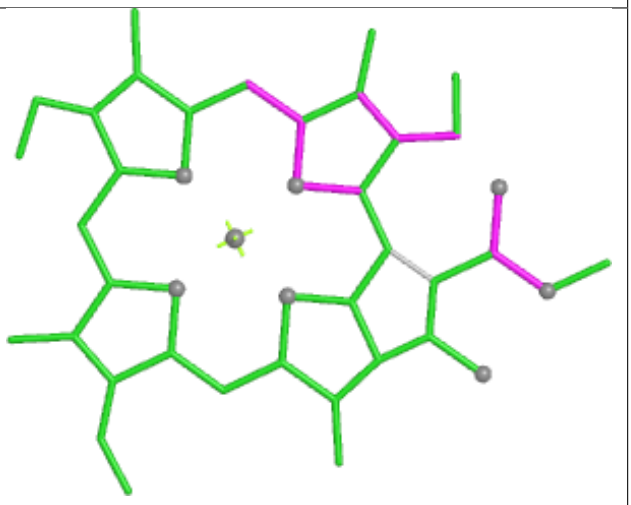


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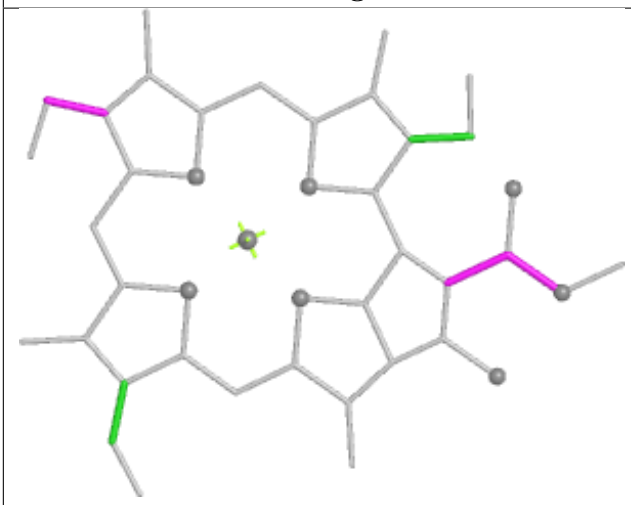
Ligand CLA s 603



Bond lengths



Bond angles

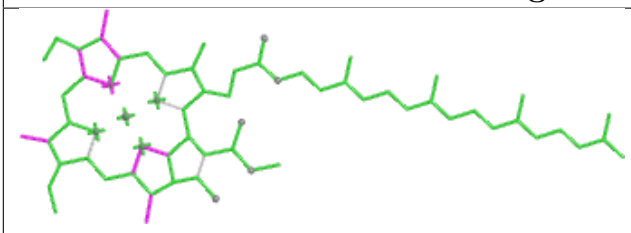


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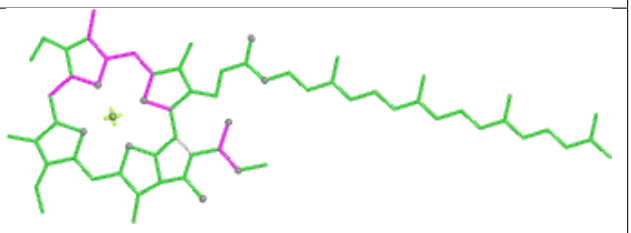


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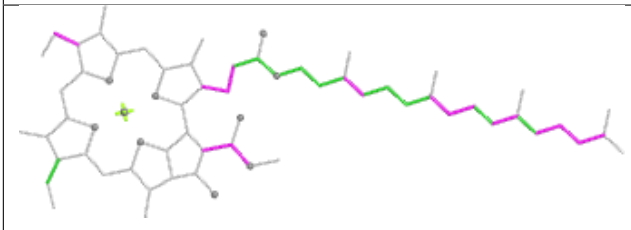
Ligand CLA 6 604



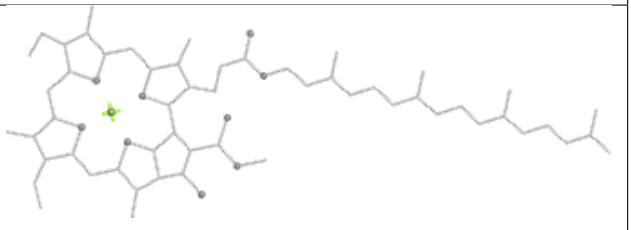
Bond lengths



Bond angles

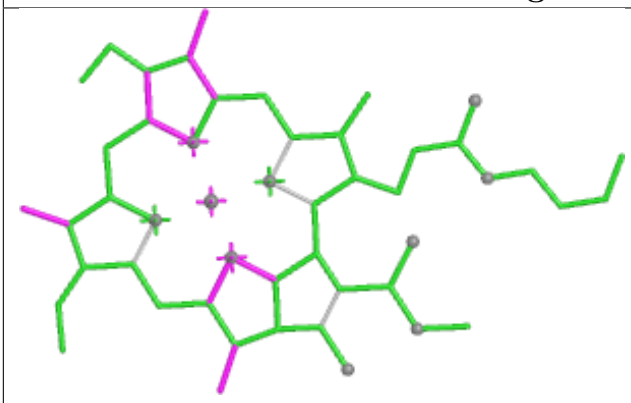


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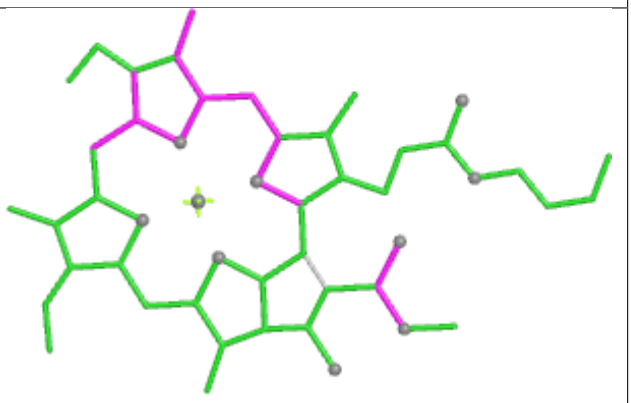


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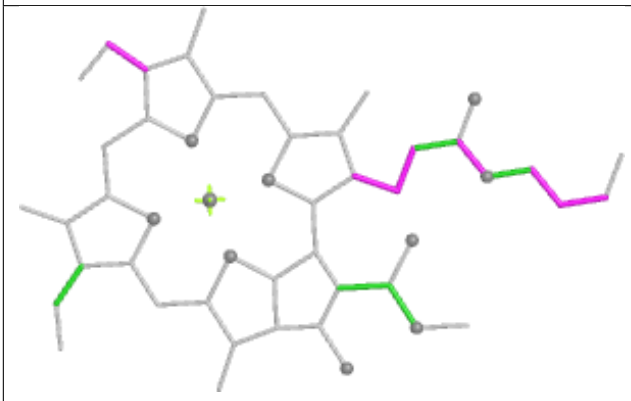
Ligand CLA S 611



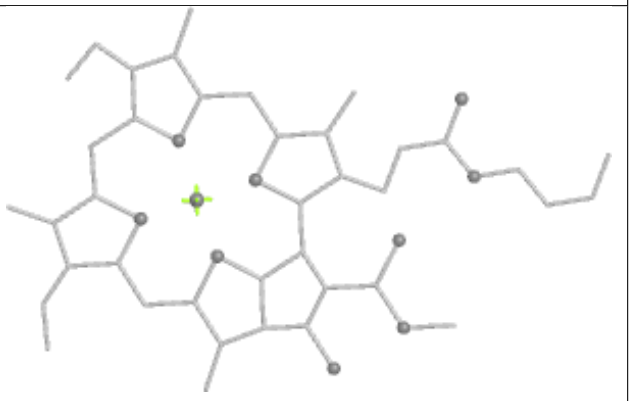
Bond lengths



Bond angles



Torsions

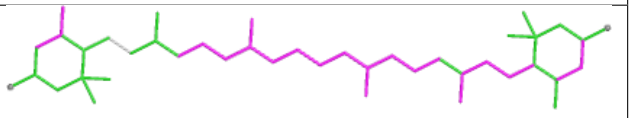


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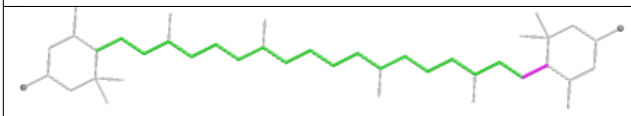
Ligand LUT s 1620



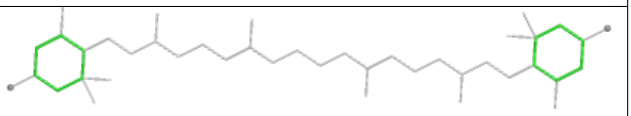
Bond lengths



Bond angles

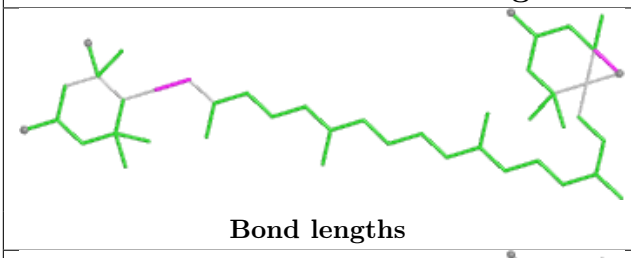


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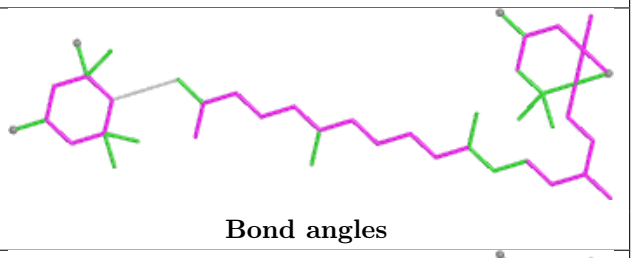


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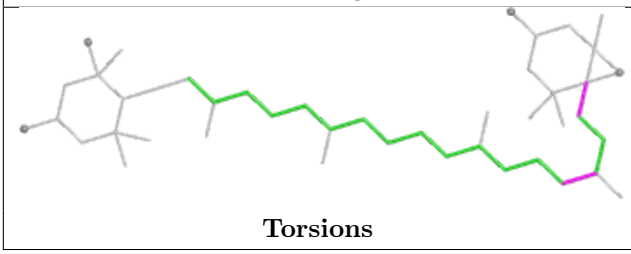
Ligand NEX G 1623



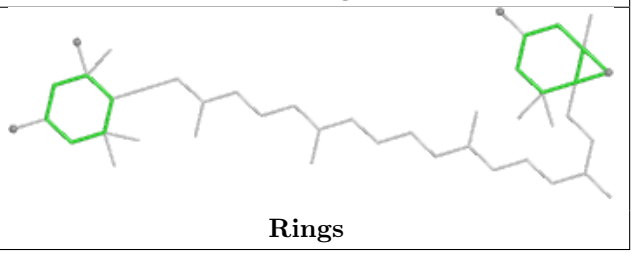
Bond lengths



Bond angles

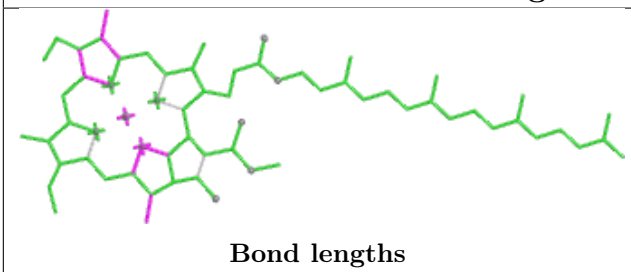


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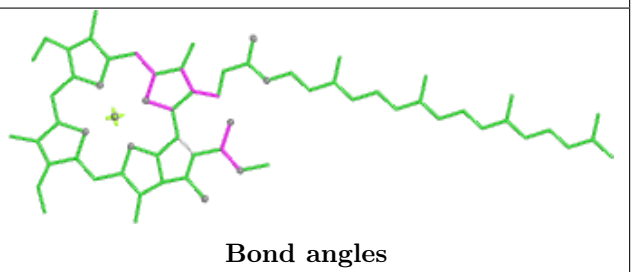


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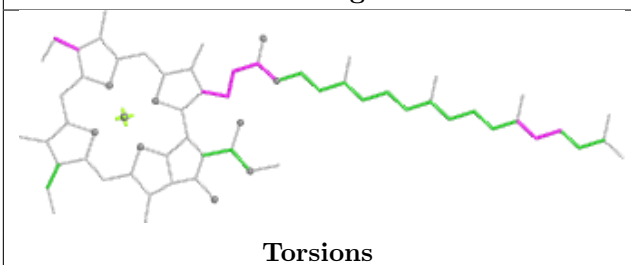
Ligand CLA 6 603



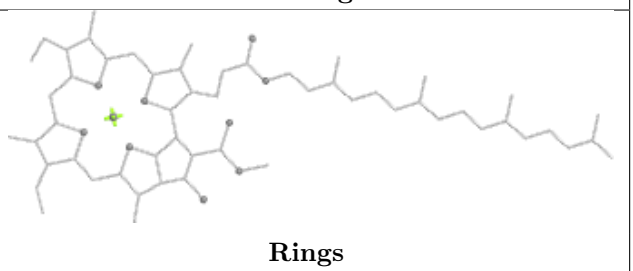
Bond lengths



Bond angles

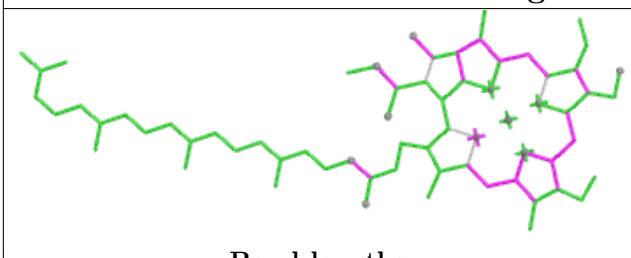


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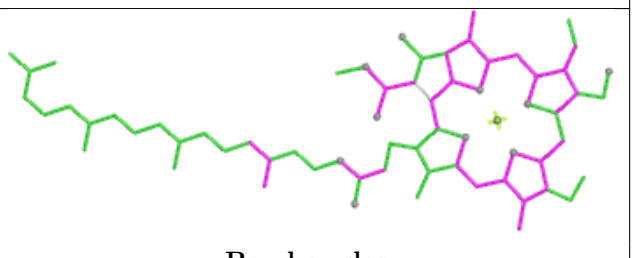


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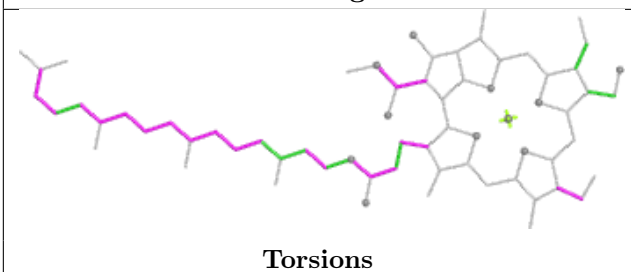
Ligand CHL 8 601



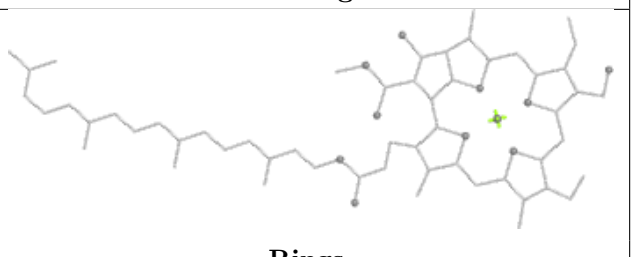
Bond lengths



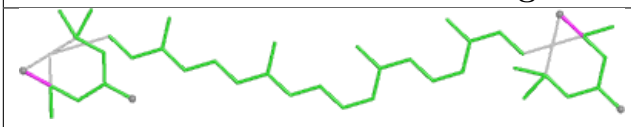
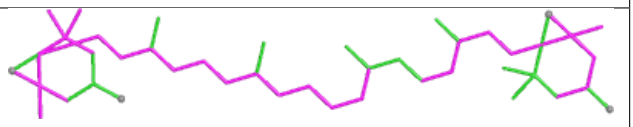
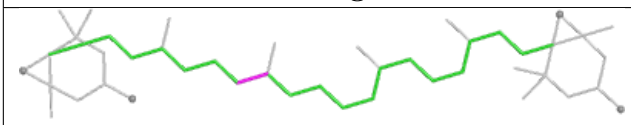
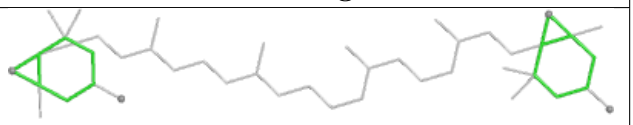
Bond angles

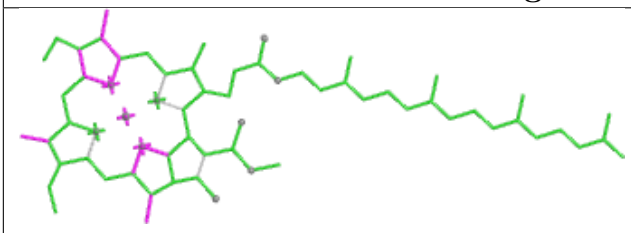
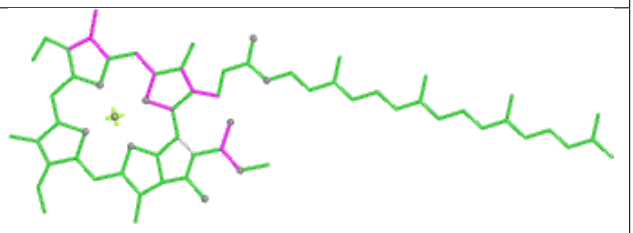
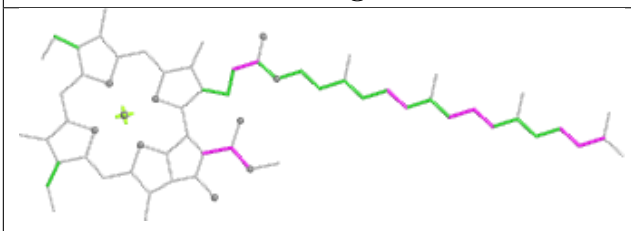
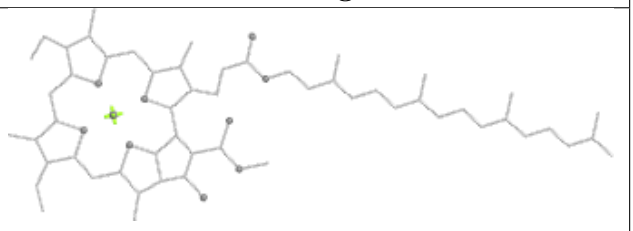


Torsions

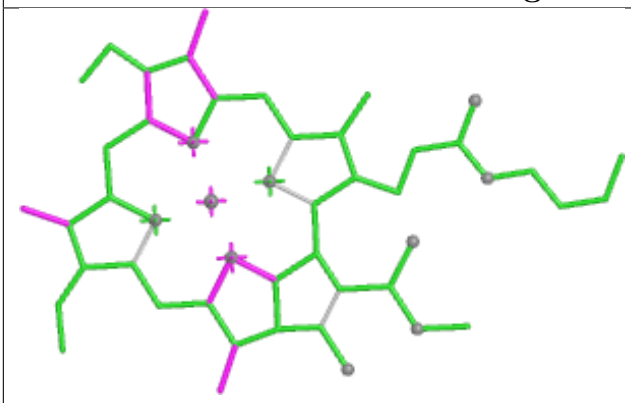


Rings

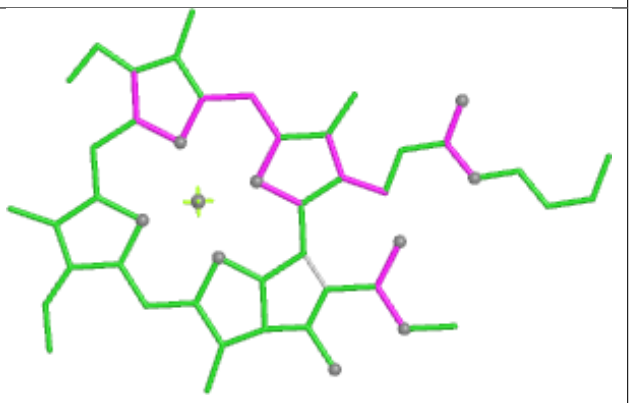
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

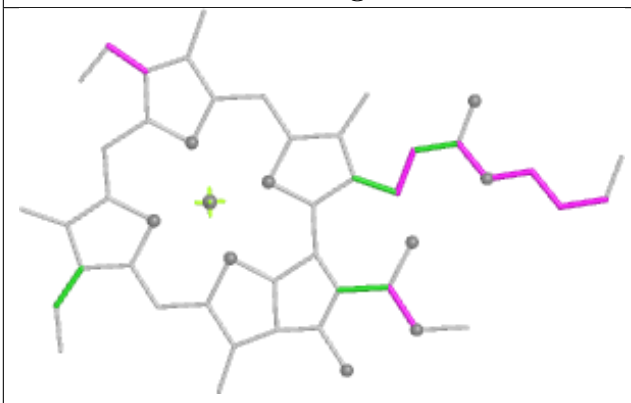
Ligand CLA R 612



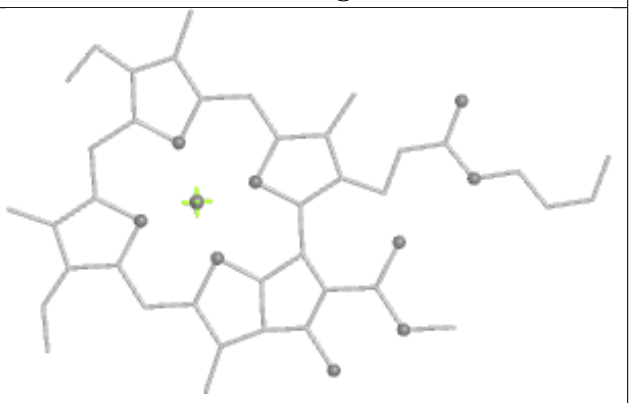
Bond lengths



Bond angles

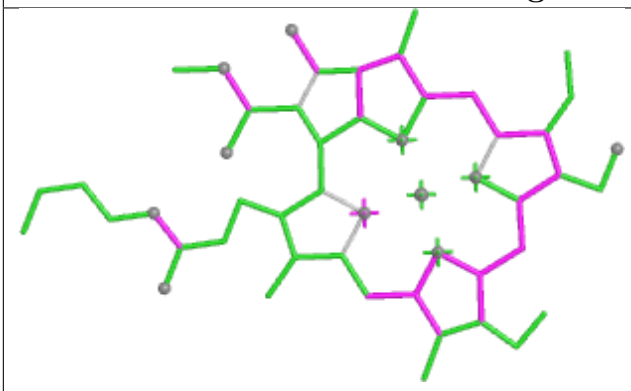


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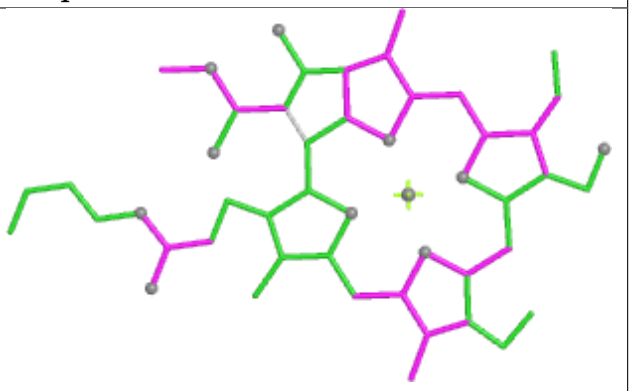


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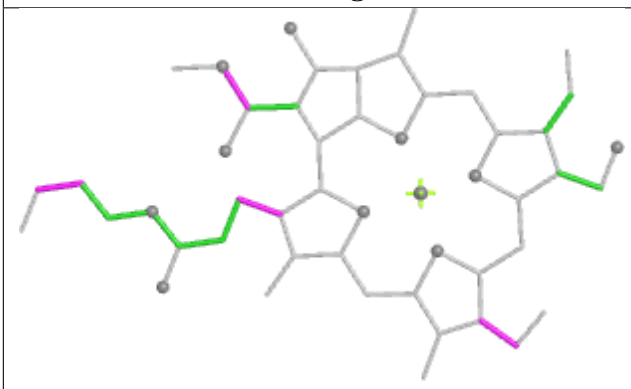
Ligand CHL q 606



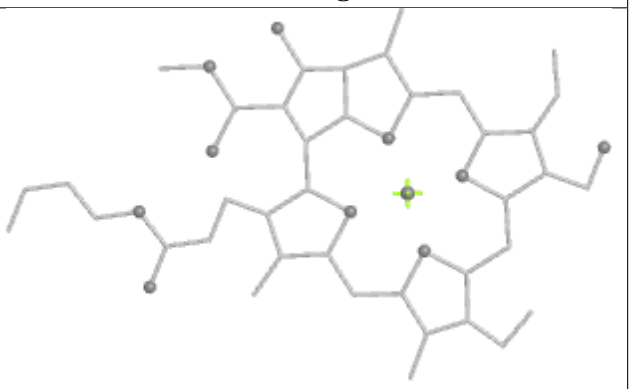
Bond lengths



Bond angles

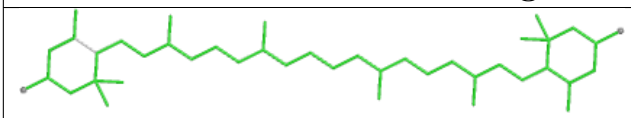


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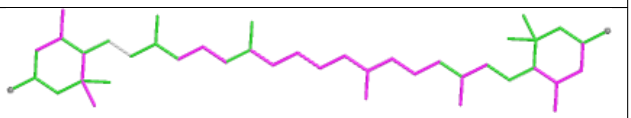


Rings

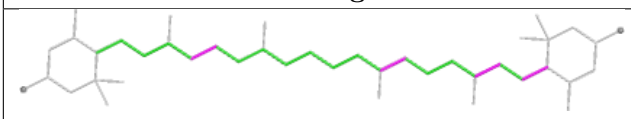
Ligand LUT 4 1621



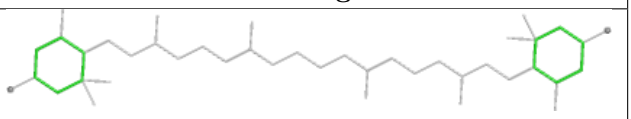
Bond lengths



Bond angles

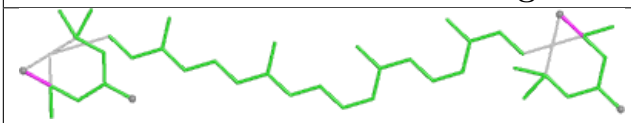


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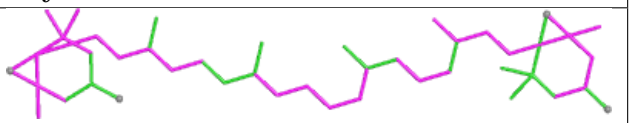


Rings

Ligand XAT y 1622



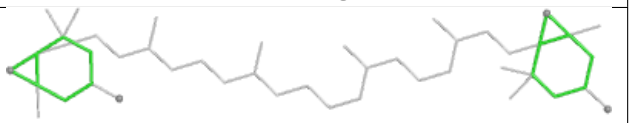
Bond lengths



Bond angles

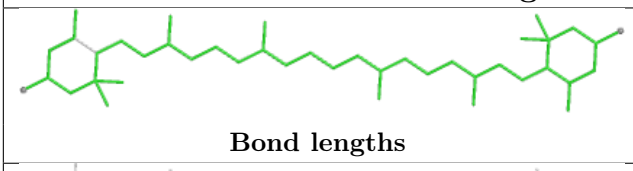


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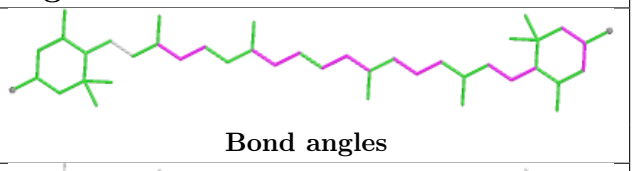


Rings

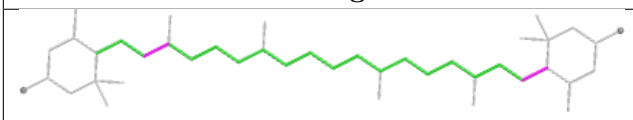
Ligand LUT g 1620



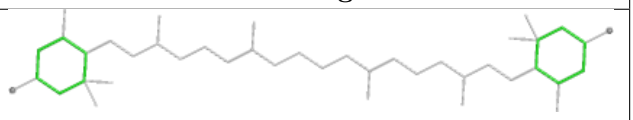
Bond lengths



Bond angles

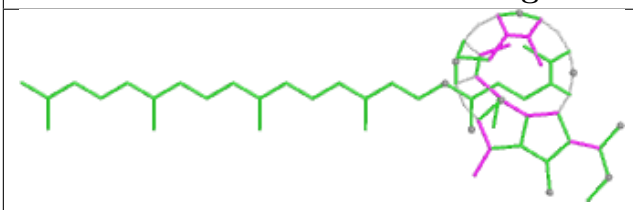


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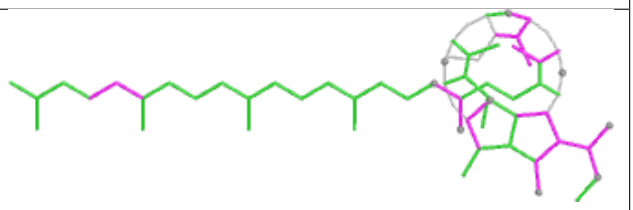


Rings

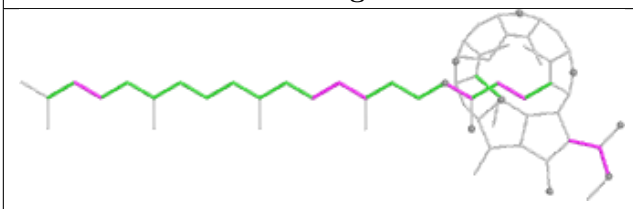
Ligand PHO A 408



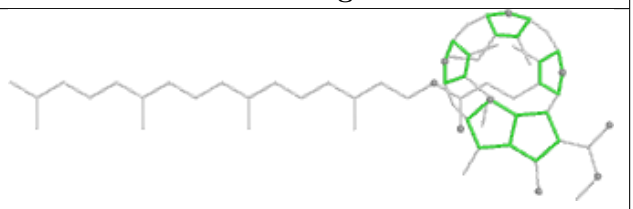
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Bond angles

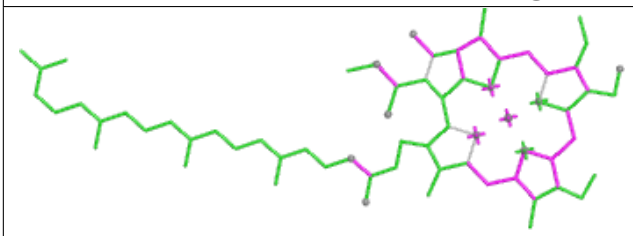


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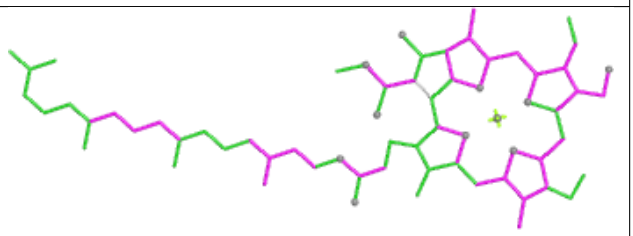


Rings

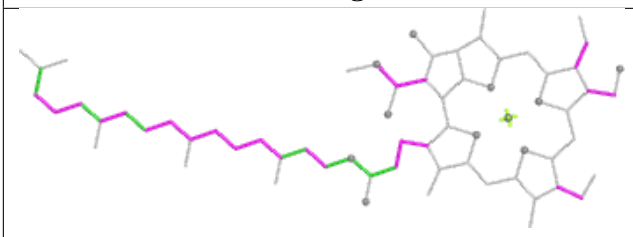
Ligand CHL 2 601



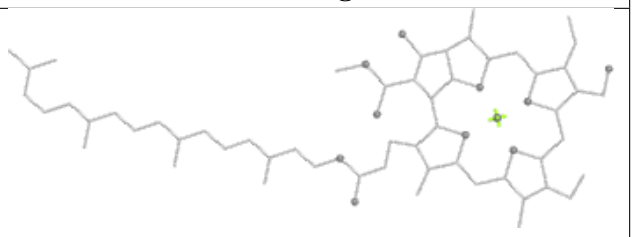
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Bond angles

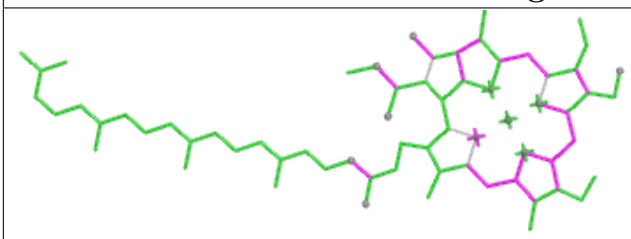


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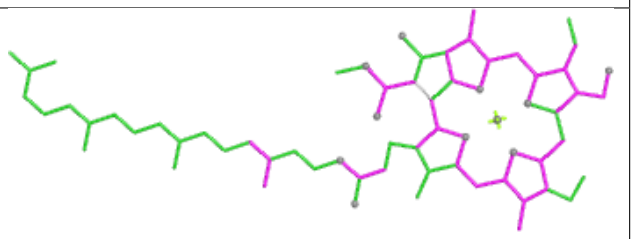


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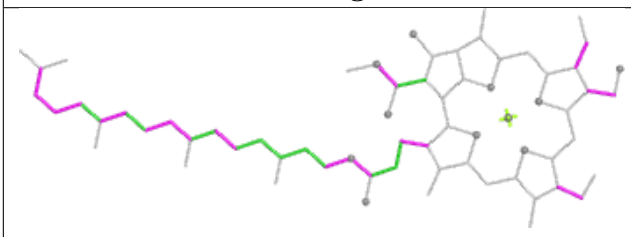
Ligand CHL 8 609



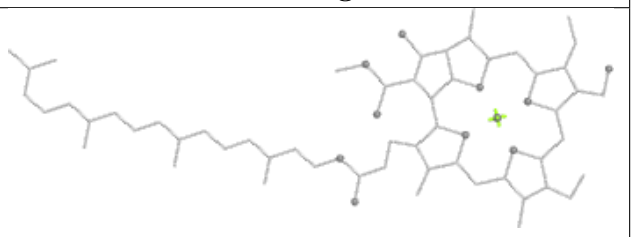
Bond lengths



Bond angles

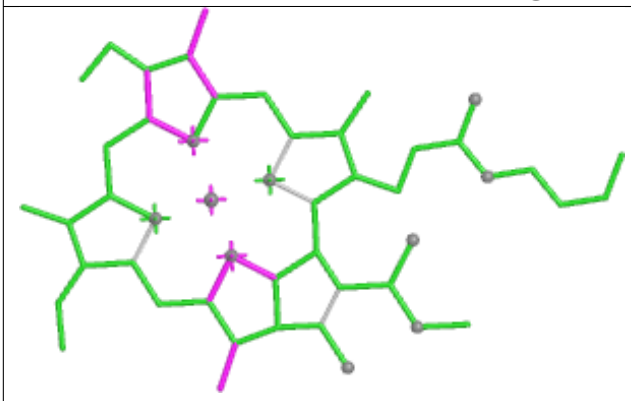


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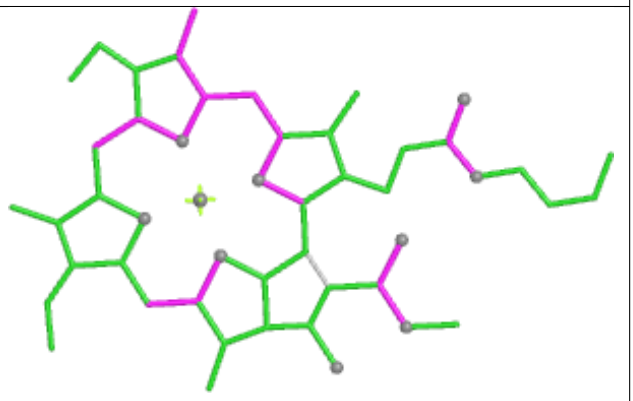


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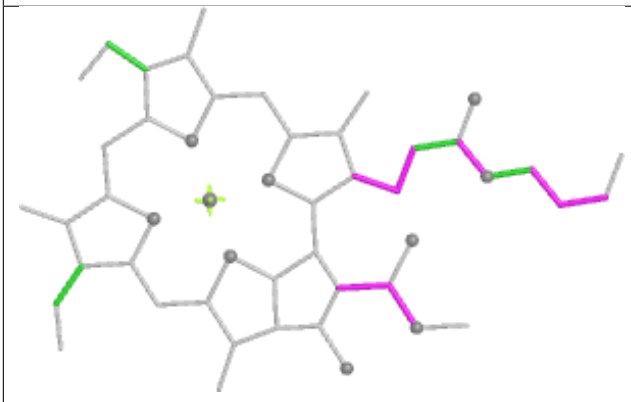
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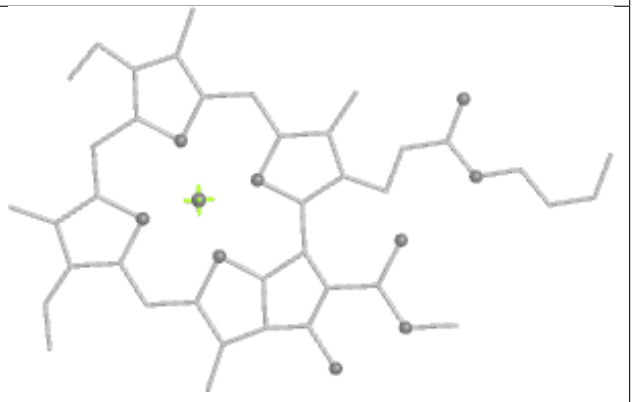
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Bond angles

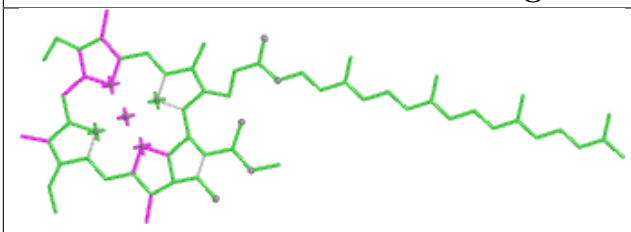


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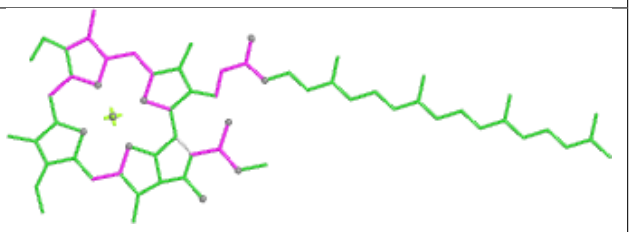


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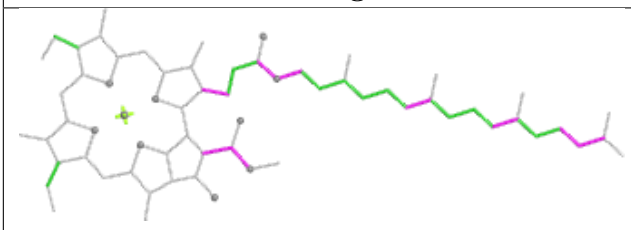
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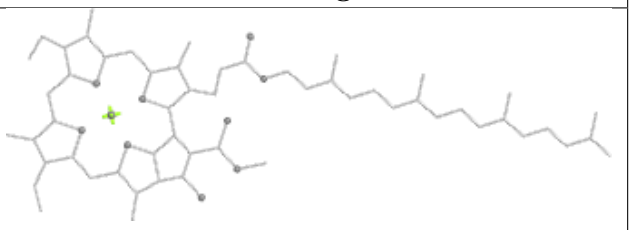
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Bond angles

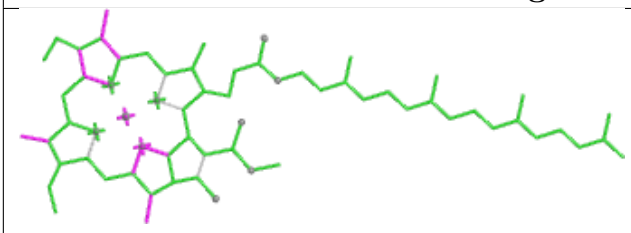


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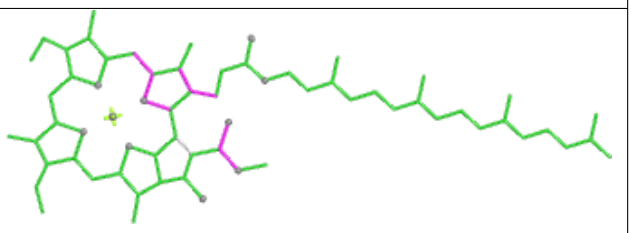


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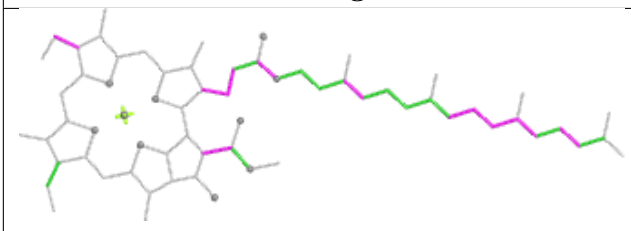
Ligand CLA 7 603



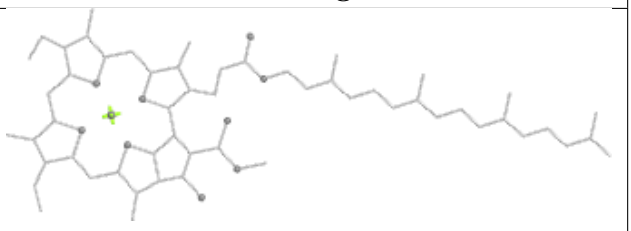
Bond lengths



Bond angles

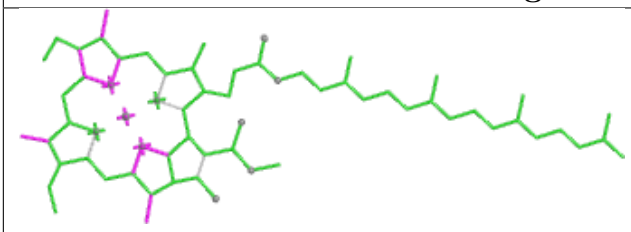


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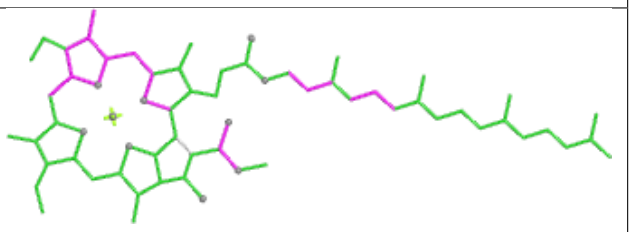


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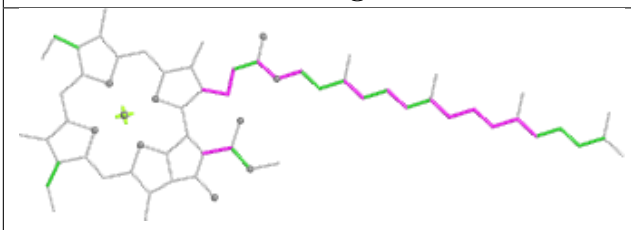
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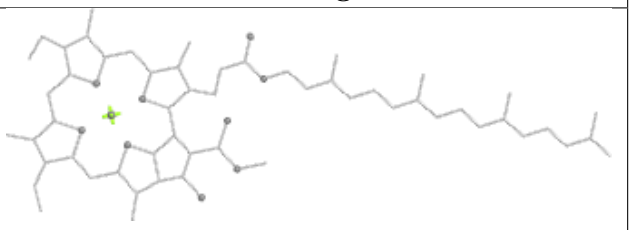
Bond lengths



Bond angles

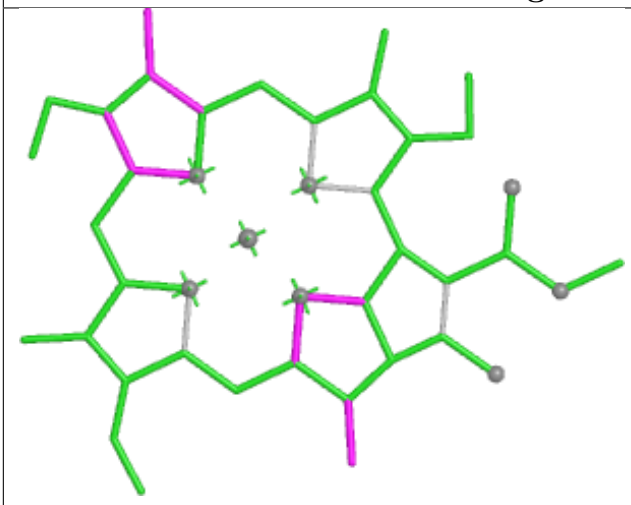


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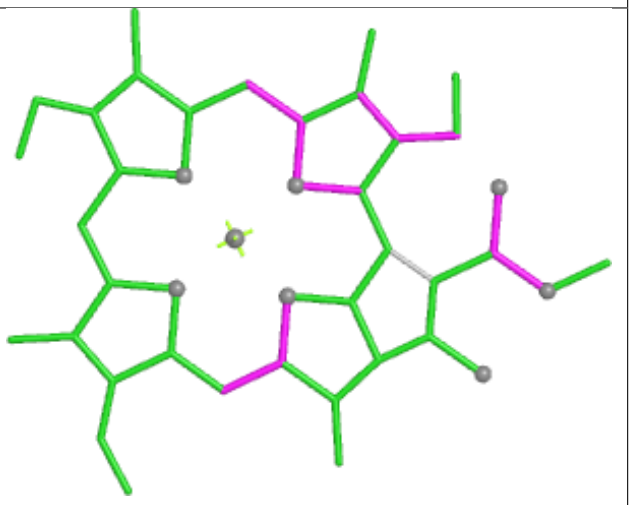


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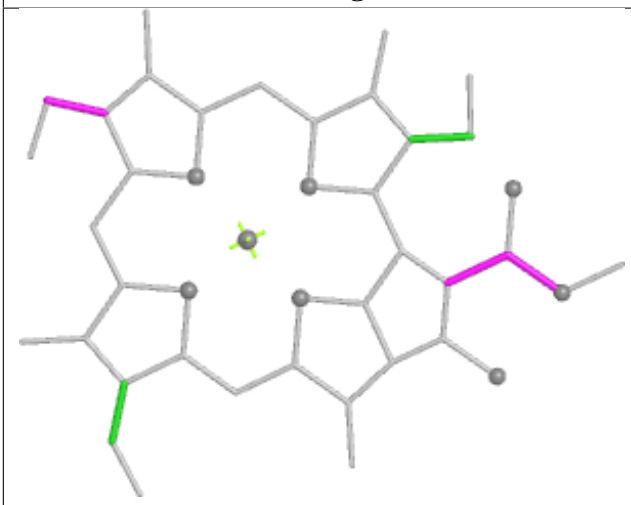
Ligand CLA S 603



Bond lengths



Bond angles

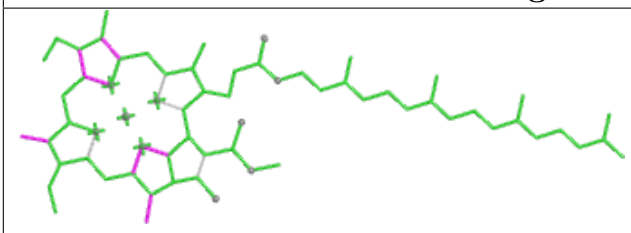


Torsions

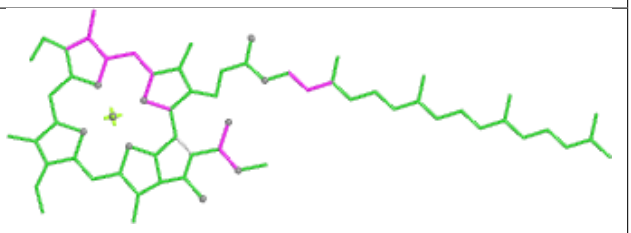


Rings

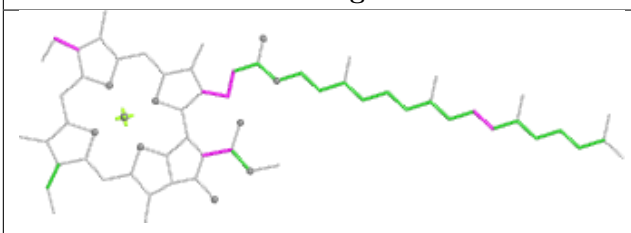
Ligand CLA 2 610



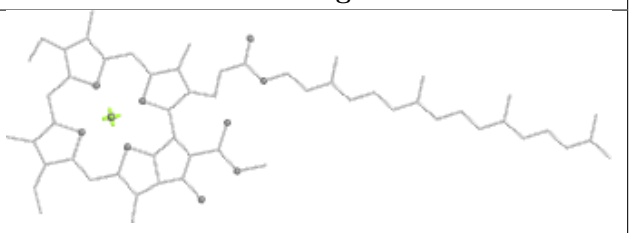
Bond lengths



Bond angles

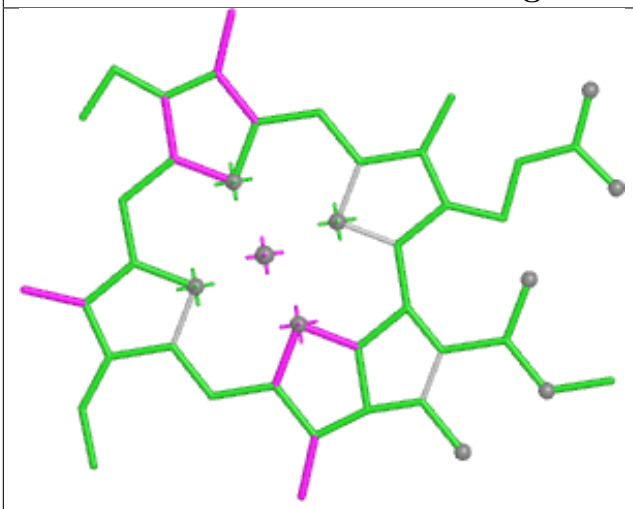


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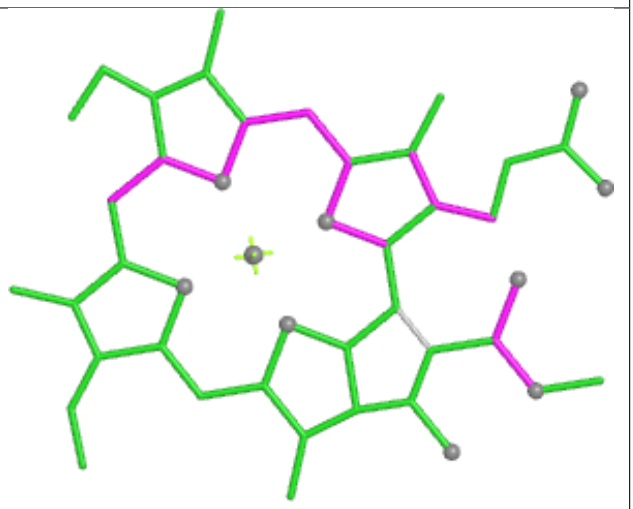


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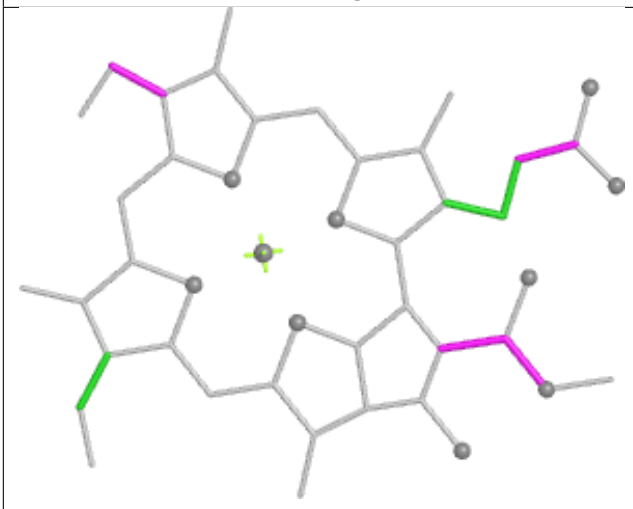
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Bond lengths



Bond angles

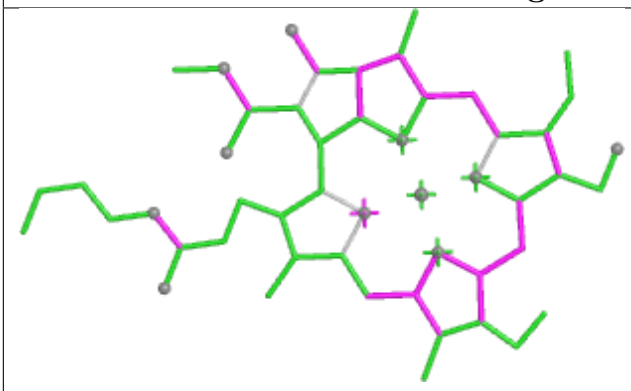


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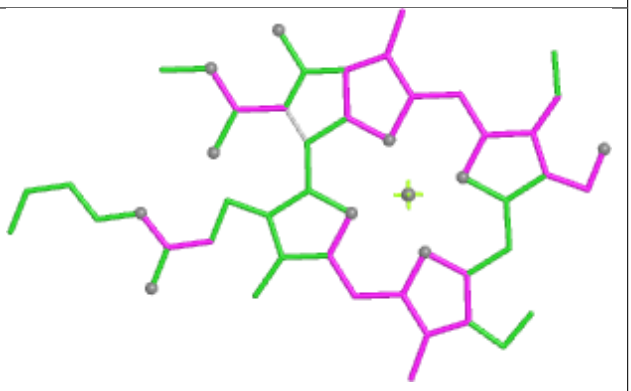


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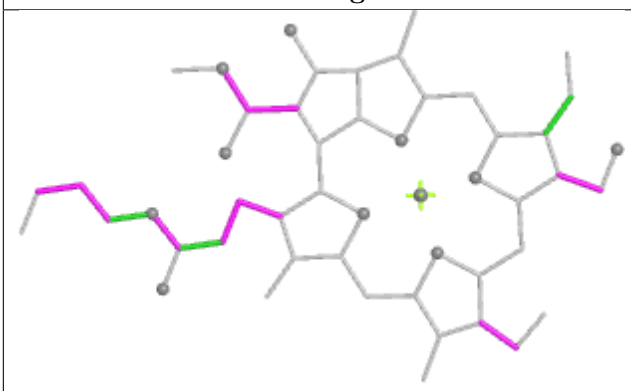
Ligand CHL 7 608



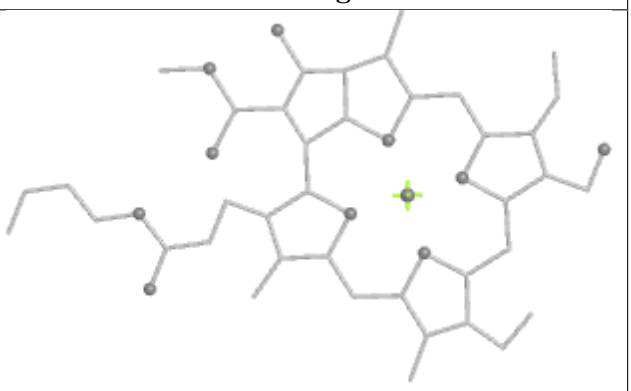
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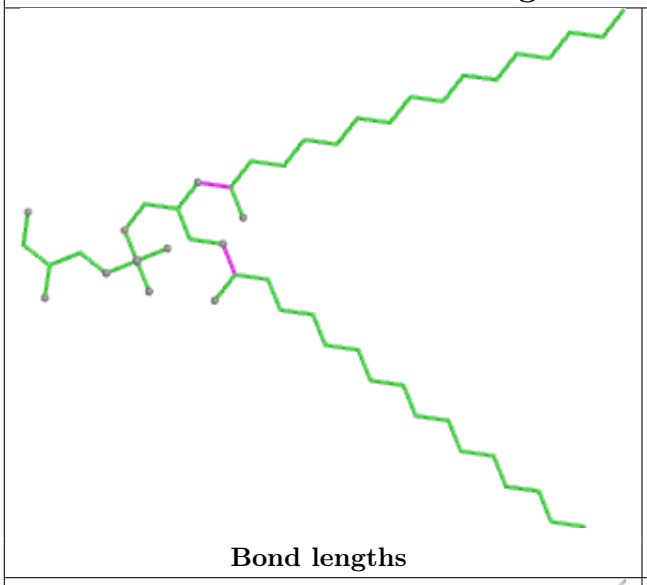


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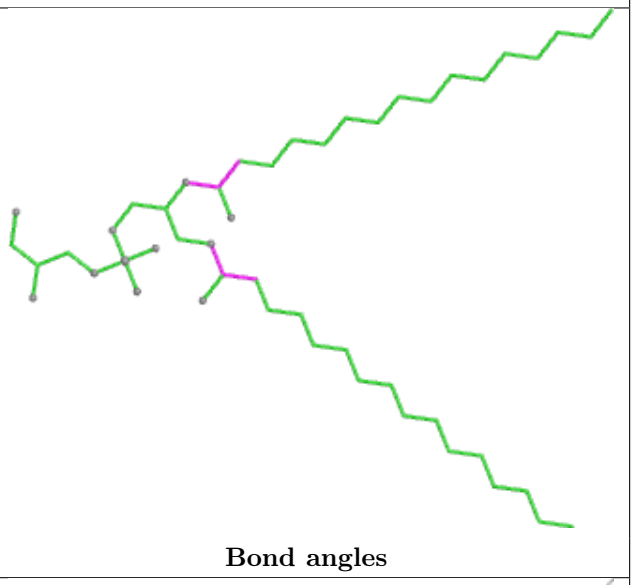


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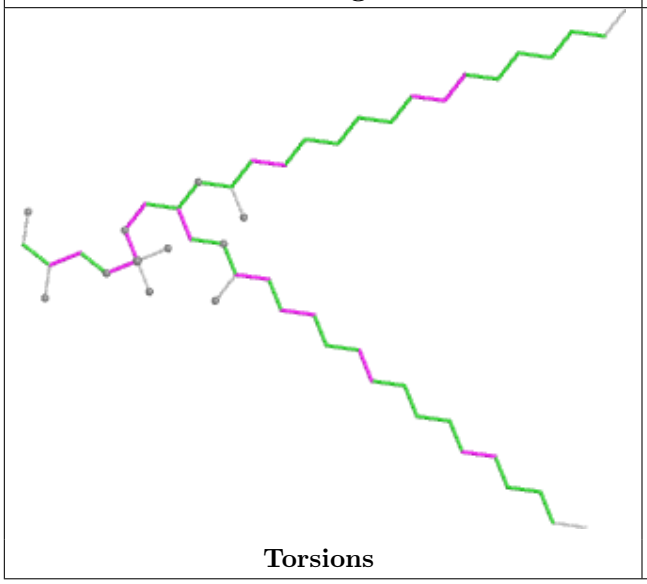
Ligand LHG 0 2630



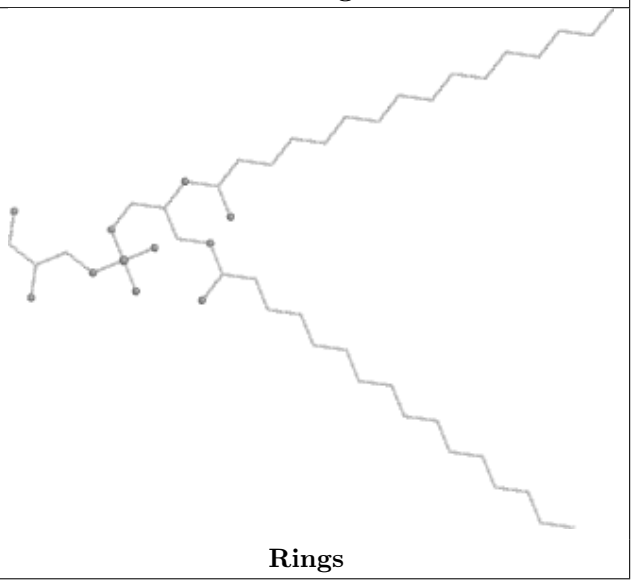
Bond lengths



Bond angles

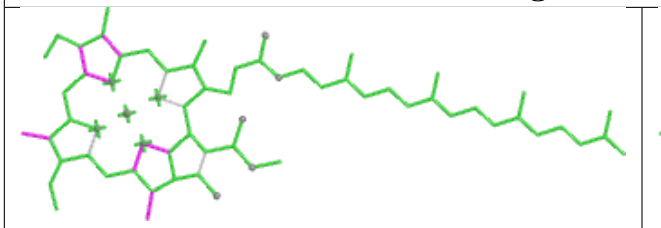


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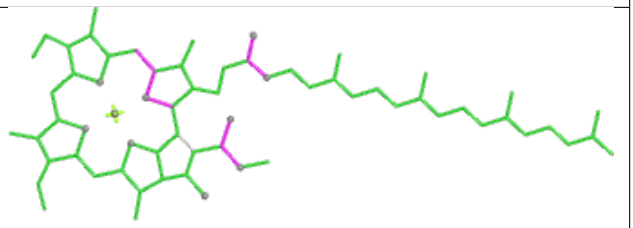


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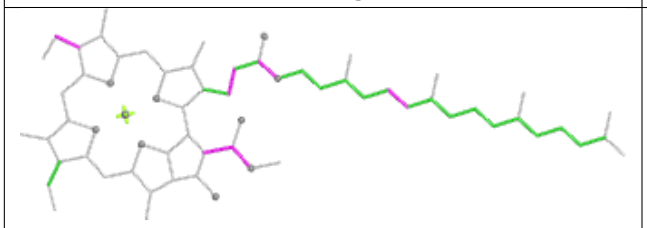
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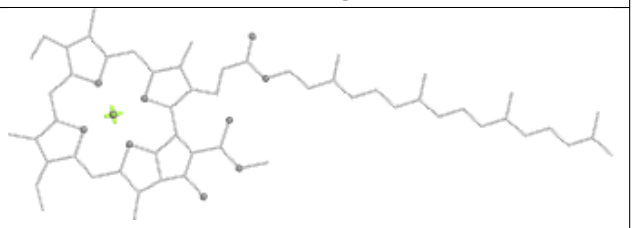
Bond lengths



Bond angles

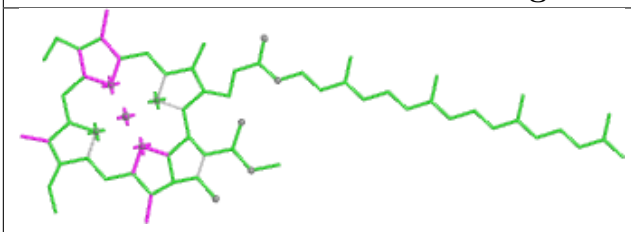


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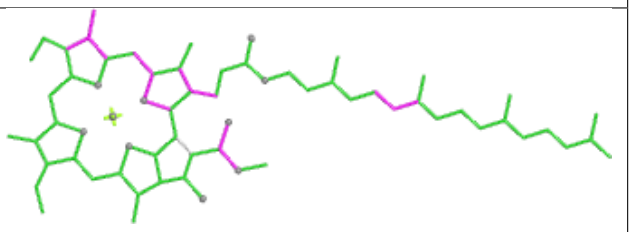


Rings

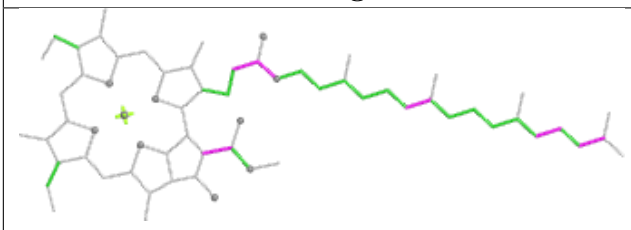
Ligand CLA c 510



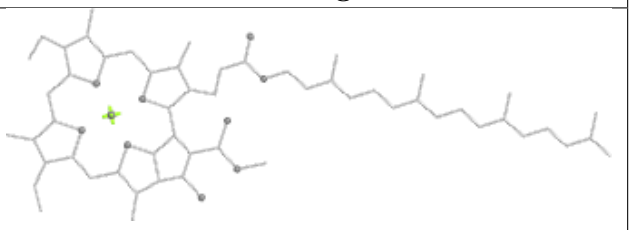
Bond lengths



Bond angles

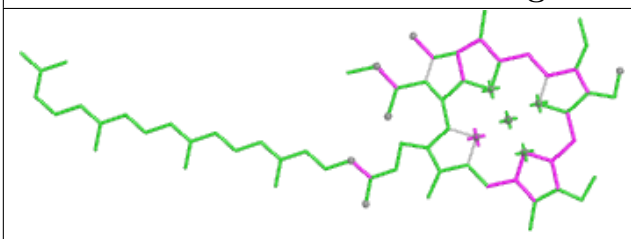


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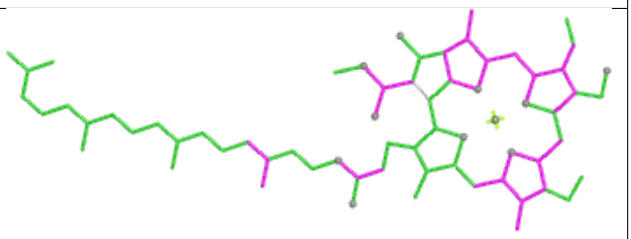


Rings

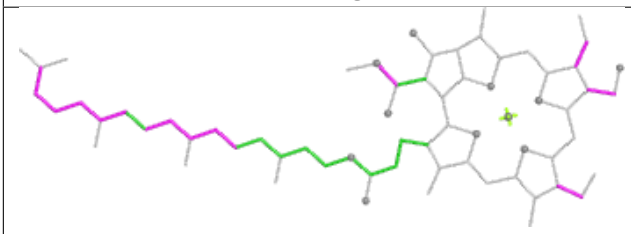
Ligand CHL 5 609



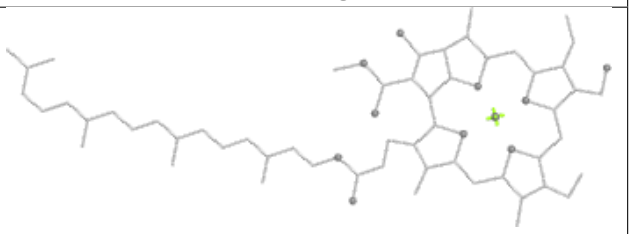
Bond lengths



Bond angles

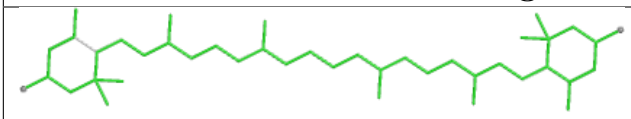


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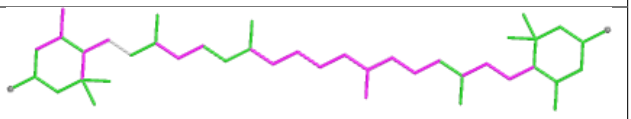


Rings

Ligand LUT n 1620



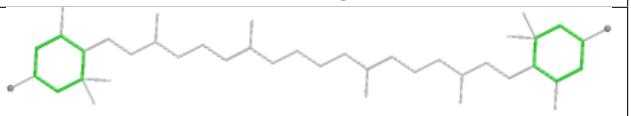
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Bond angles

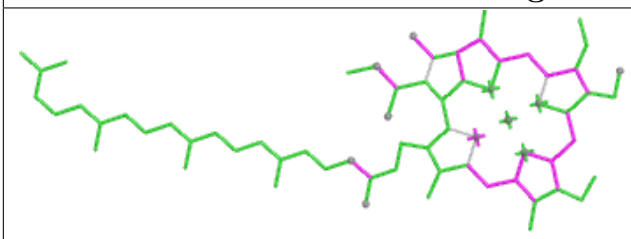


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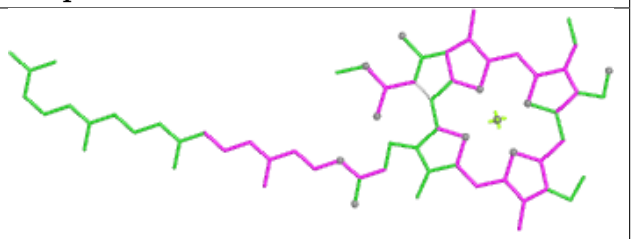


Rings

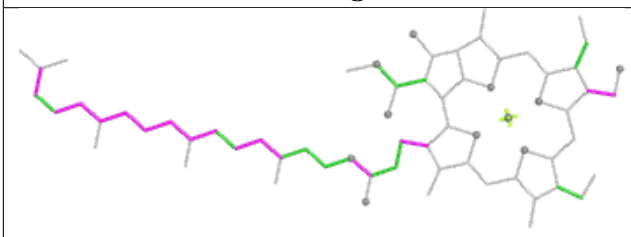
Ligand CHL q 601



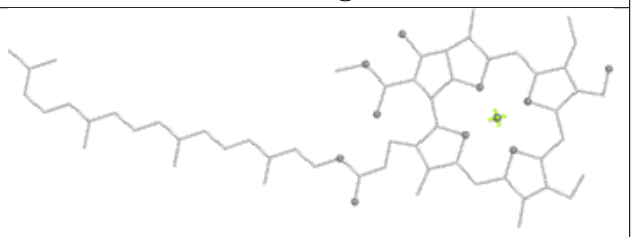
Bond lengths



Bond angles

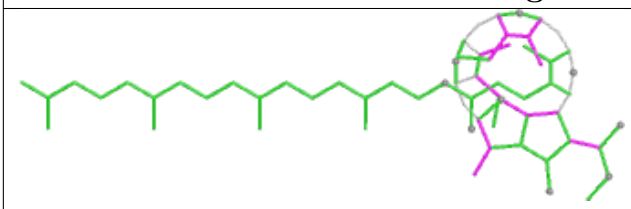


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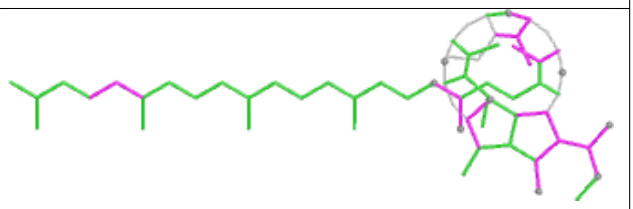


Rings

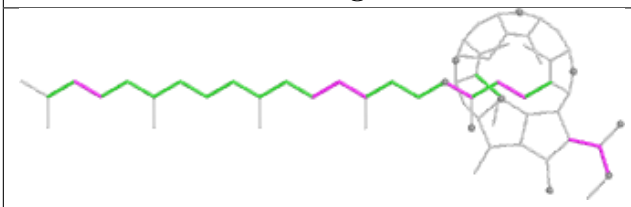
Ligand PHO a 408



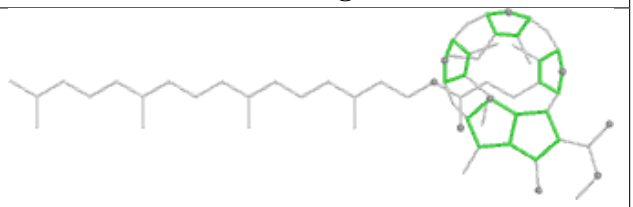
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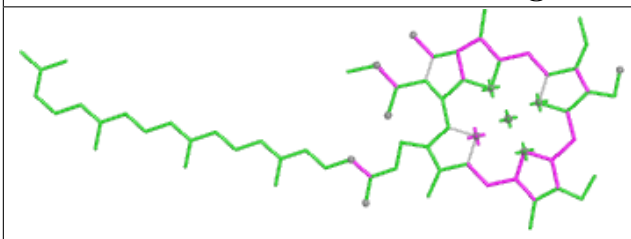


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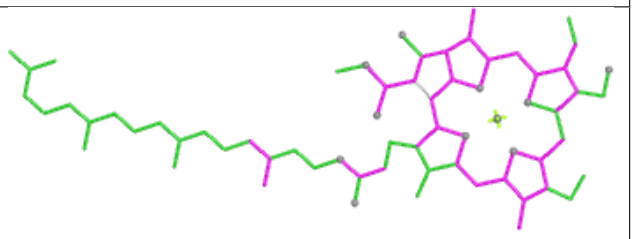


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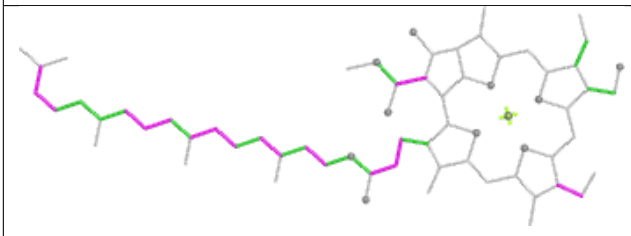
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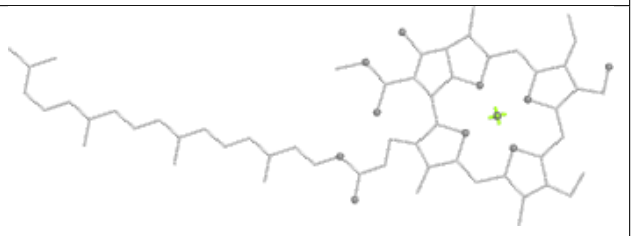
Bond lengths



Bond angles

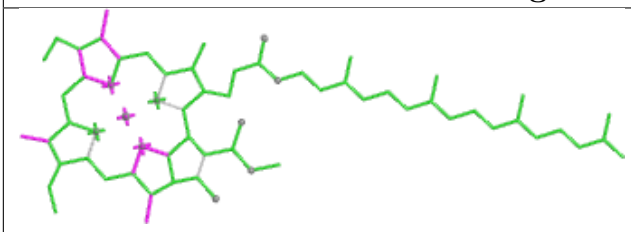


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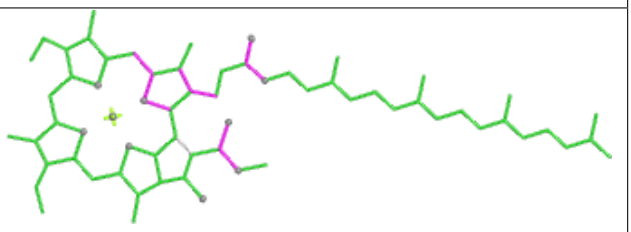


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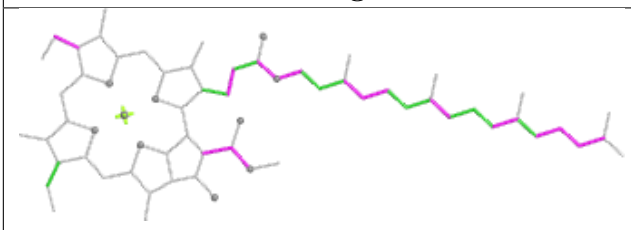
Ligand CLA c 513



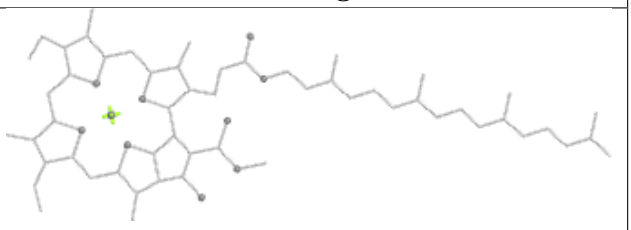
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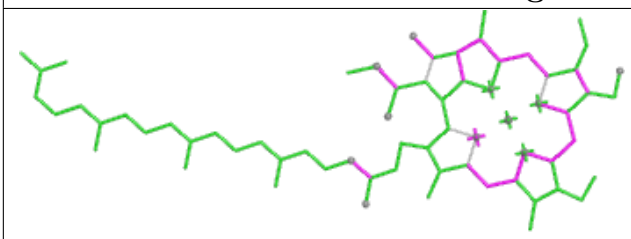


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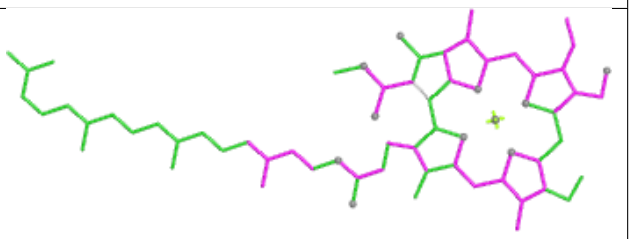


Rings

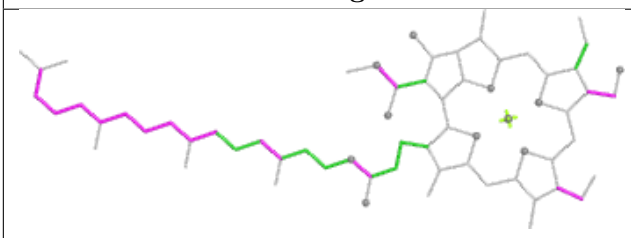
Ligand CHL n 609



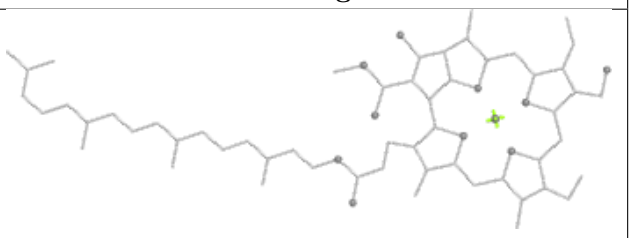
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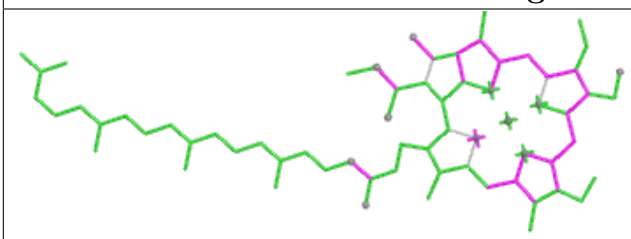


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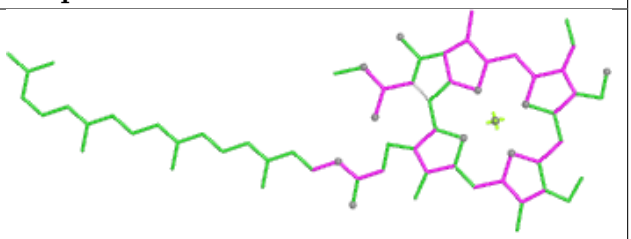


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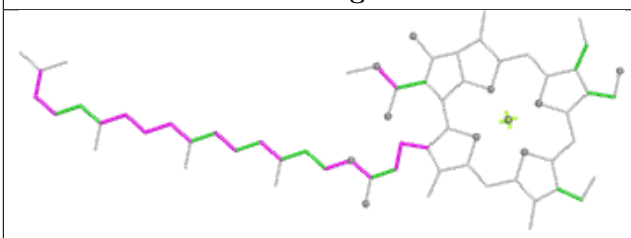
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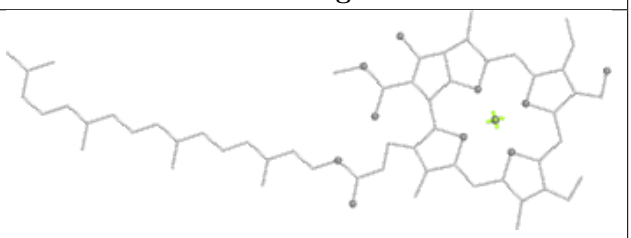
Bond lengths



Bond angles

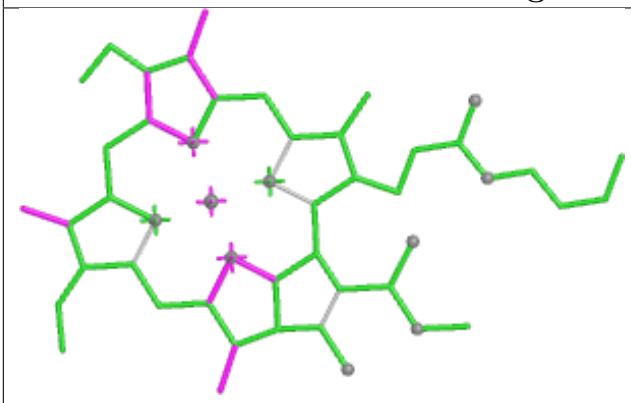


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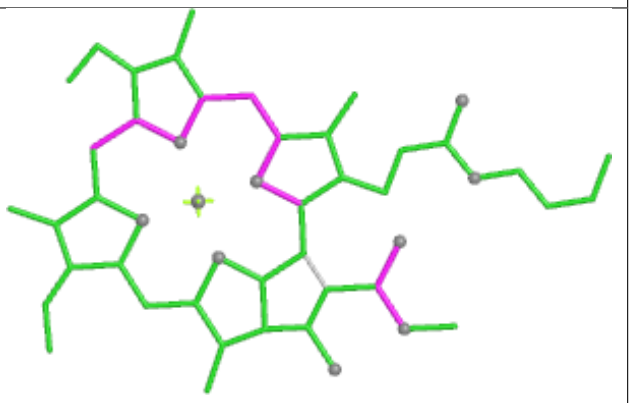


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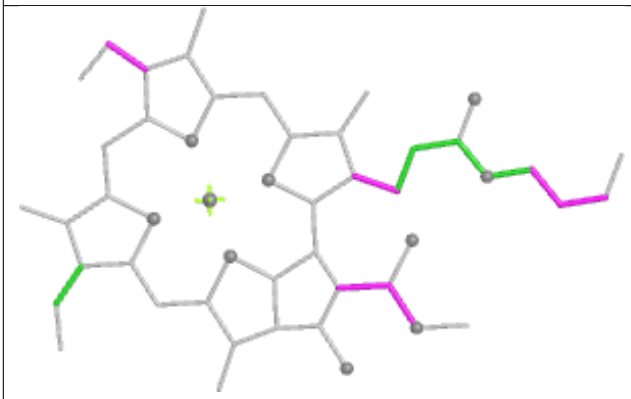
Ligand CLA n 611



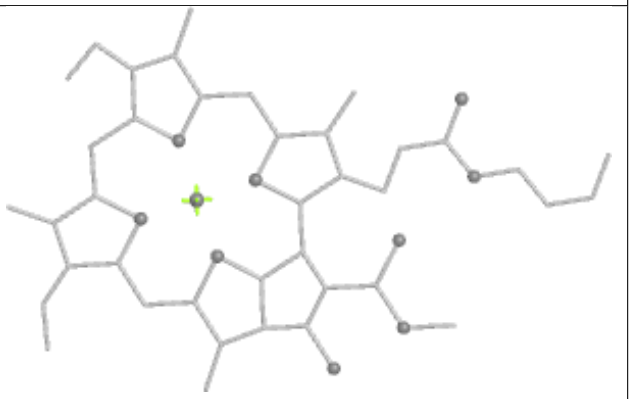
Bond lengths



Bond angles



Torsions

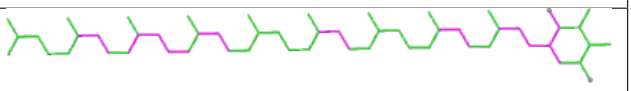


Rings

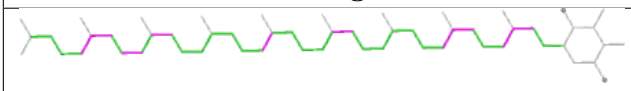
Ligand PL9 d 405



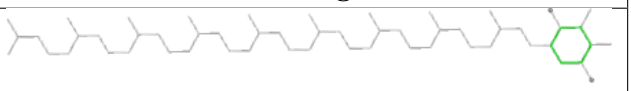
Bond lengths



Bond angles

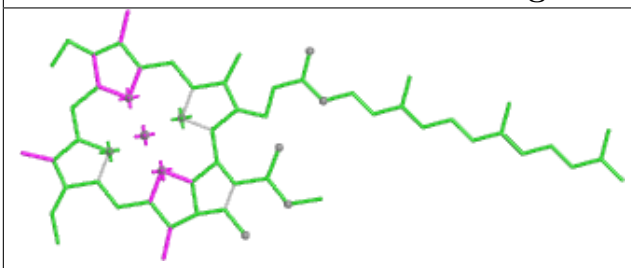


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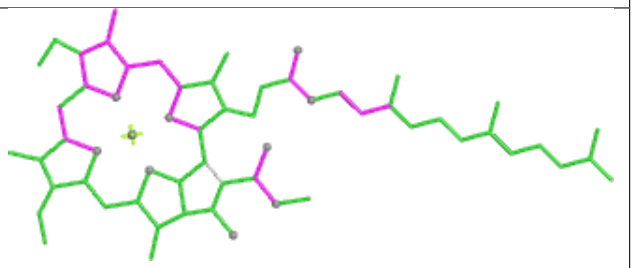


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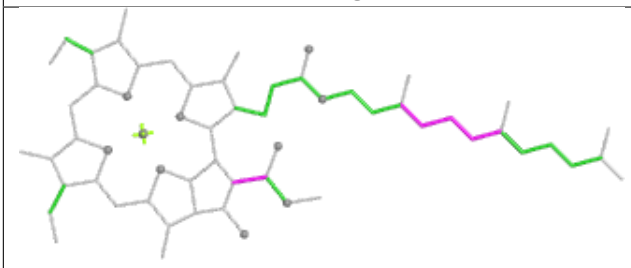
Ligand CLA a 410



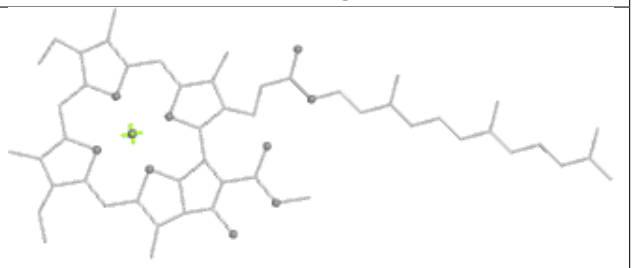
Bond lengths



Bond angles

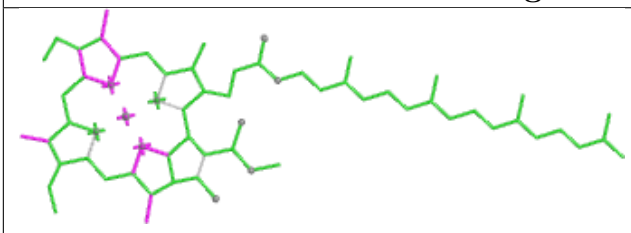


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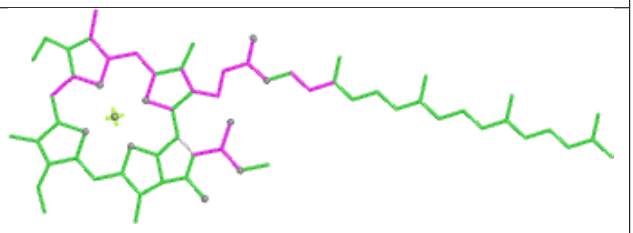


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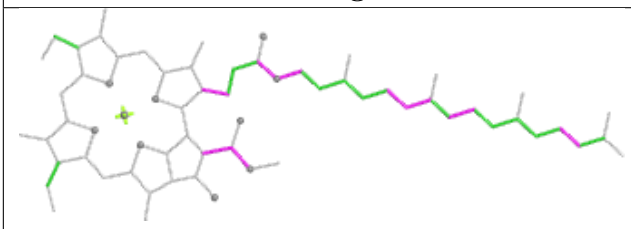
Ligand CLA B 605



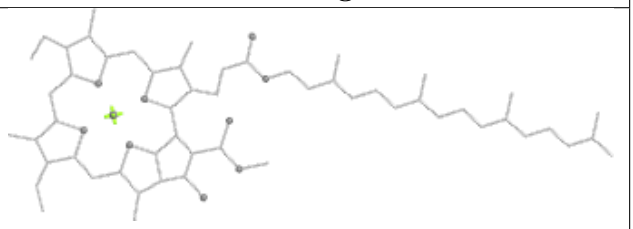
Bond lengths



Bond angles

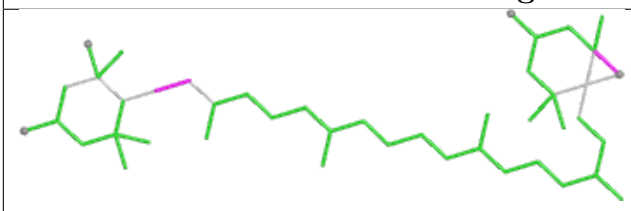


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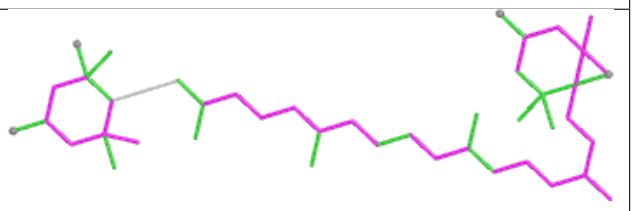


Rings

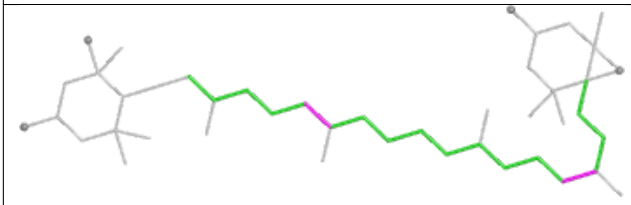
Ligand NEX 1 1623



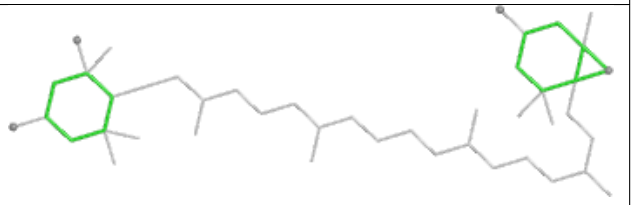
Bond lengths



Bond angles

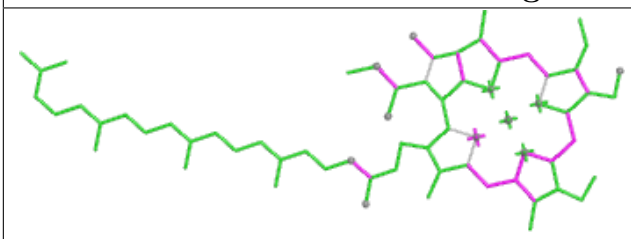


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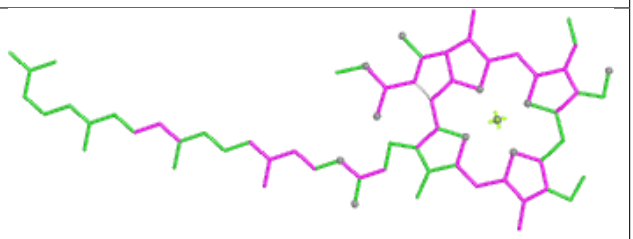


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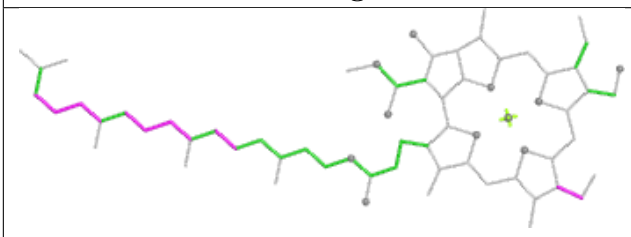
Ligand CHL N 601



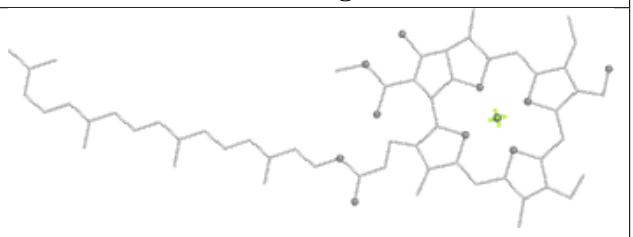
Bond lengths



Bond angles

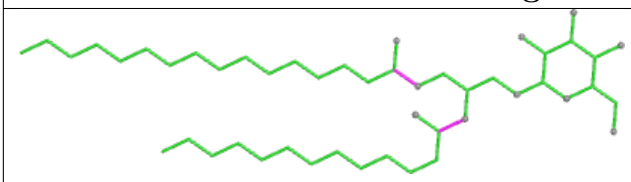


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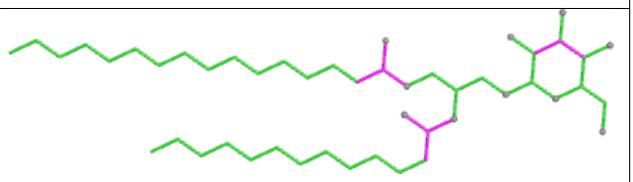


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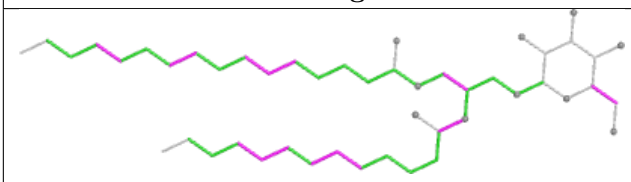
Ligand LMG h 102



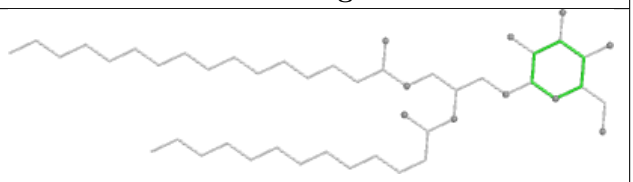
Bond lengths



Bond angles

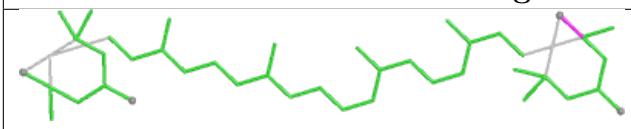


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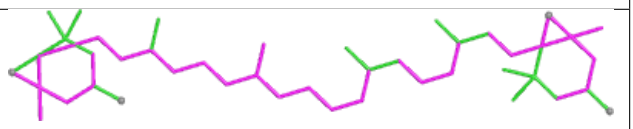


Rings

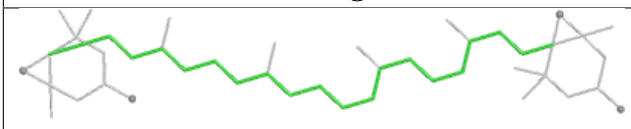
Ligand XAT G 1622



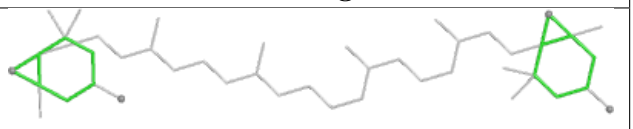
Bond lengths



Bond angles

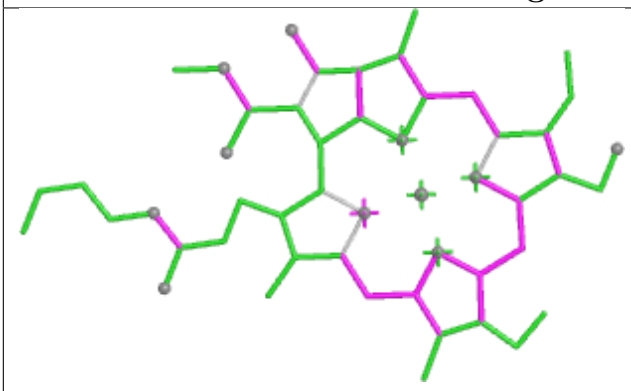


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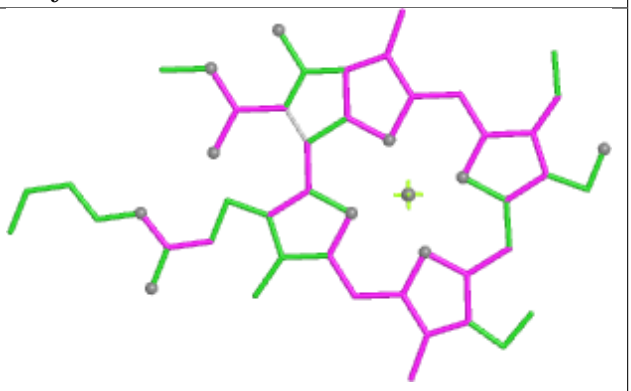


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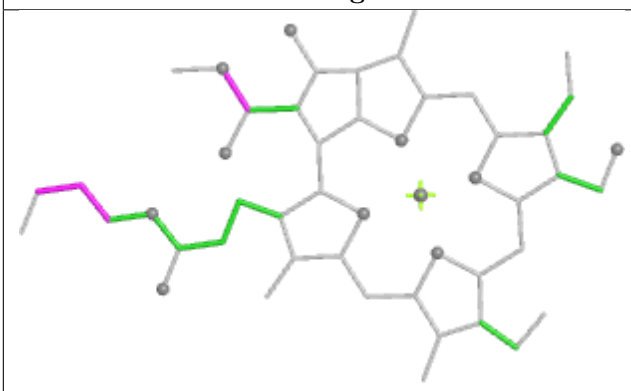
Ligand CHL y 608



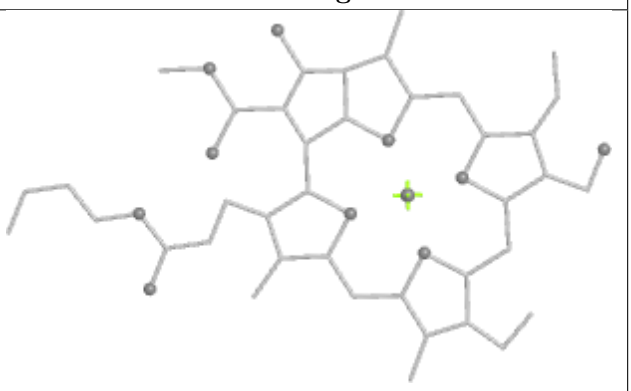
Bond lengths



Bond angles

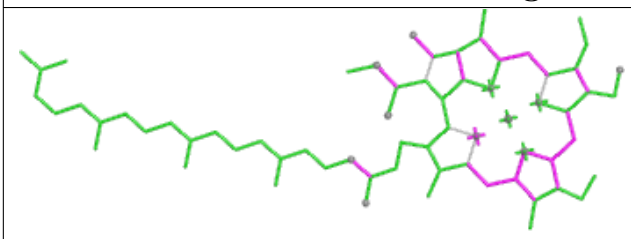


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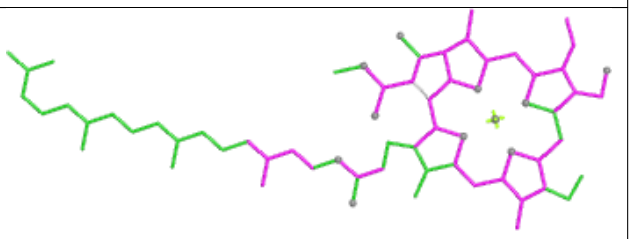


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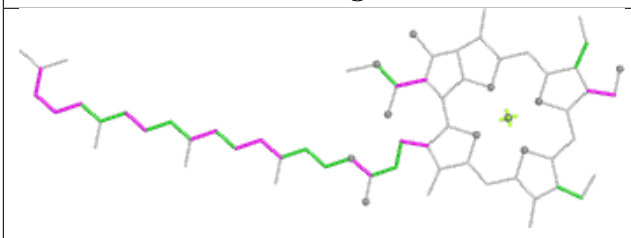
Ligand CHL G 601



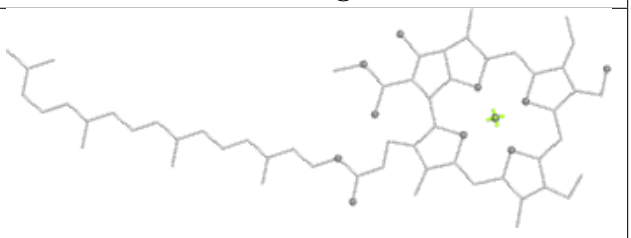
Bond lengths



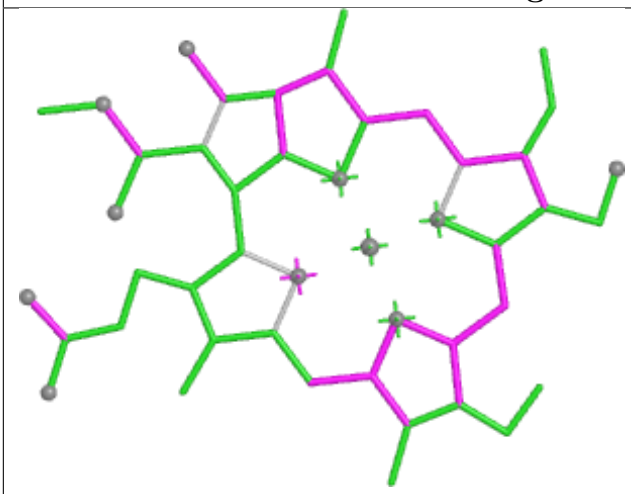
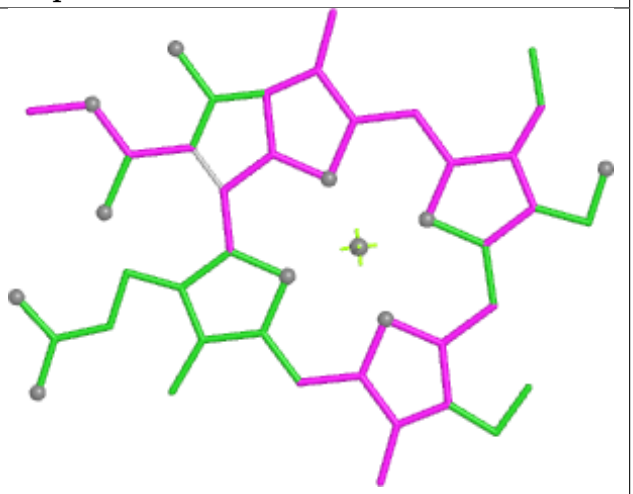
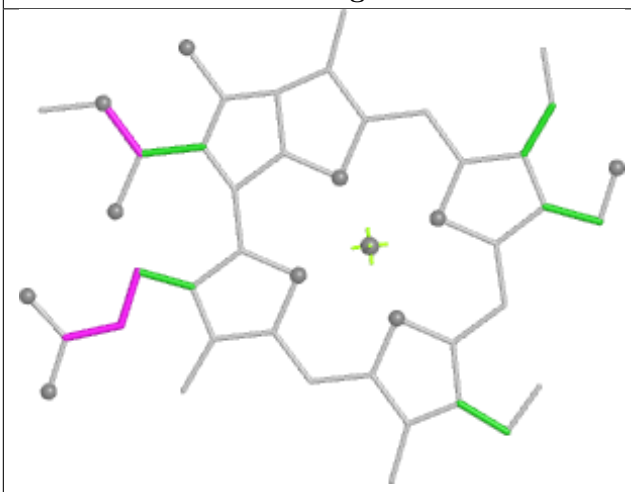
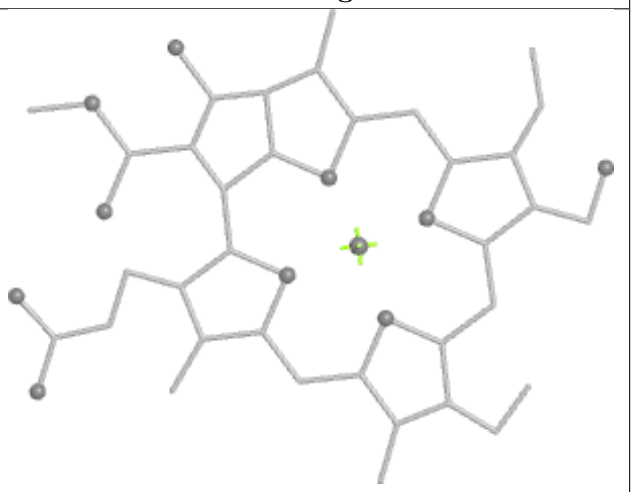
Bond angles

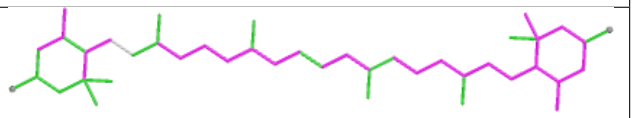
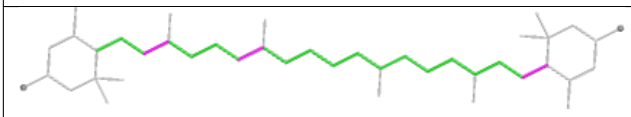
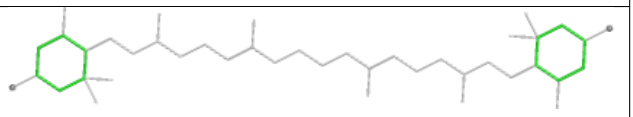


Torsions

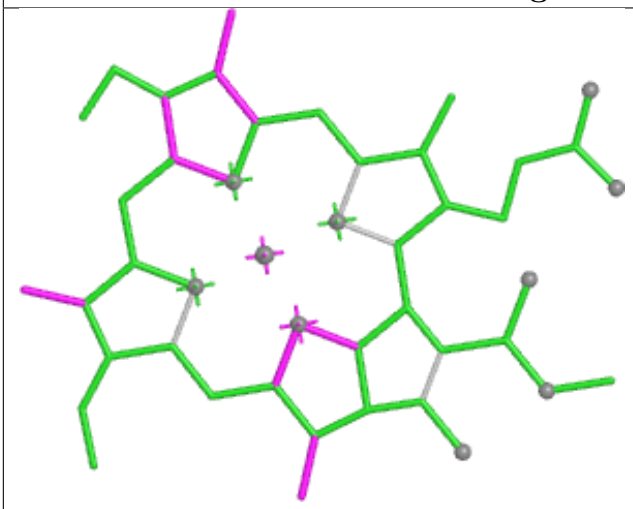


Rings

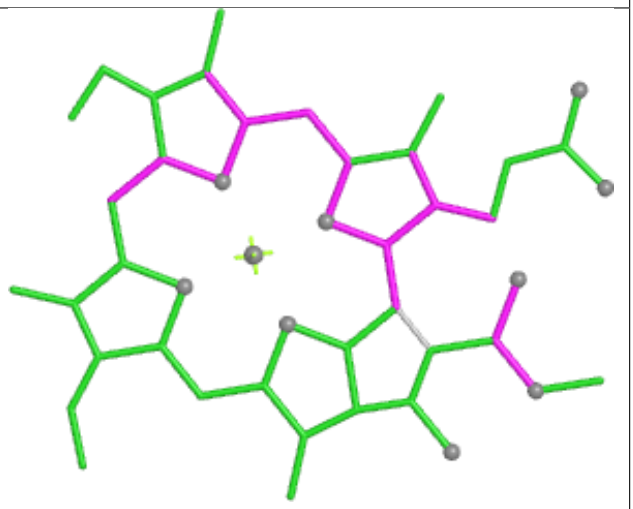
Ligand CHL p 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 4 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

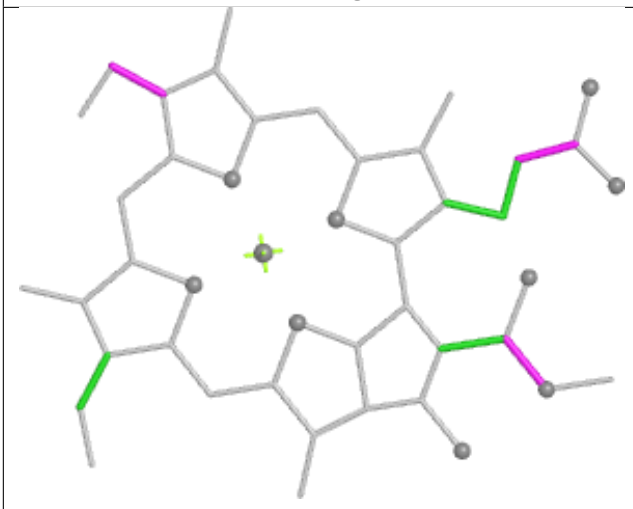
Ligand CLA s 612



Bond lengths



Bond angles

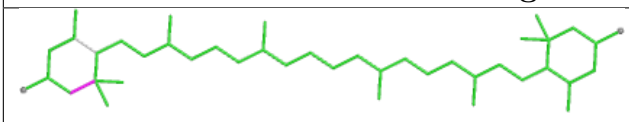


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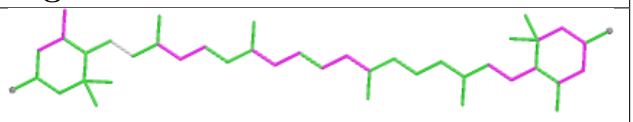


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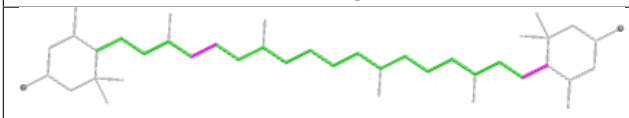
Ligand LUT g 1621



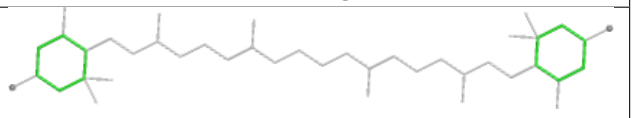
Bond lengths



Bond angles

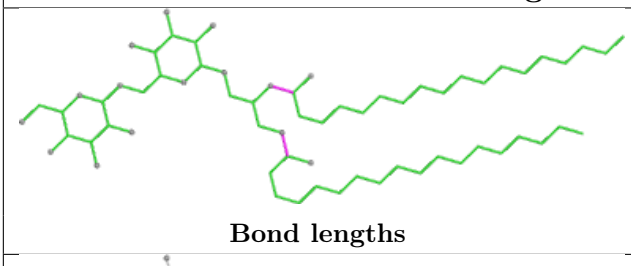


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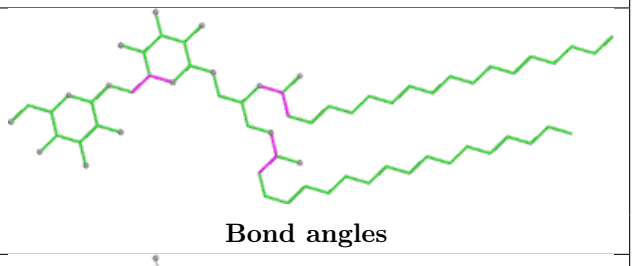


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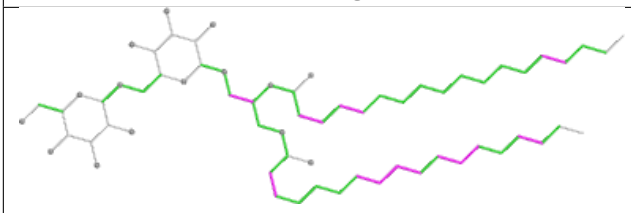
Ligand DGD c 523



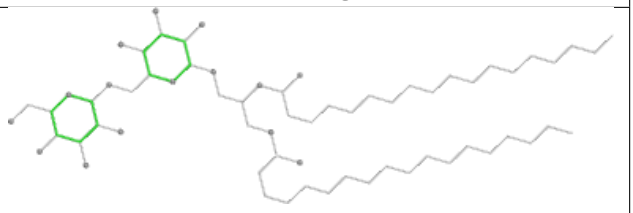
Bond lengths



Bond angles

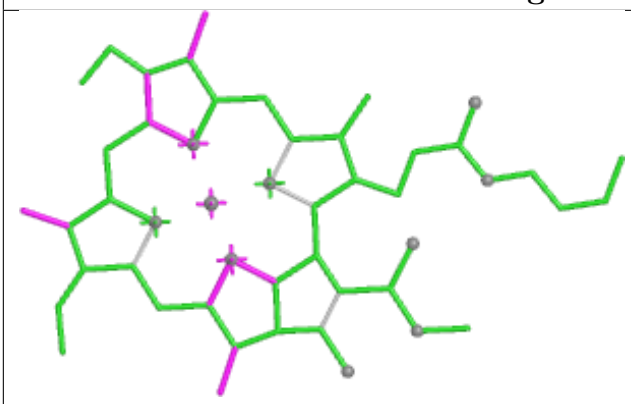


Torsions

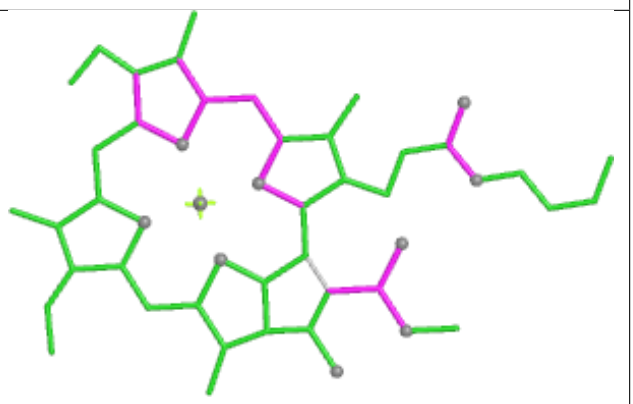


Rings

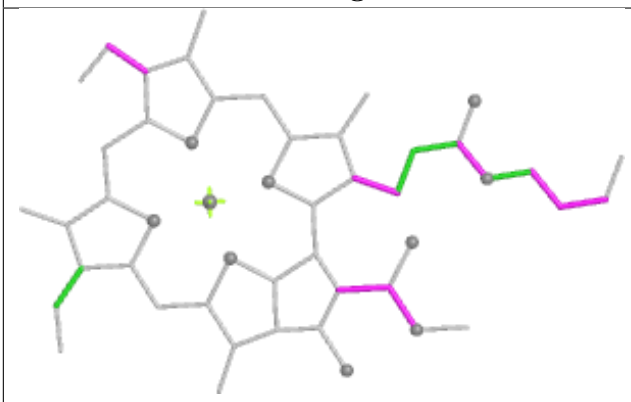
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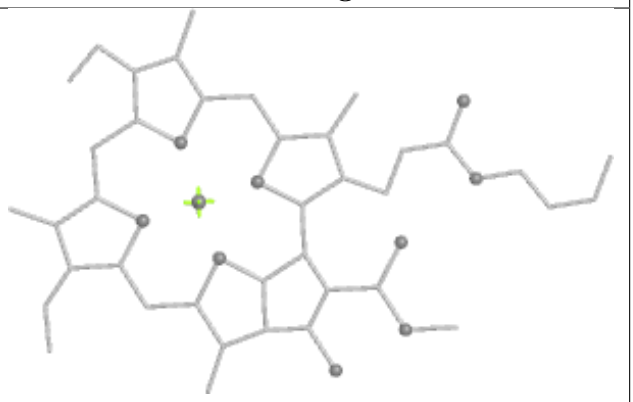
Bond lengths



Bond angles

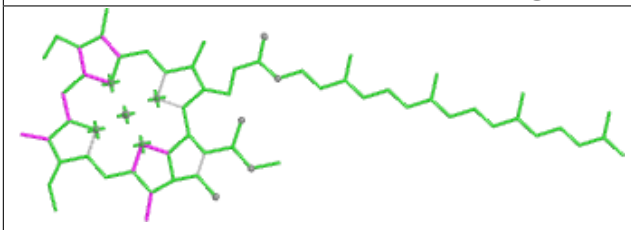


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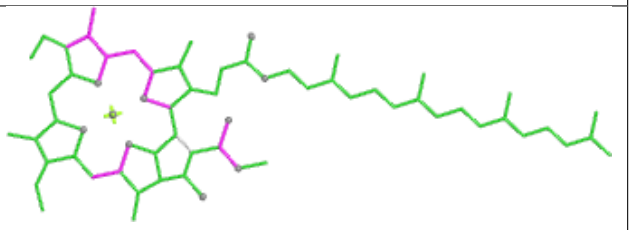


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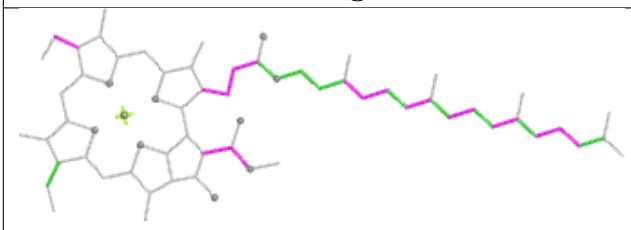
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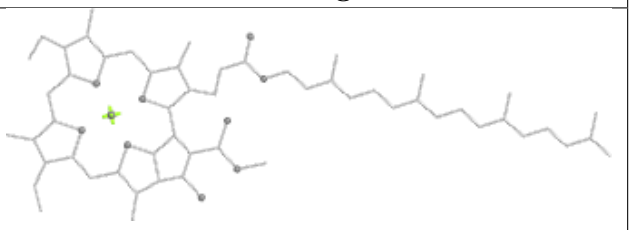
Bond lengths



Bond angles

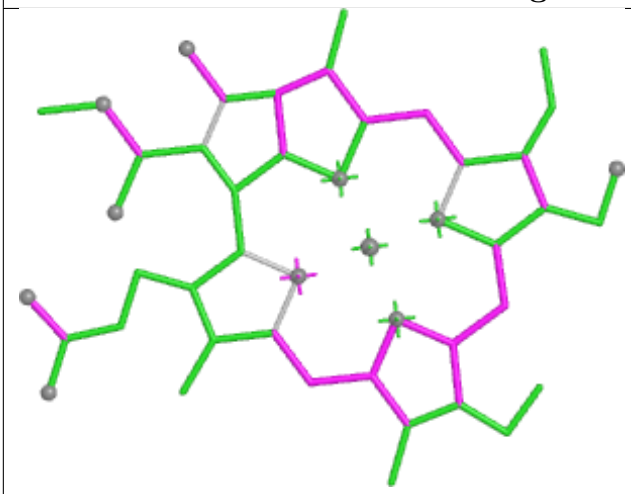


Torsions



Rings

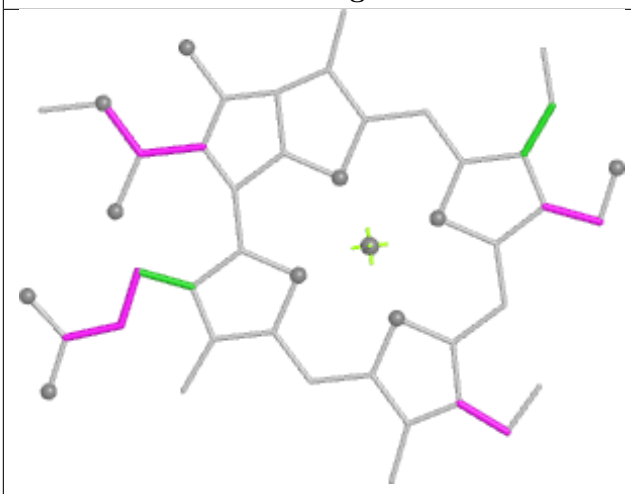
Ligand CHL s 601



Bond lengths



Bond angles

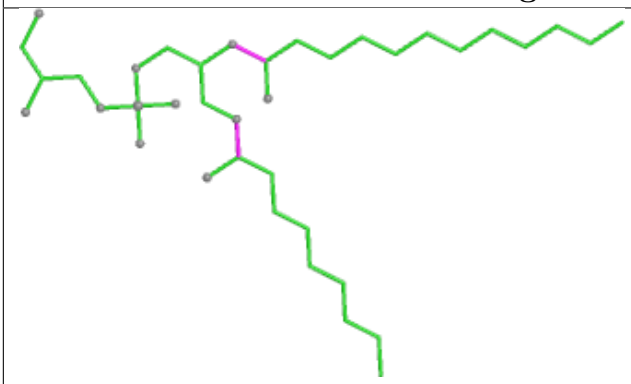


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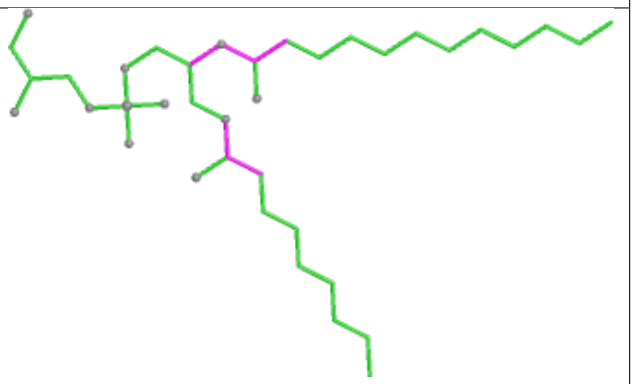


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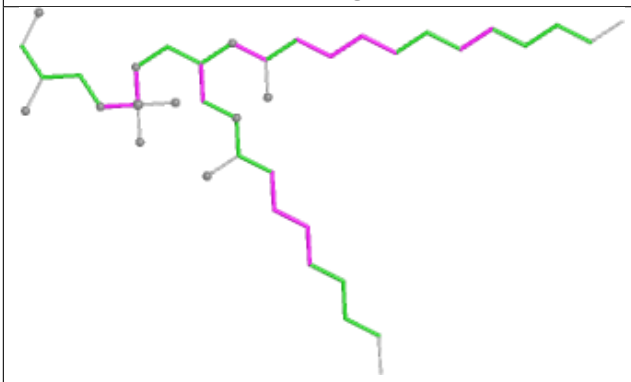
Ligand LHG r 2630



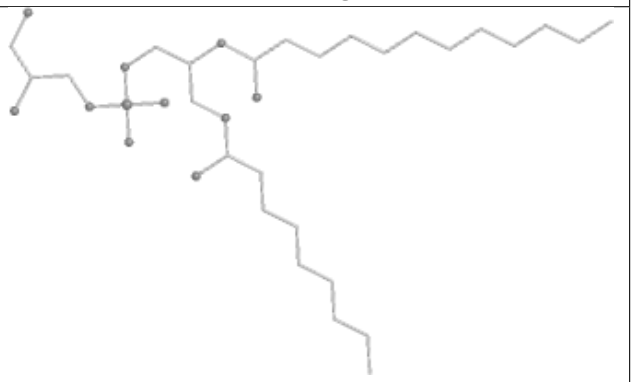
Bond lengths



Bond angles

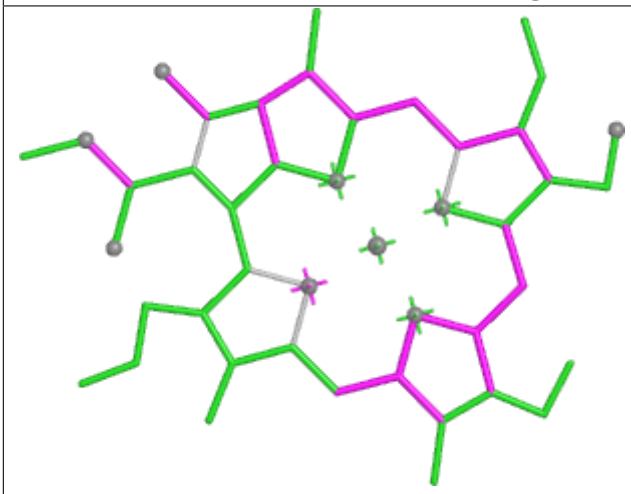


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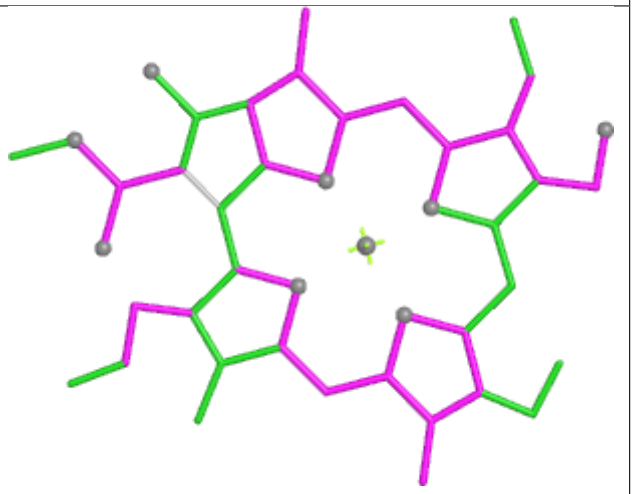


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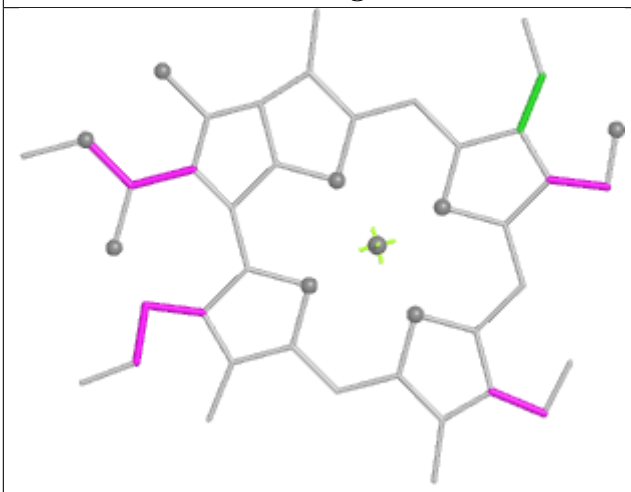
Ligand CHL S 606



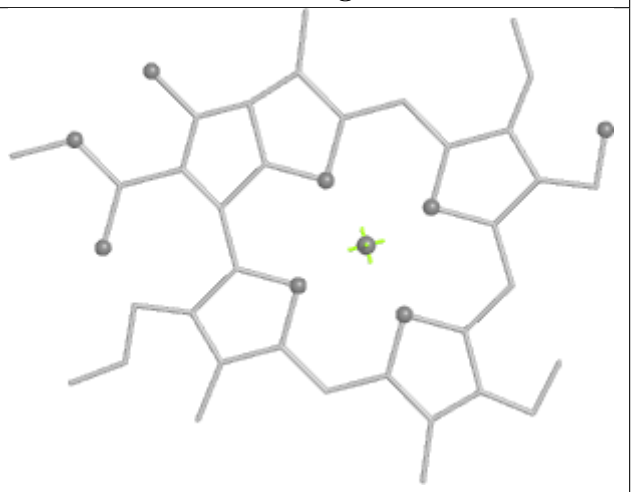
Bond lengths



Bond angles

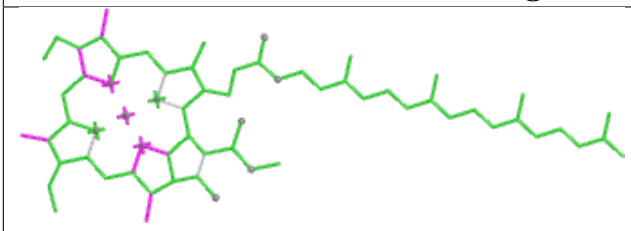


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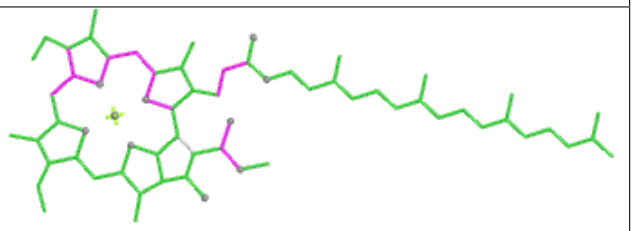


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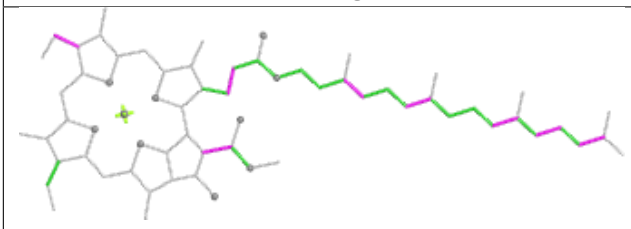
Ligand CLA B 604



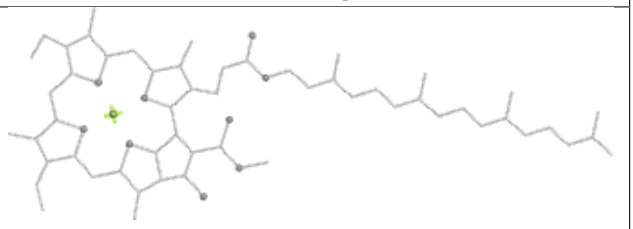
Bond lengths



Bond angles

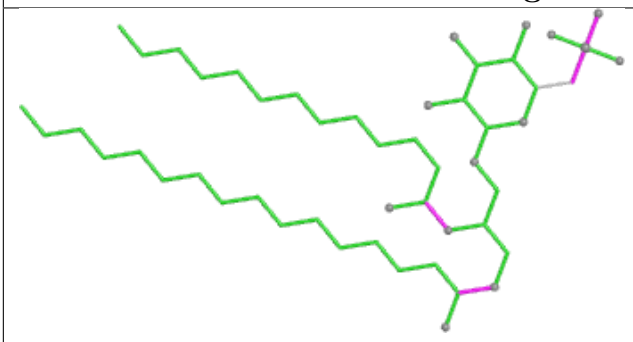


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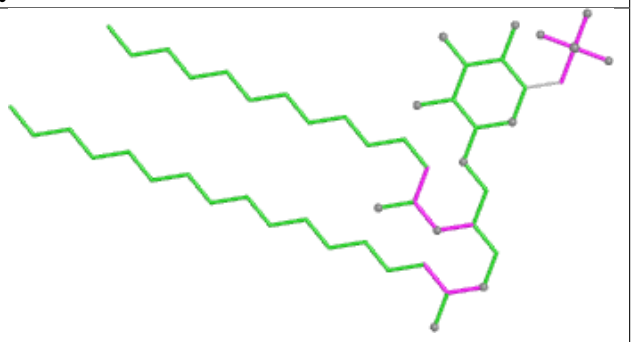


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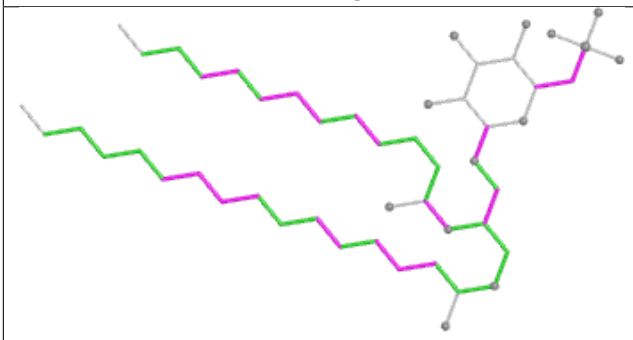
Ligand SQD A 412



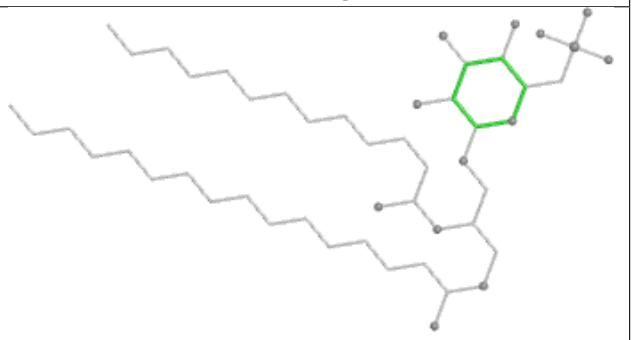
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Bond angles

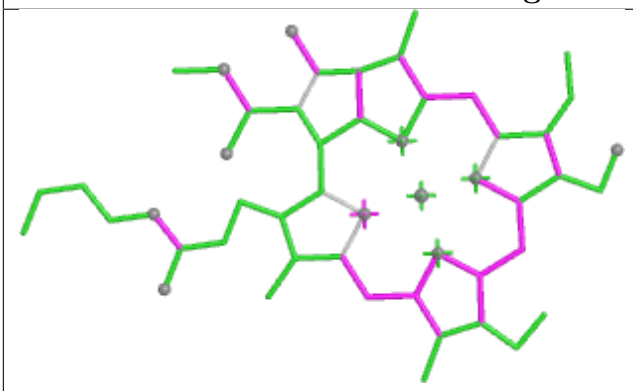


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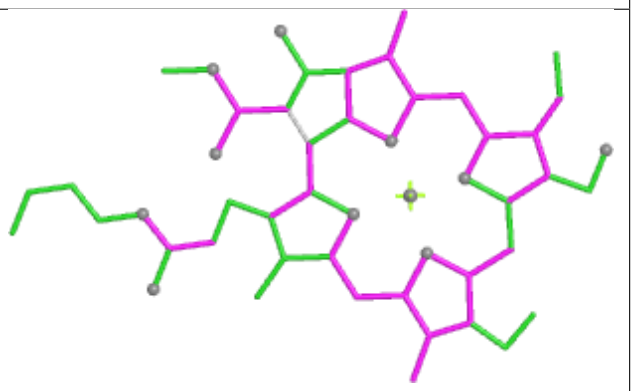


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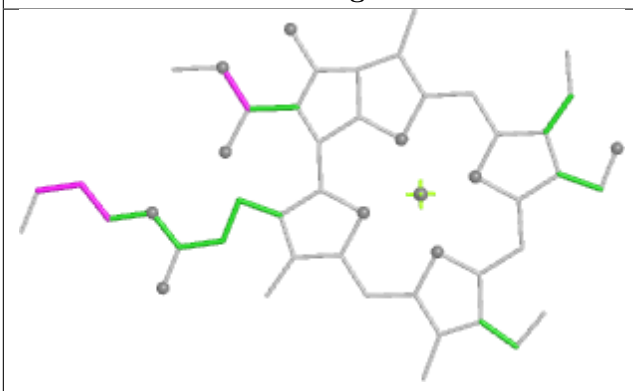
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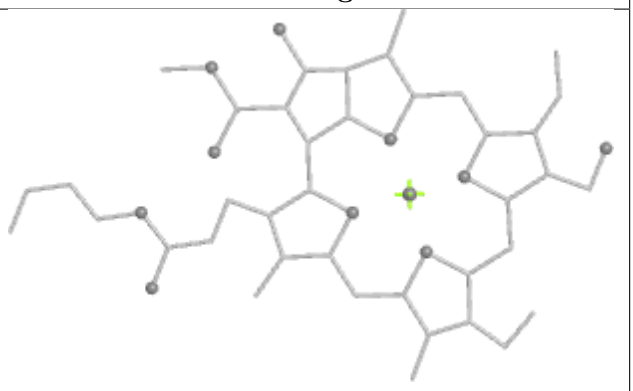
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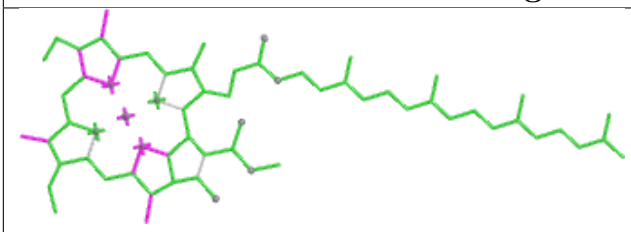


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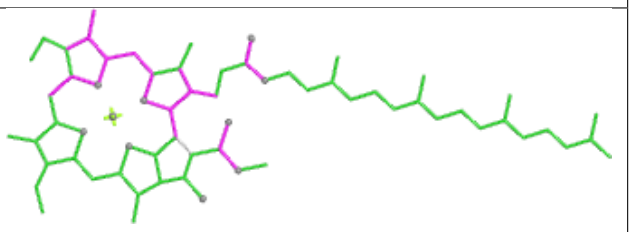


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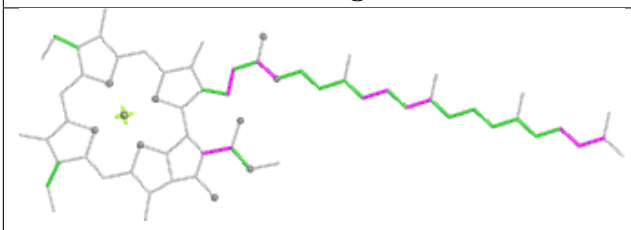
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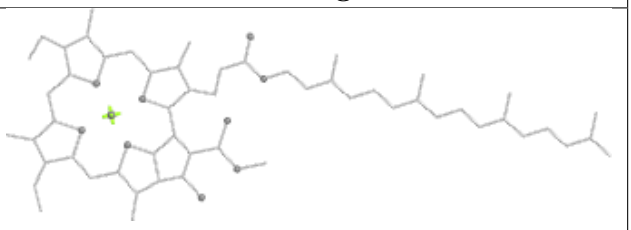
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Bond angles

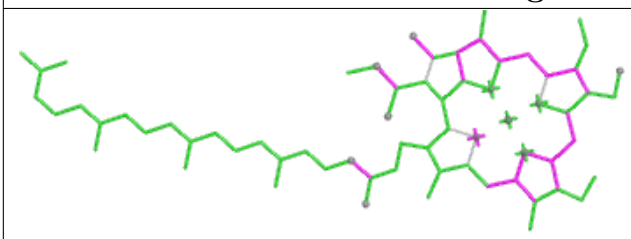


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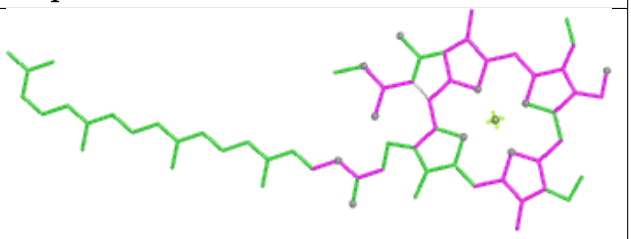


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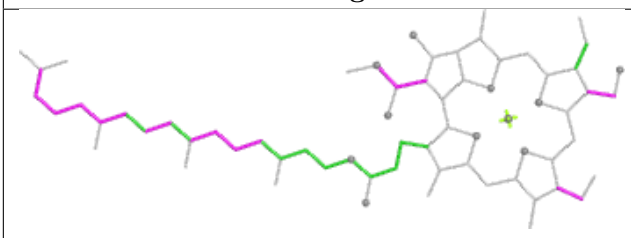
Ligand CHL p 605



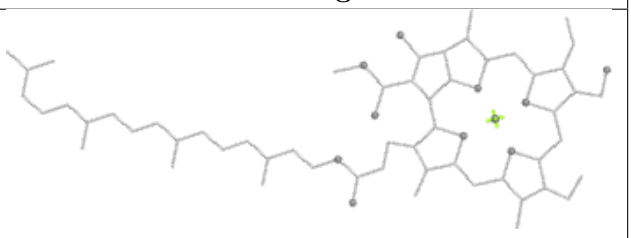
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Bond angles

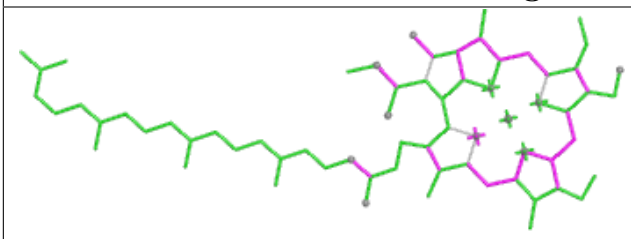


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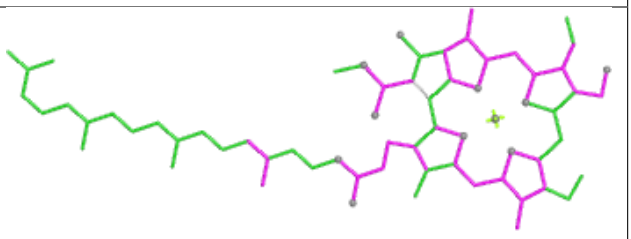


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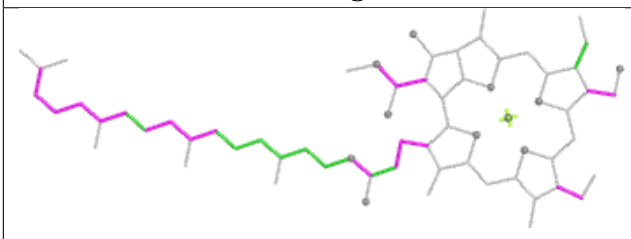
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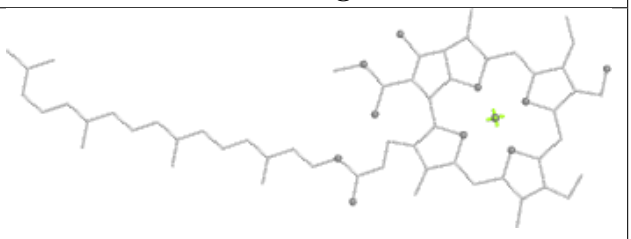
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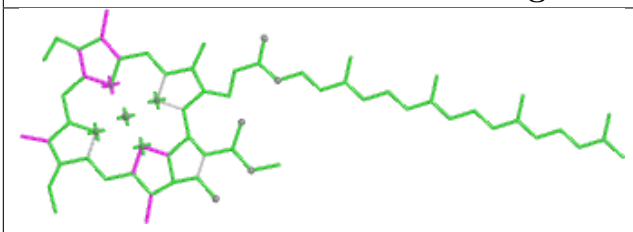


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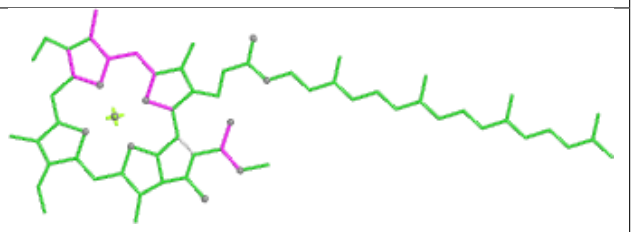


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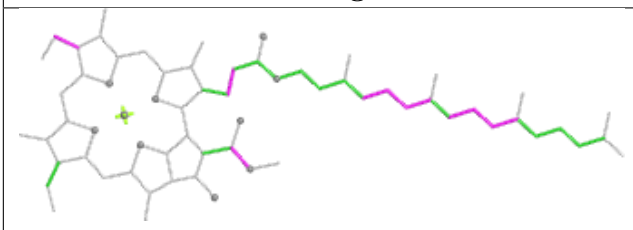
Ligand CLA 0 602



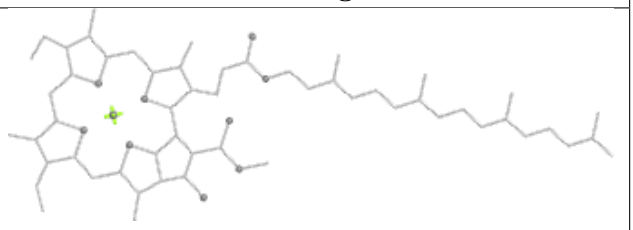
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Bond angles

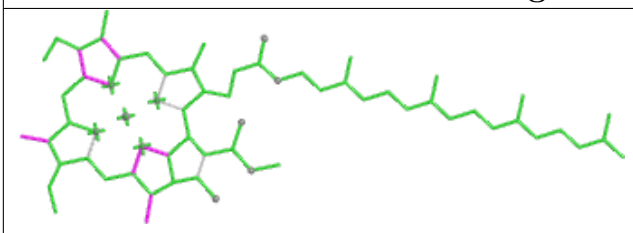


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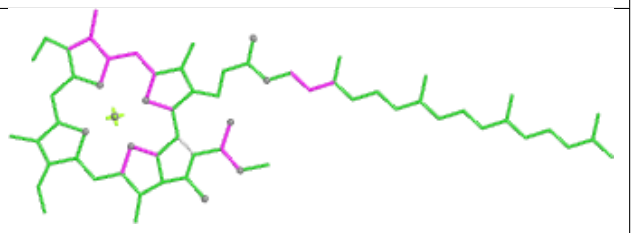


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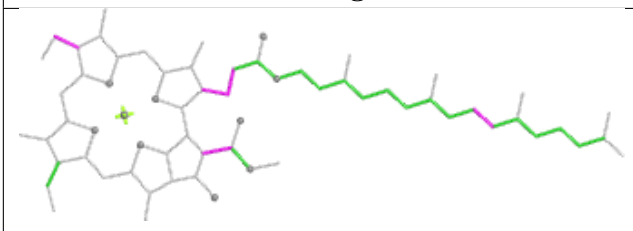
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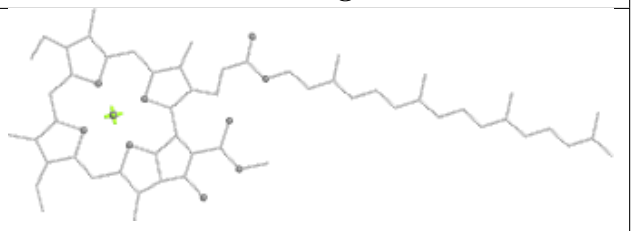
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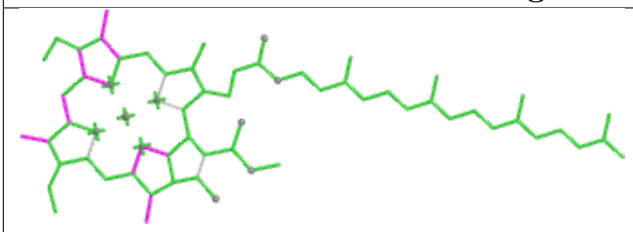


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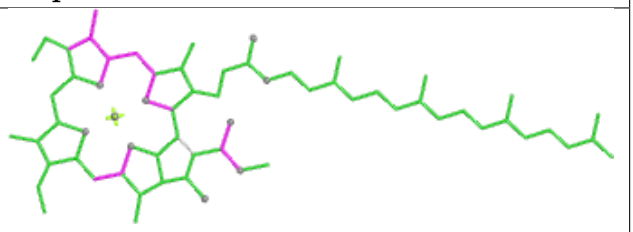


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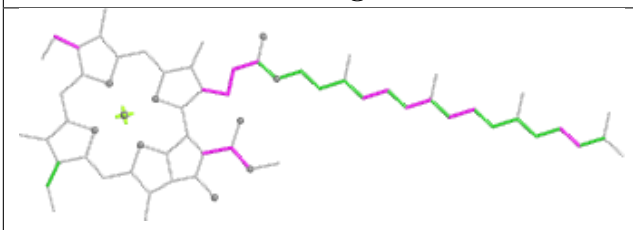
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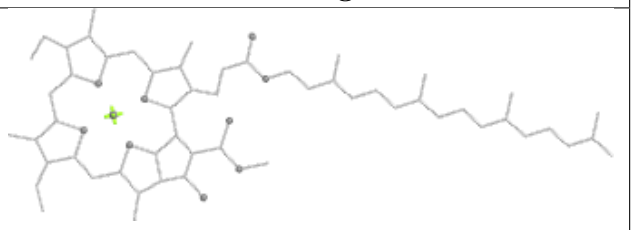
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Bond angles

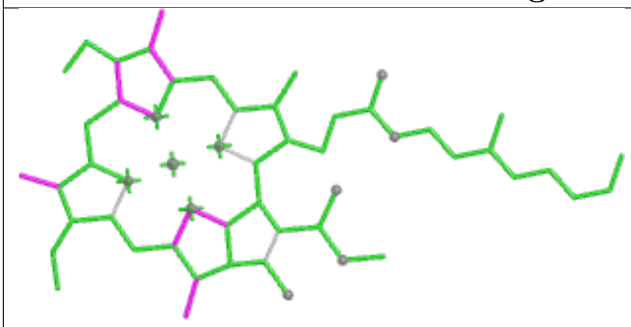


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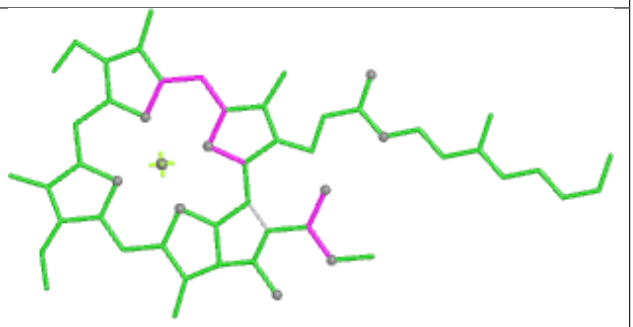


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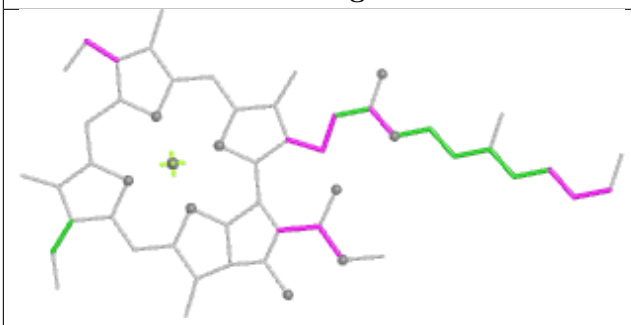
Ligand CLA 1 614



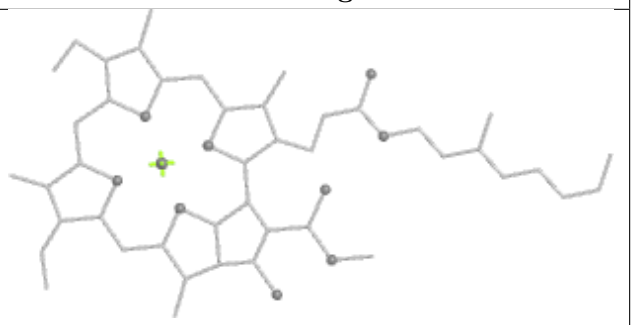
Bond lengths



Bond angles

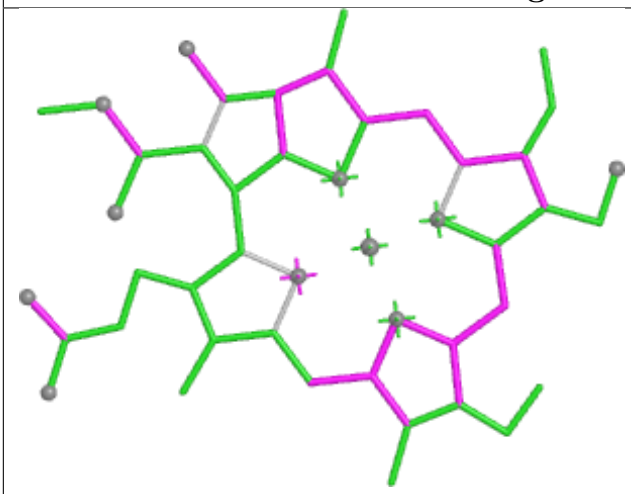


Torsions

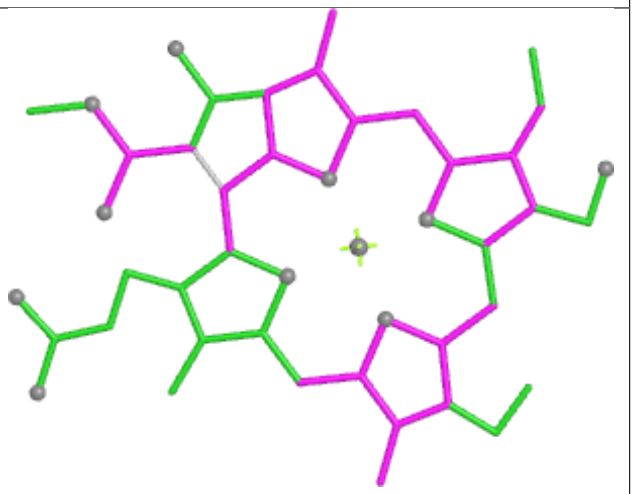


Rings

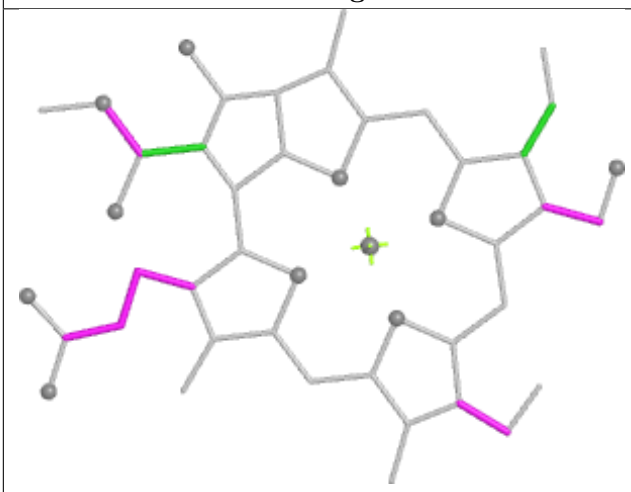
Ligand CHL 8 606



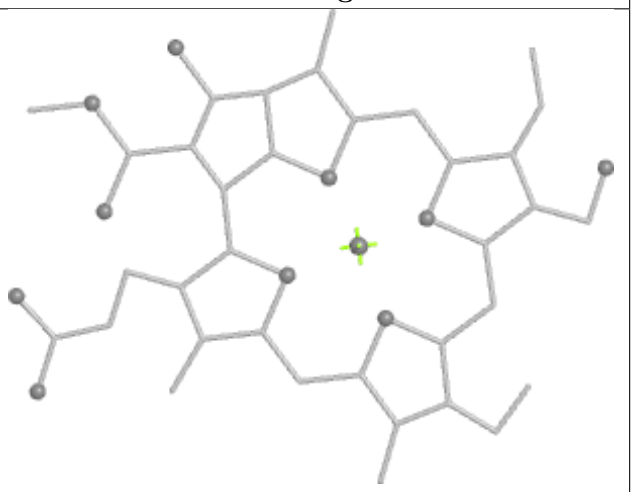
Bond lengths



Bond angles

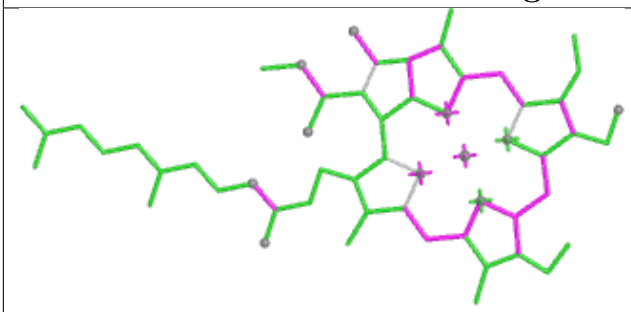


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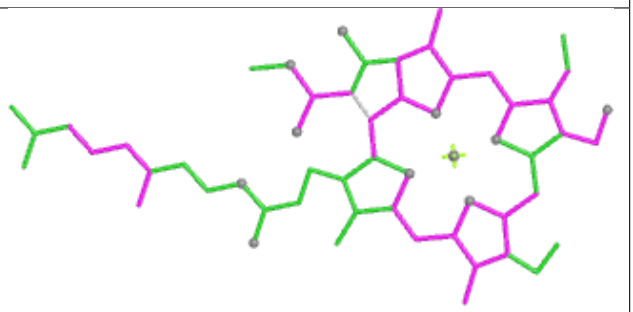


Rings

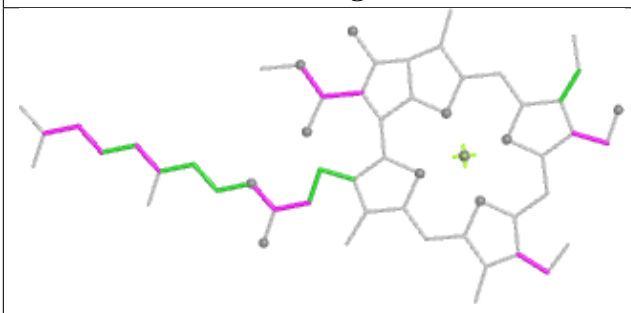
Ligand CHL R 607



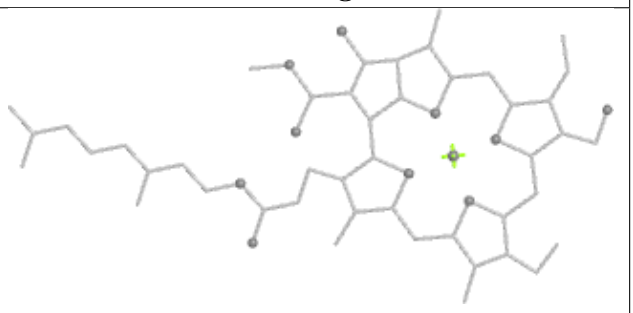
Bond lengths



Bond angles

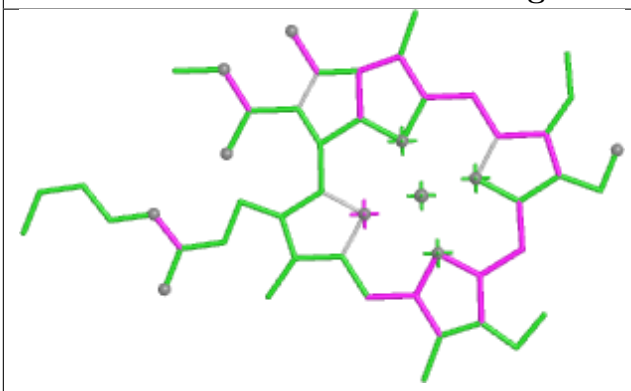


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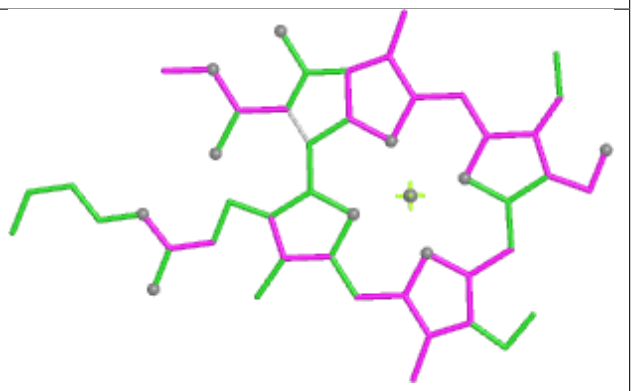


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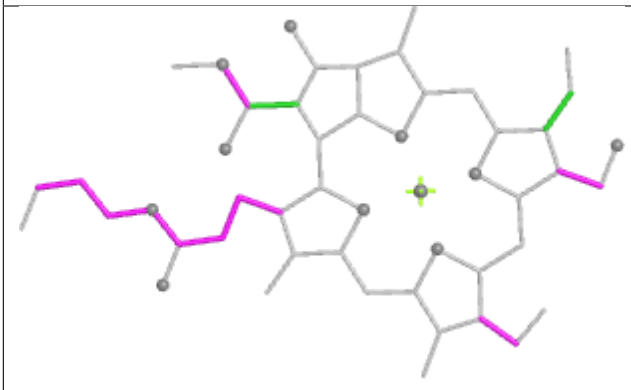
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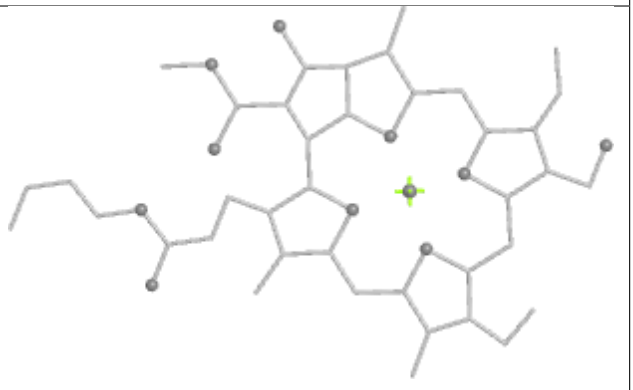
Bond lengths



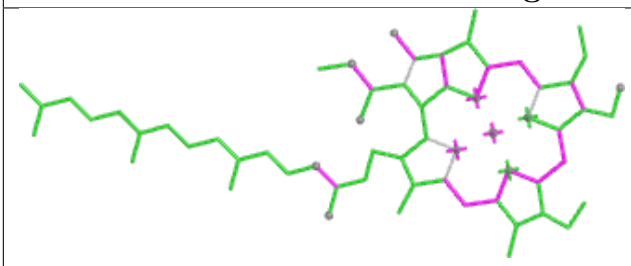
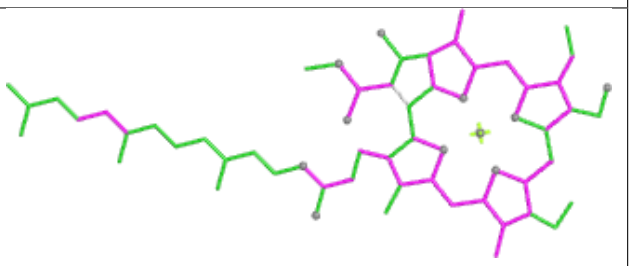
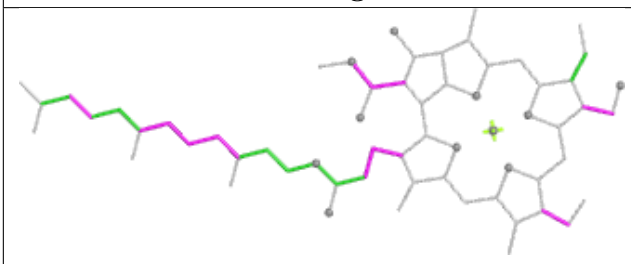
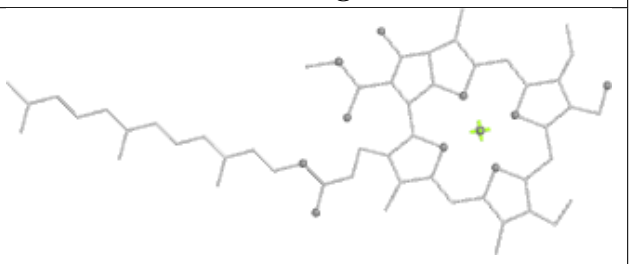
Bond angles

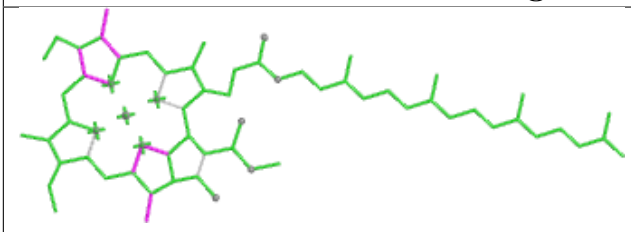
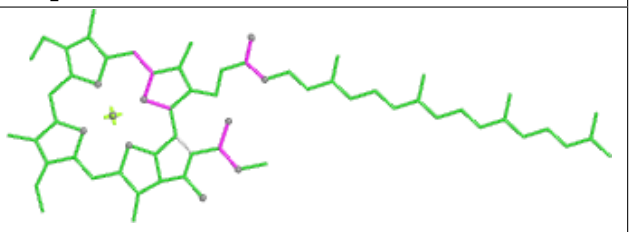
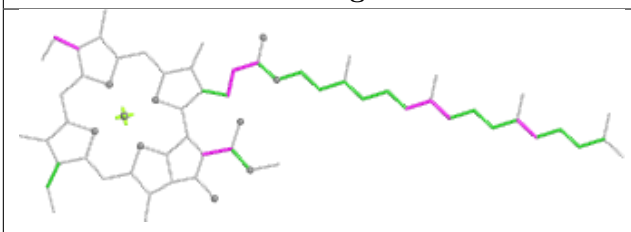
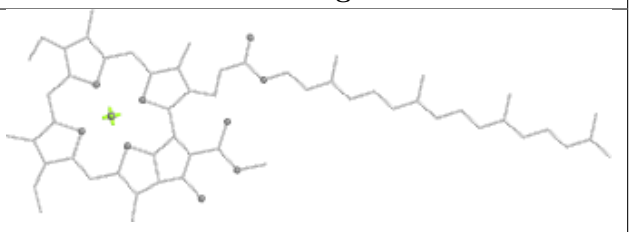


Torsions

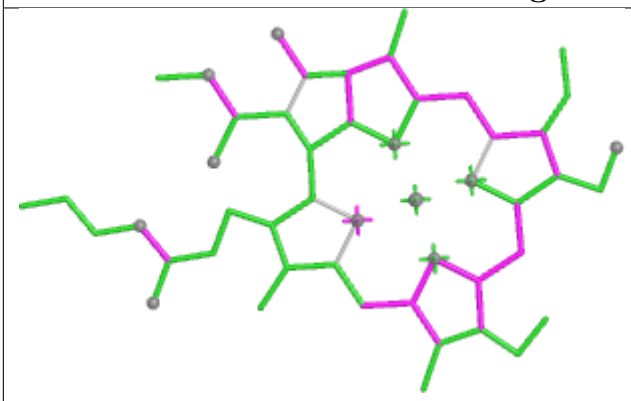


Rings

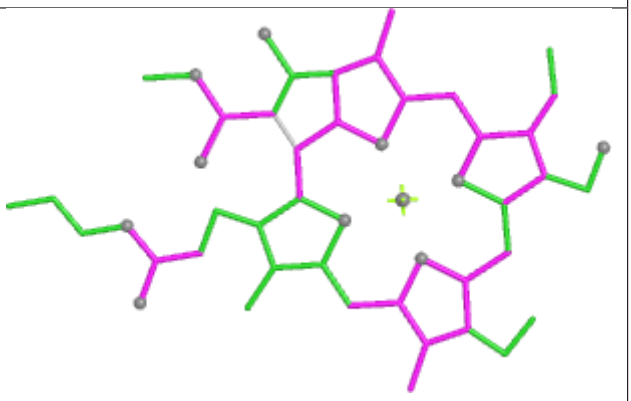
Ligand CHL R 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

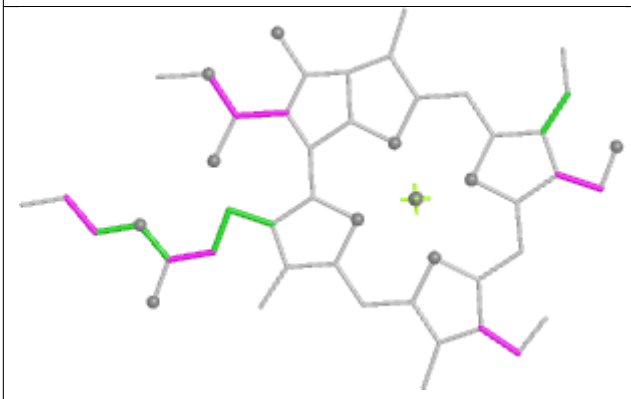
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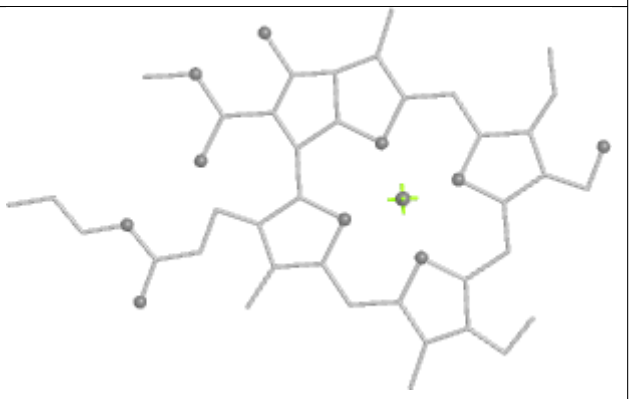
Bond lengths



Bond angles

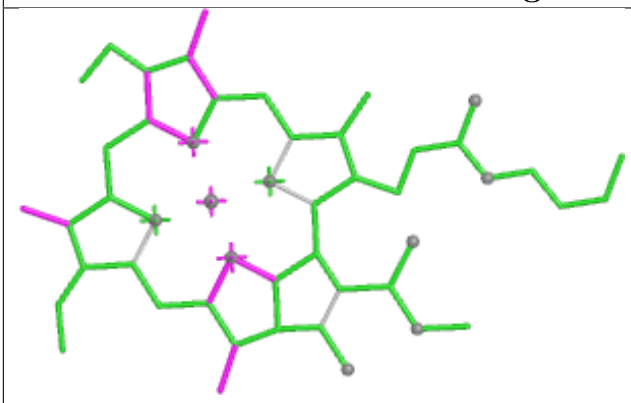


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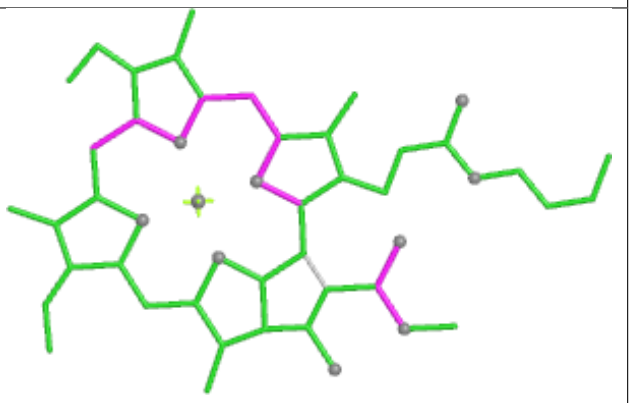


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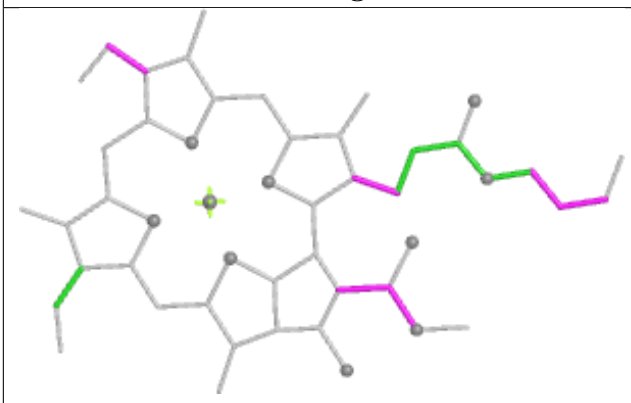
Ligand CLA N 611



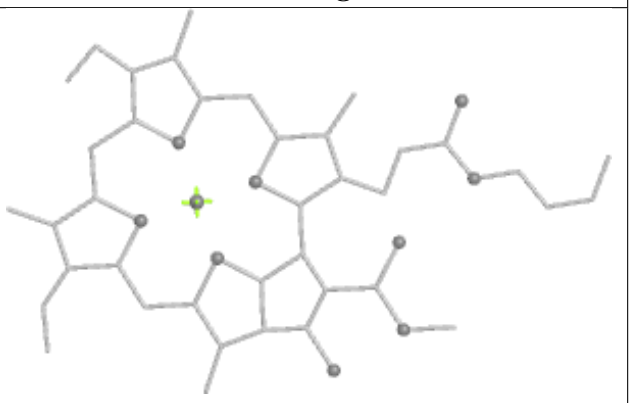
Bond lengths



Bond angles

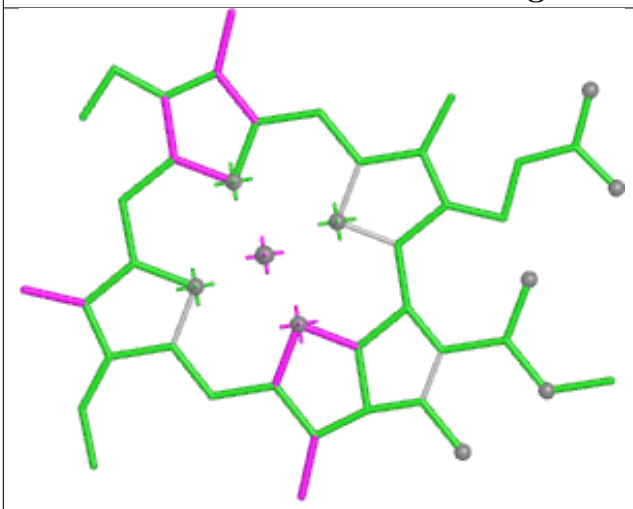


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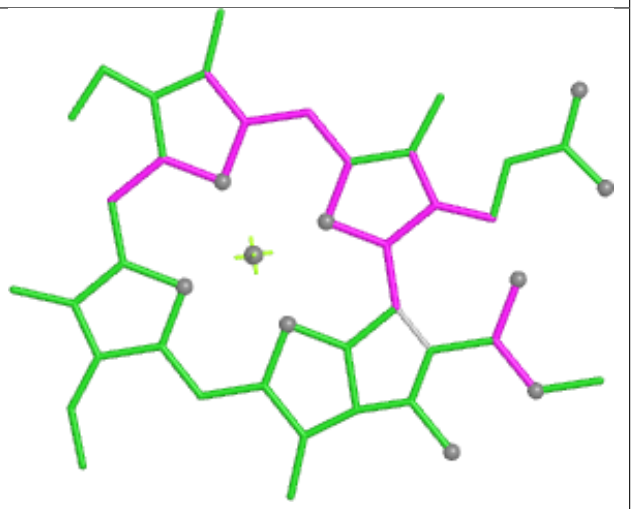


Rings

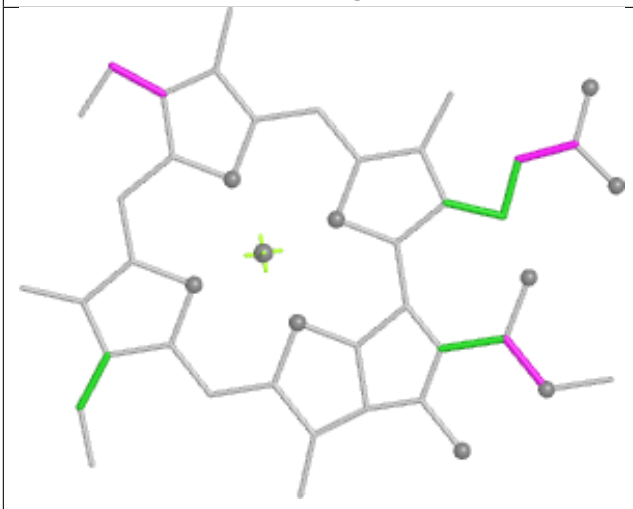
Ligand CLA S 612



Bond lengths



Bond angles

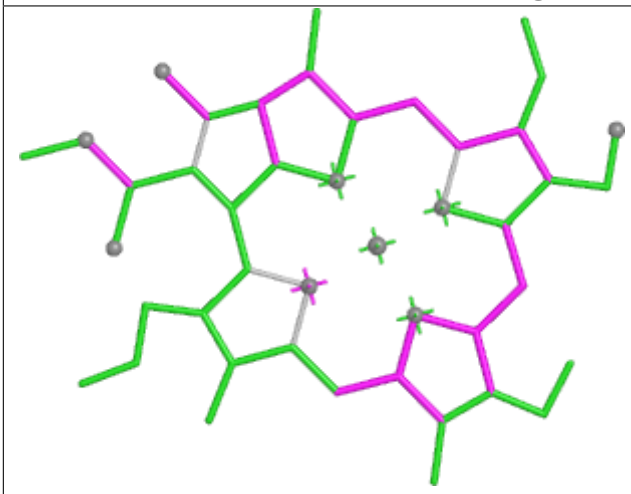


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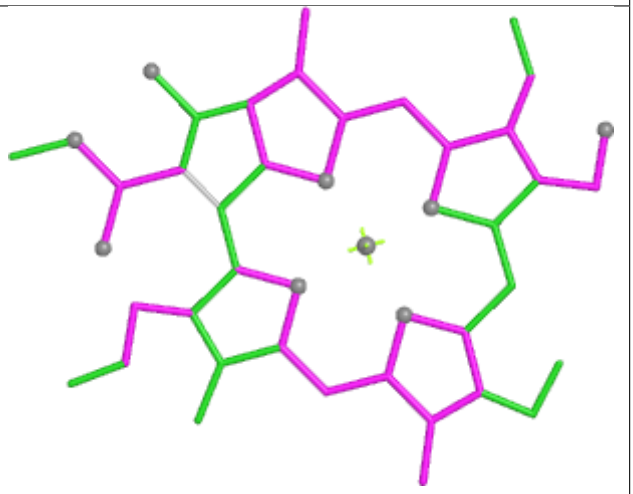


Rings

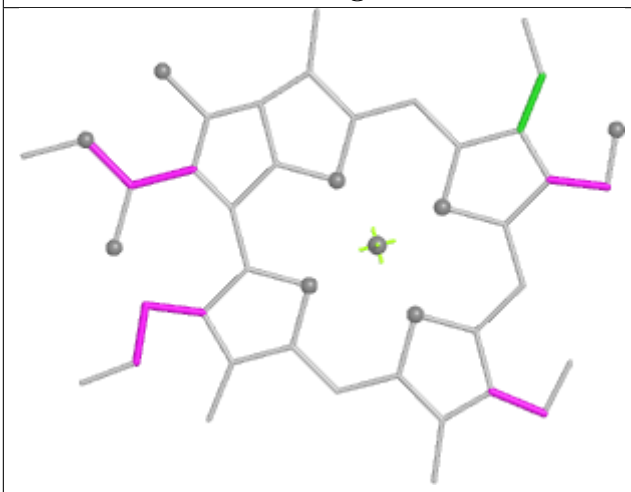
Ligand CHL s 606



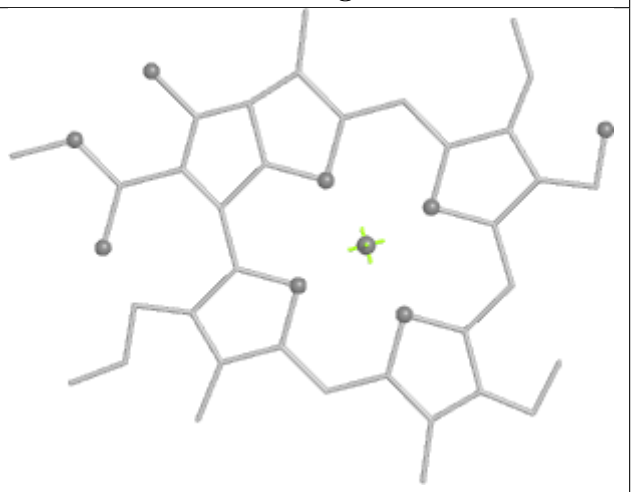
Bond lengths



Bond angles

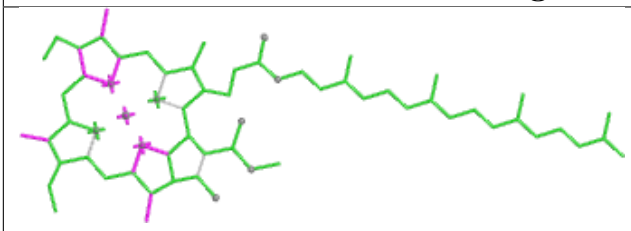


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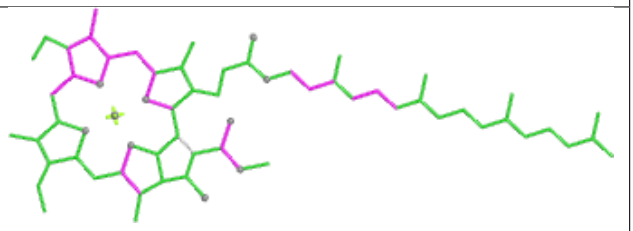


Rings

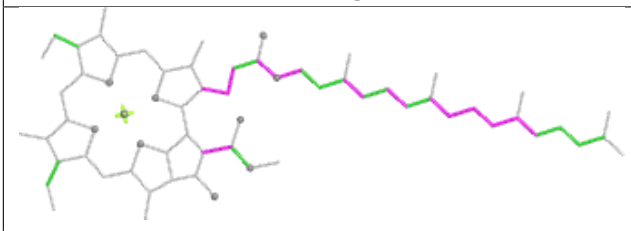
Ligand CLA c 505



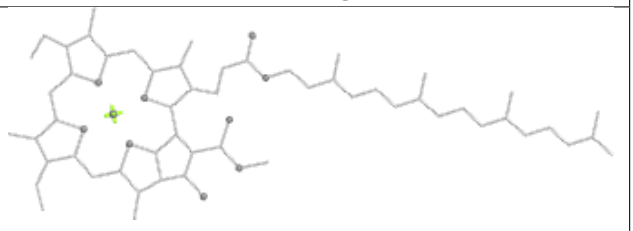
Bond lengths



Bond angles

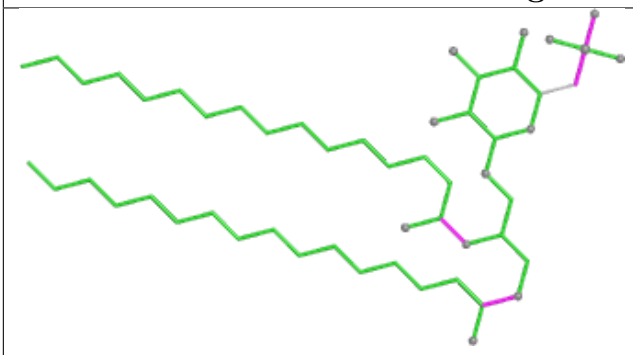


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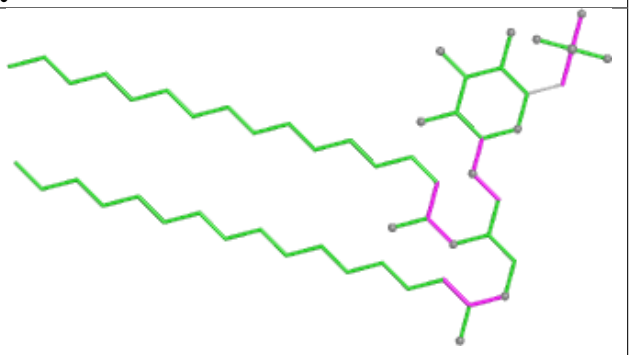


Rings

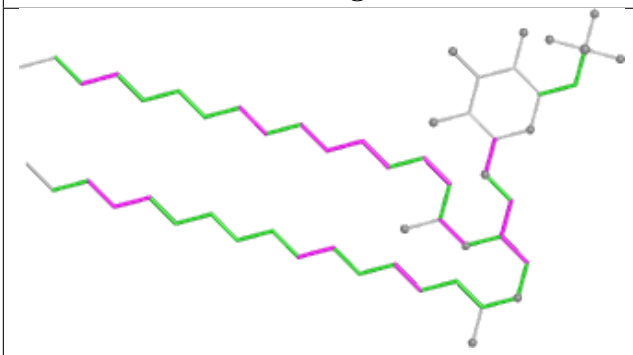
Ligand SQD b 621



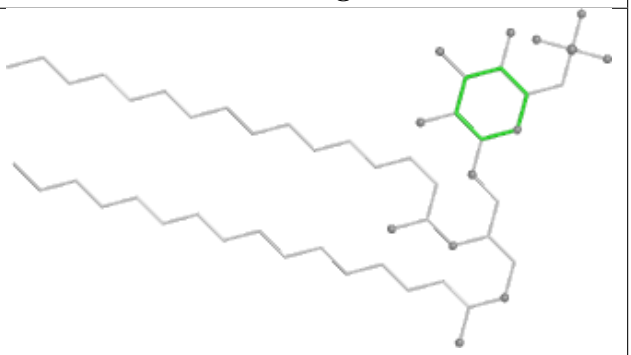
Bond lengths



Bond angles

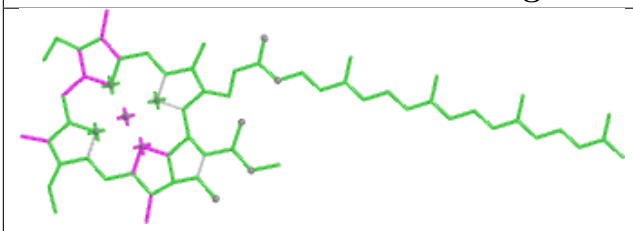


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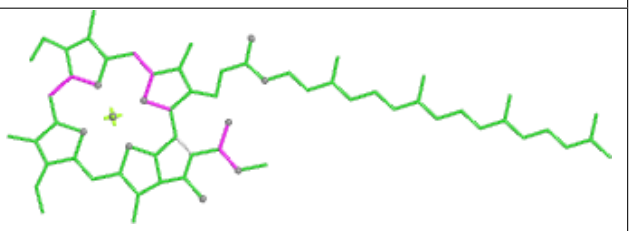


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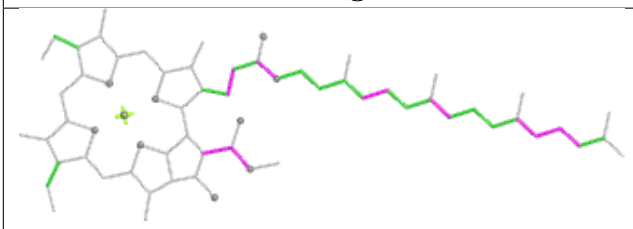
Ligand CLA G 613



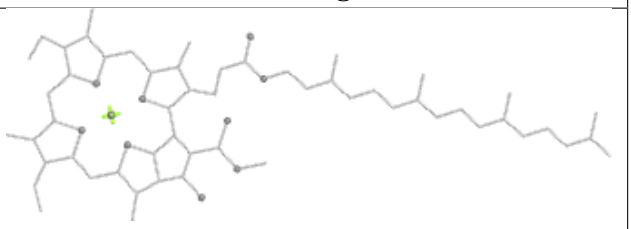
Bond lengths



Bond angles

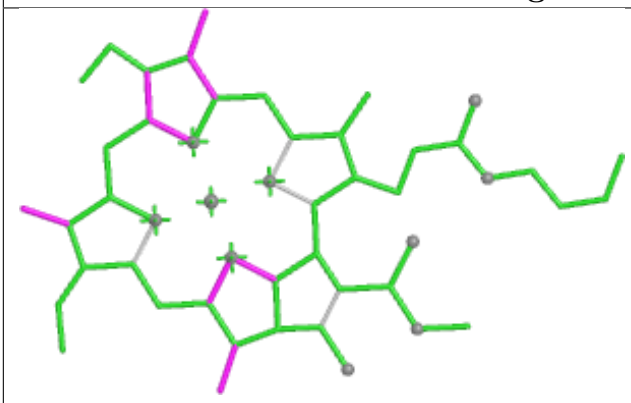


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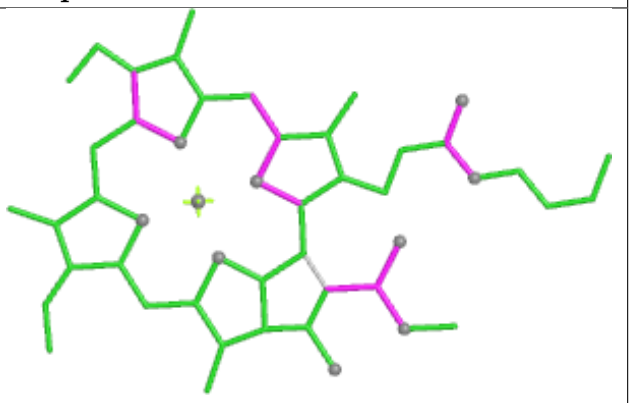


Rings

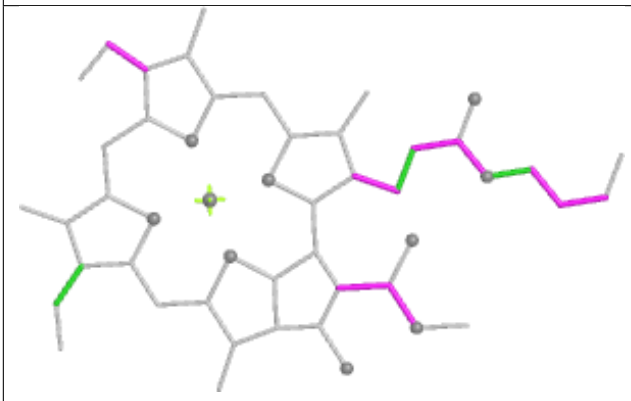
Ligand CLA q 604



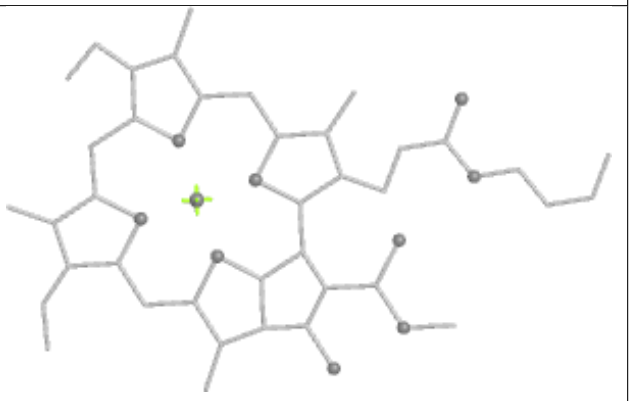
Bond lengths



Bond angles

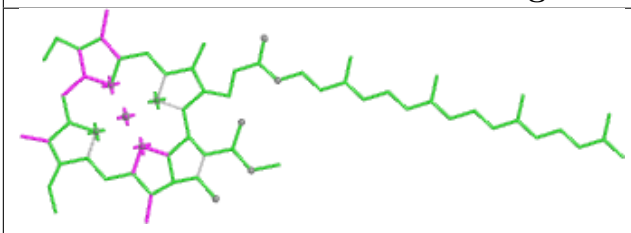


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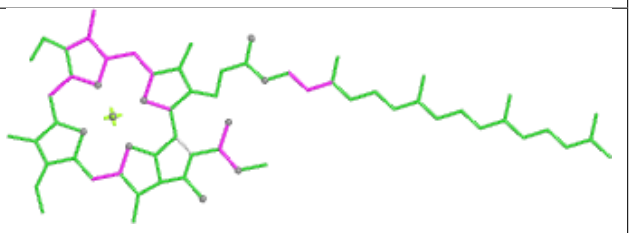


Rings

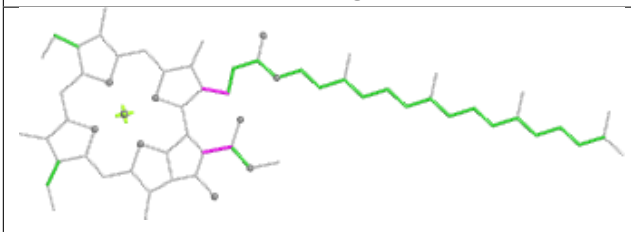
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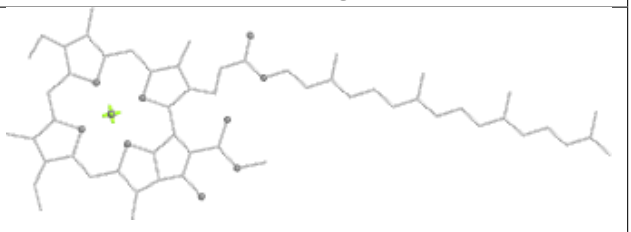
Bond lengths



Bond angles

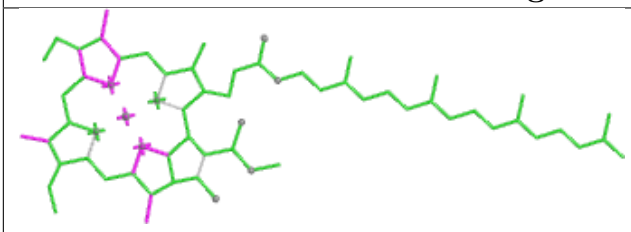


Torsions

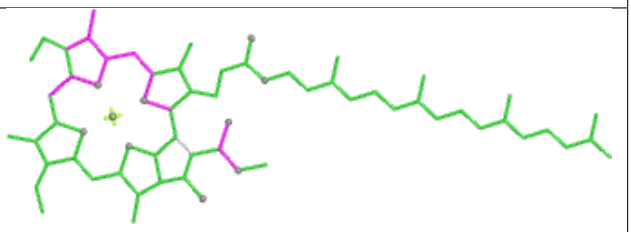


Rings

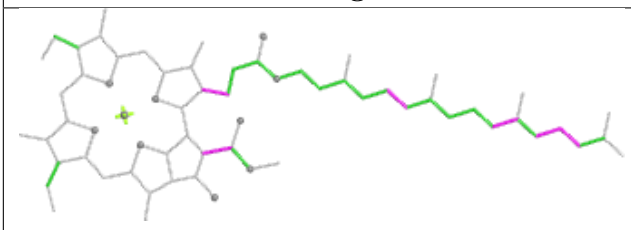
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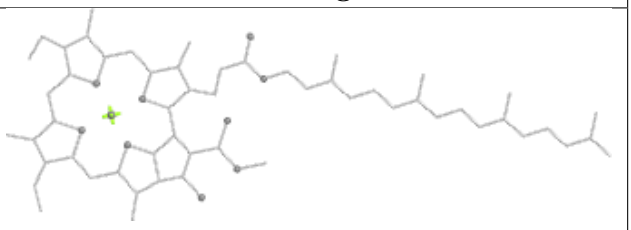
Bond lengths



Bond angles

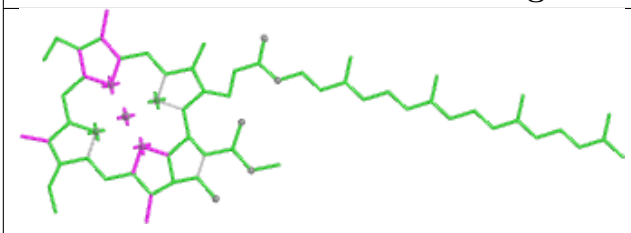


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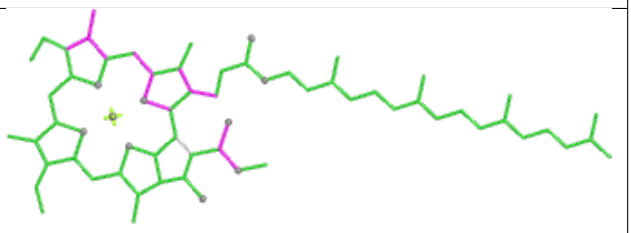


Rings

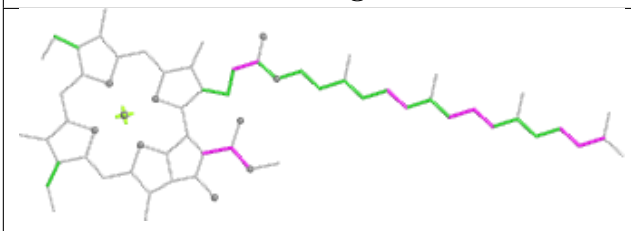
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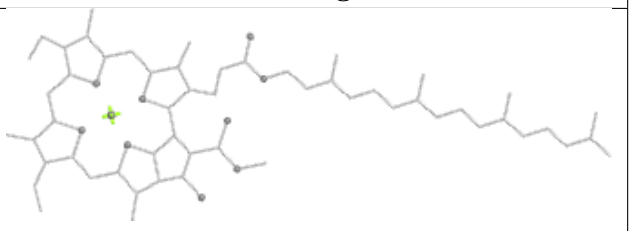
Bond lengths



Bond angles

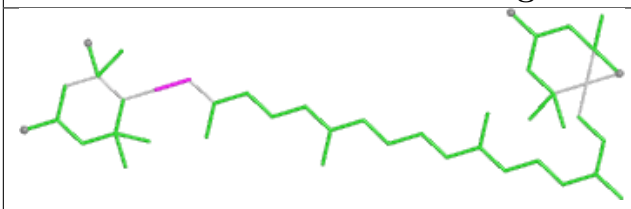


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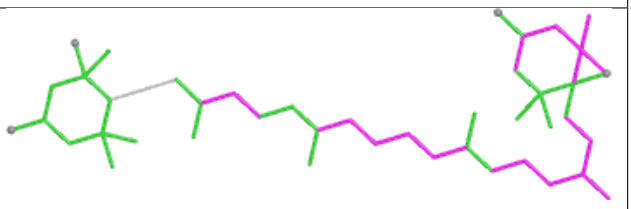


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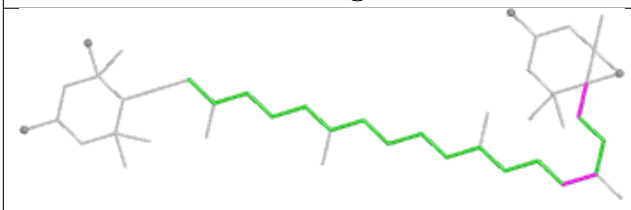
Ligand NEX 6 1623



Bond lengths



Bond angles

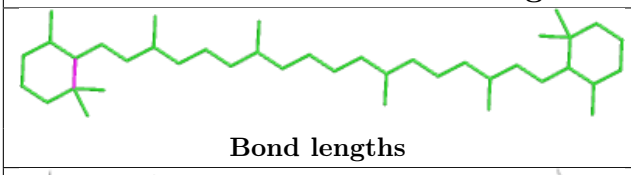


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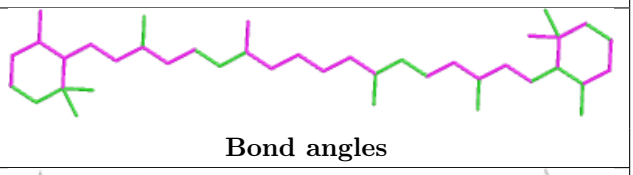


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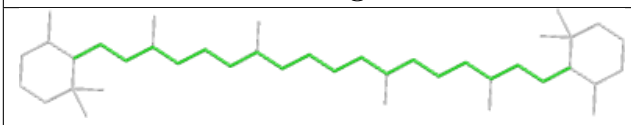
Ligand BCR b 619



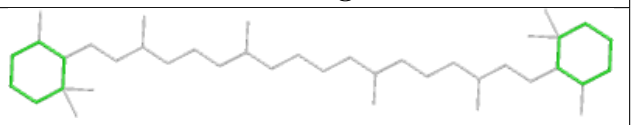
Bond lengths



Bond angles

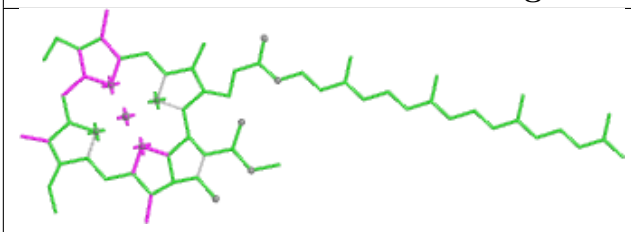


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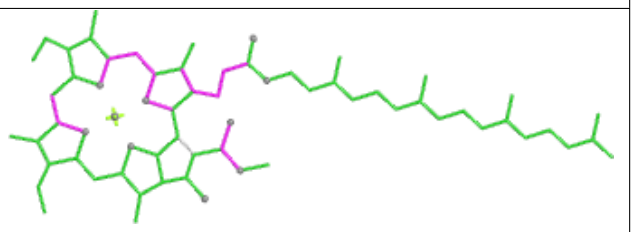


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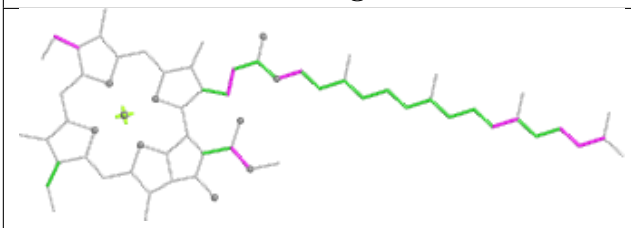
Ligand CLA B 611



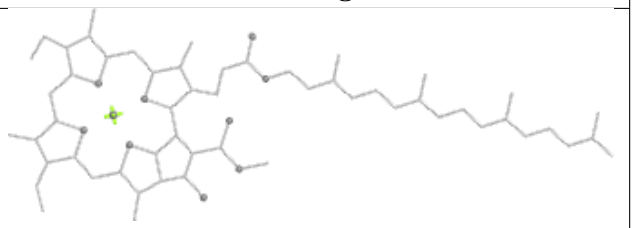
Bond lengths



Bond angles

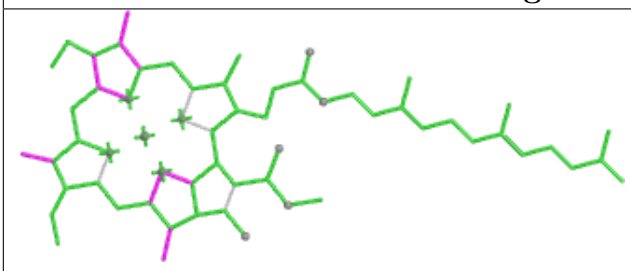


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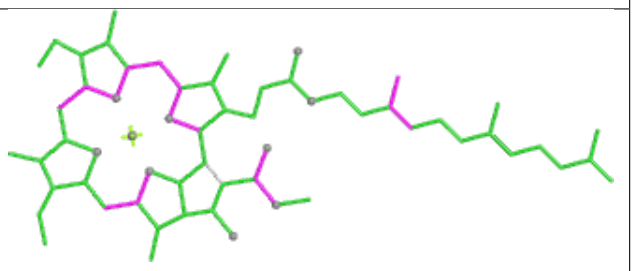


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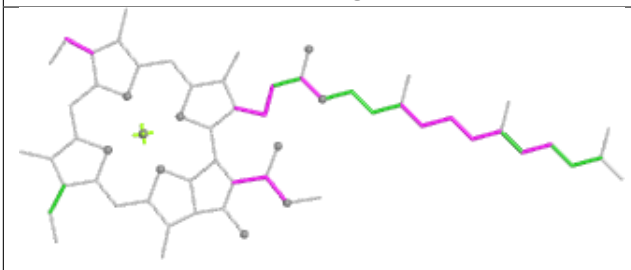
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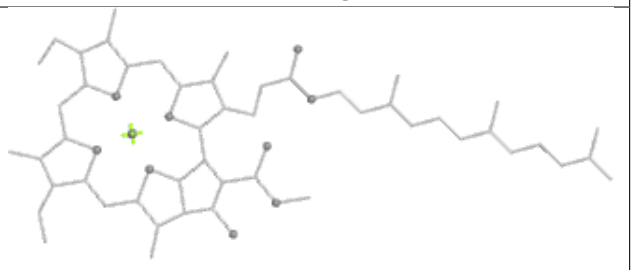
Bond lengths



Bond angles

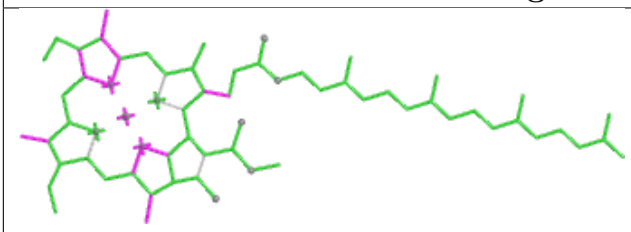


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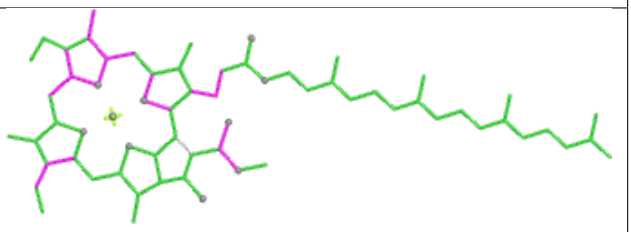


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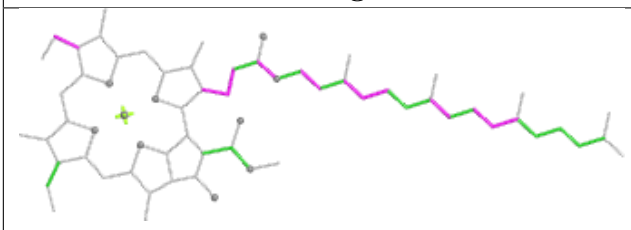
Ligand CLA d 402



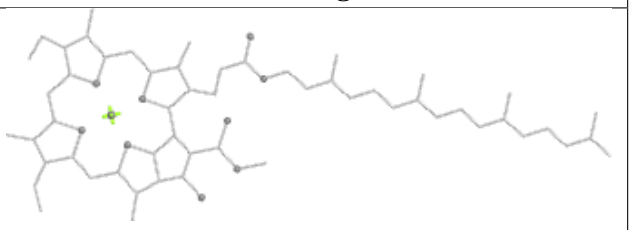
Bond lengths



Bond angles

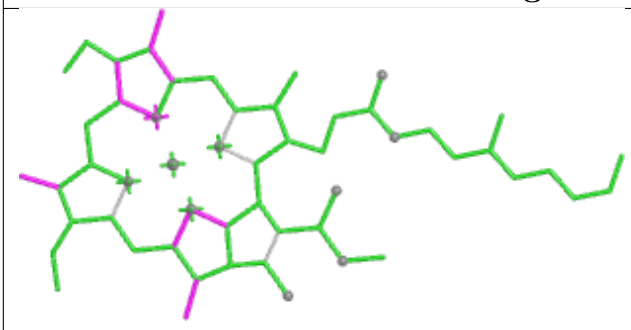


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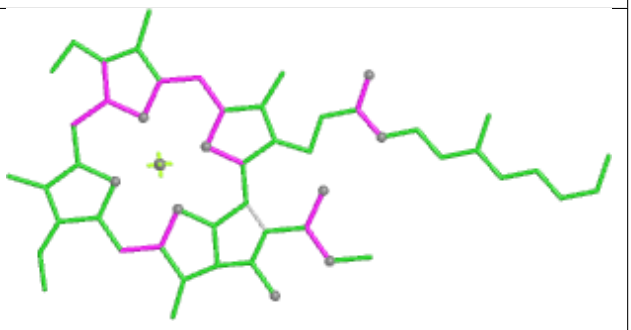


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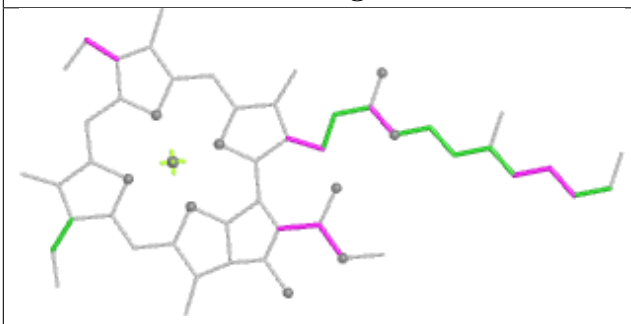
Ligand CLA Y 614



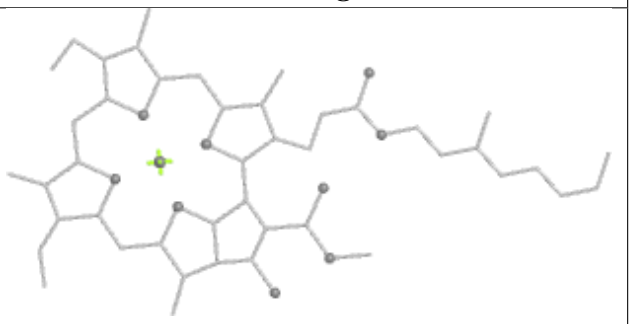
Bond lengths



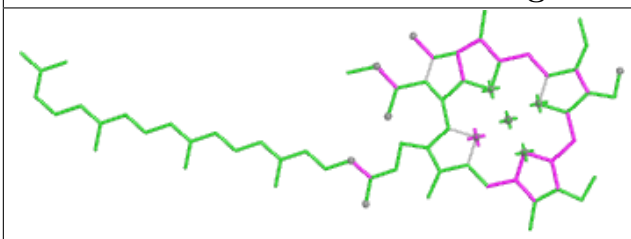
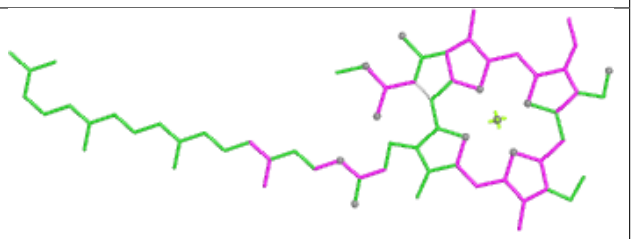
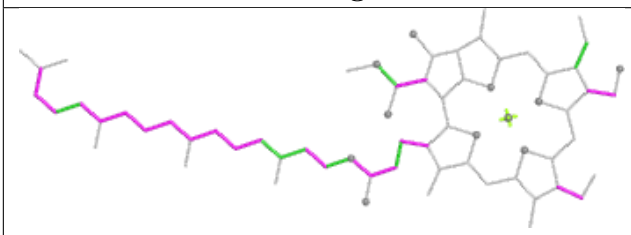
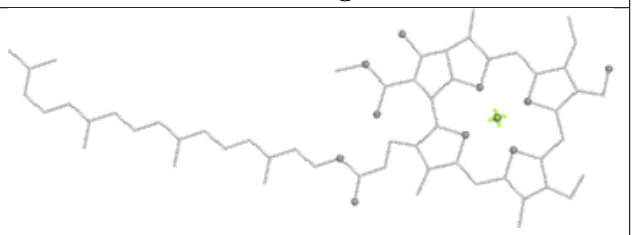
Bond angles

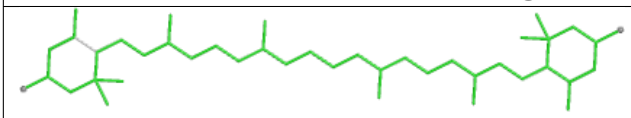
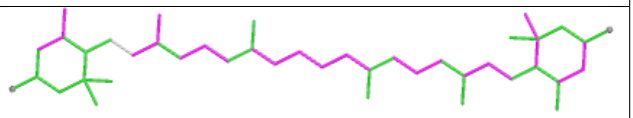
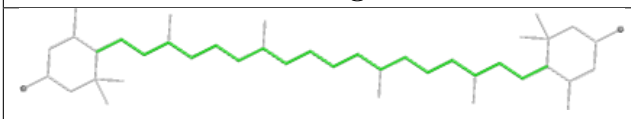
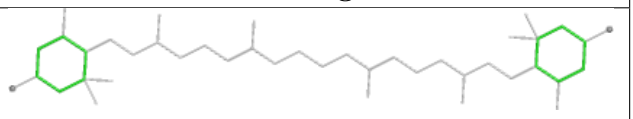


Torsions

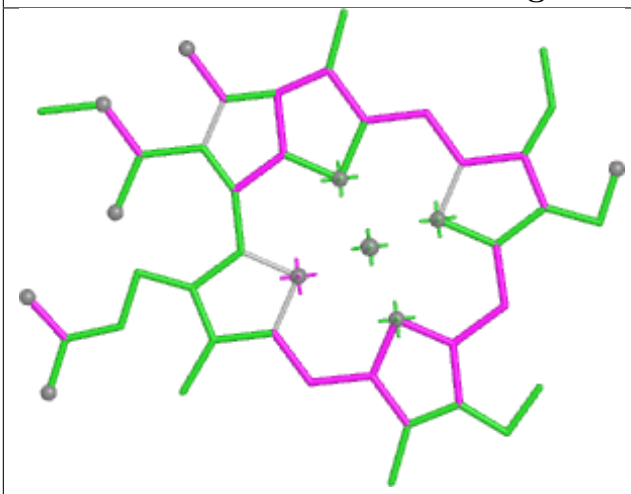


Rings

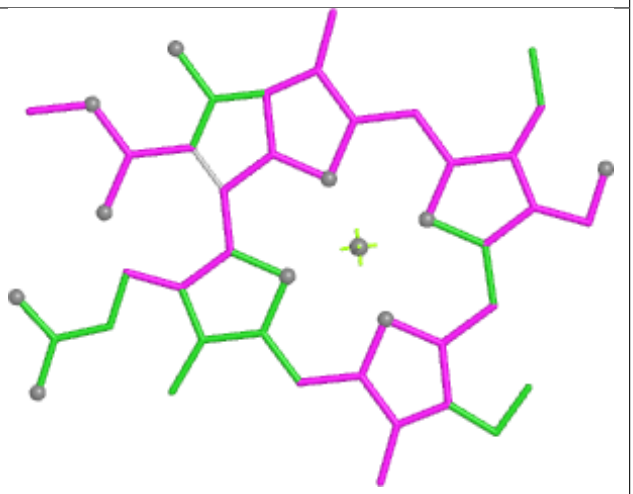
Ligand CHL 3 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

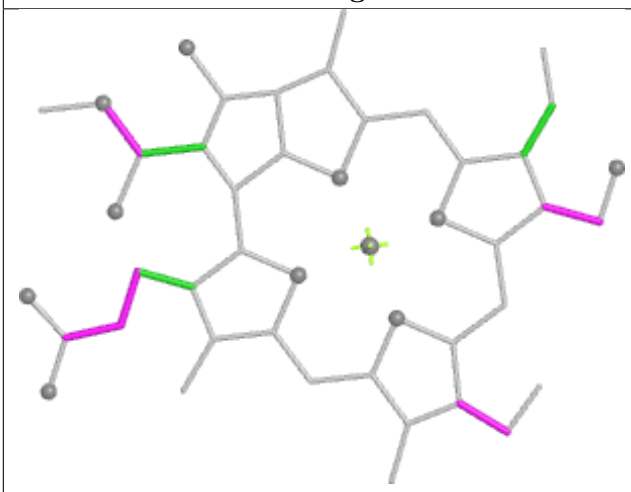
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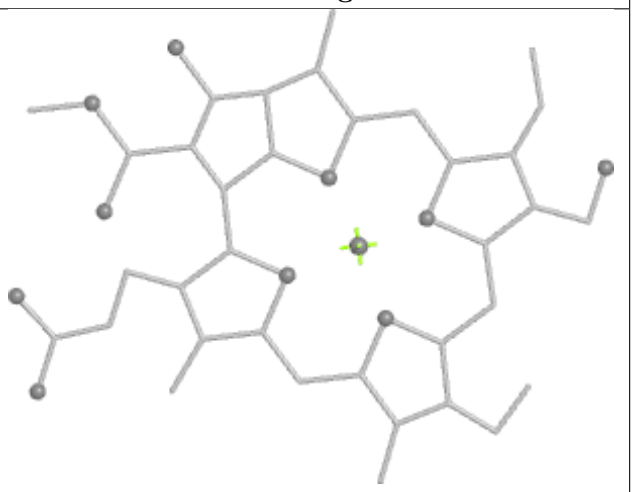
Bond lengths



Bond angles

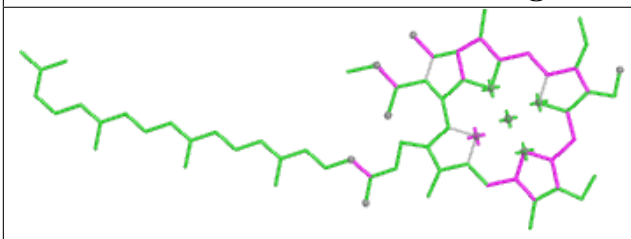


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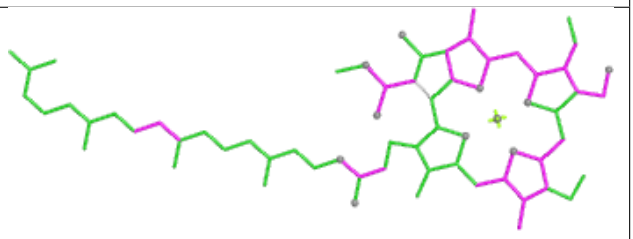


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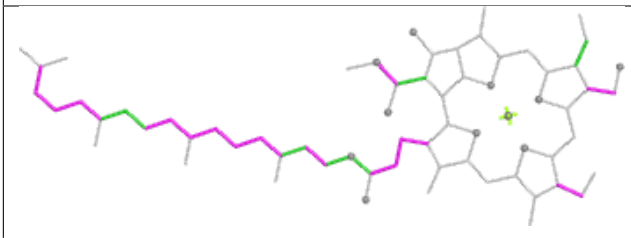
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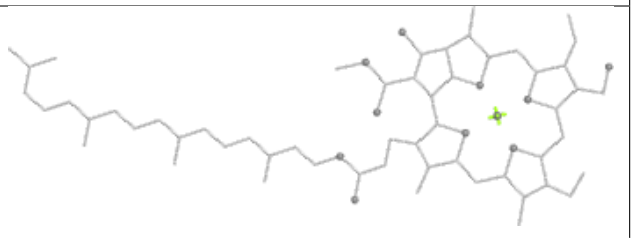
Bond lengths



Bond angles

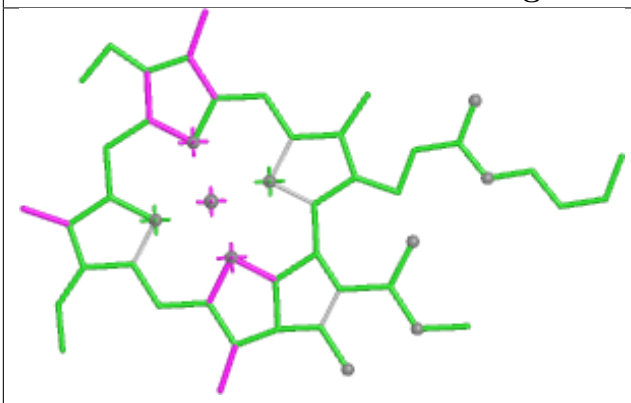


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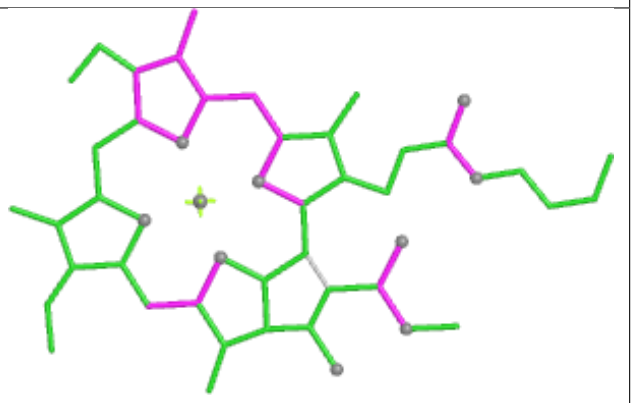


Rings

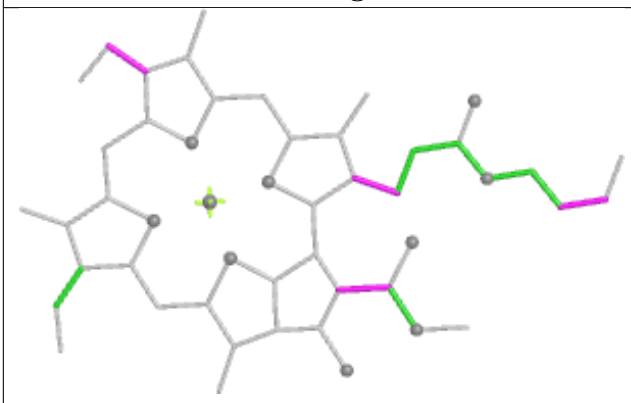
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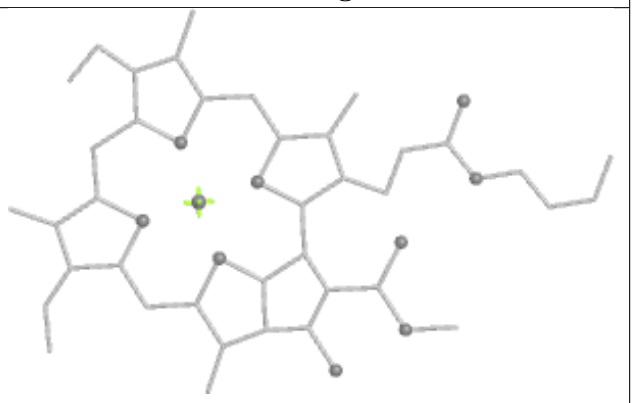
Bond lengths



Bond angles

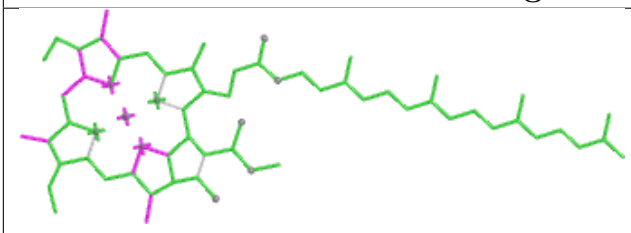


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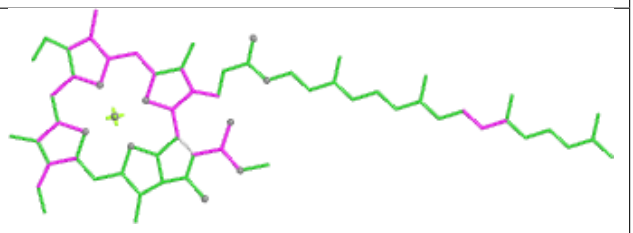


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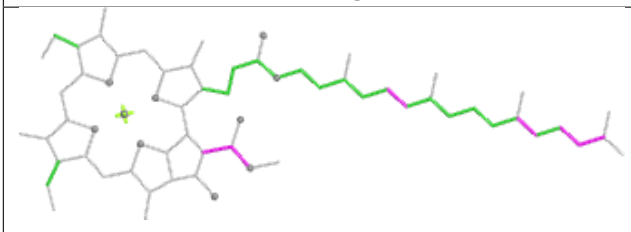
Ligand CLA B 616



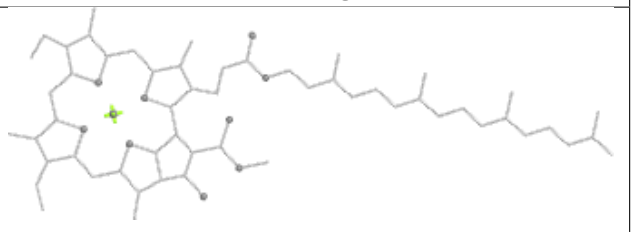
Bond lengths



Bond angles

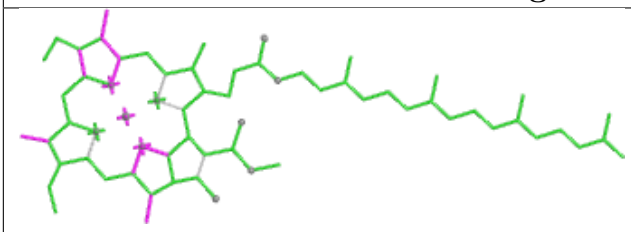


Torsions

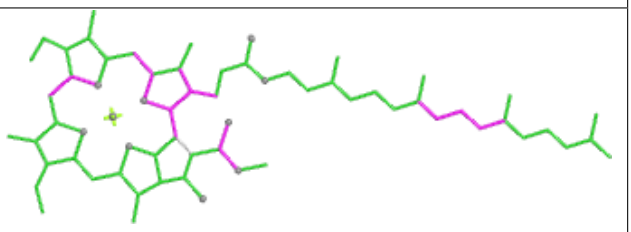


Rings

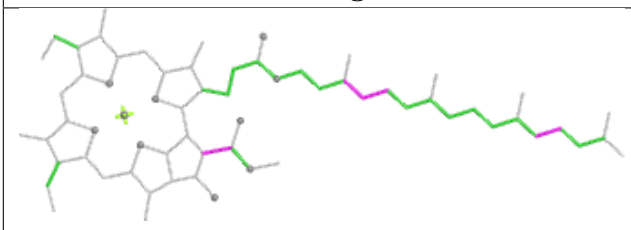
Ligand CLA c 509



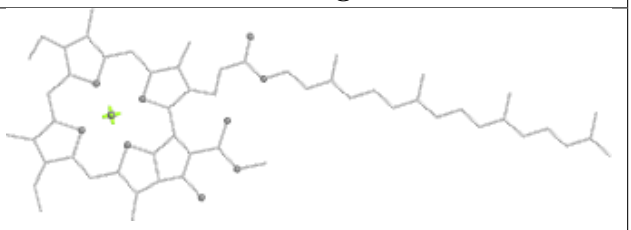
Bond lengths



Bond angles

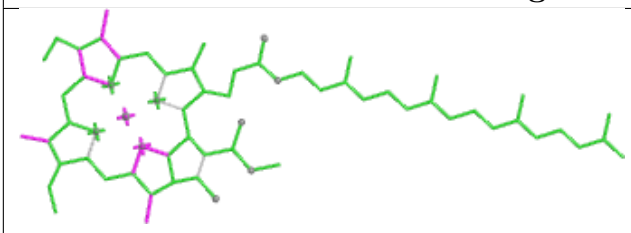


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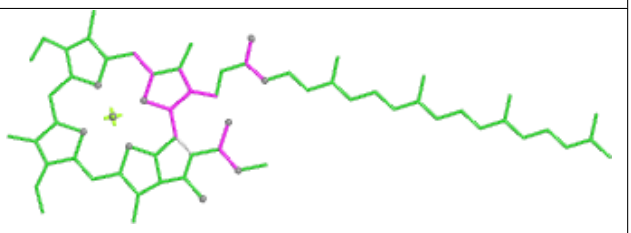


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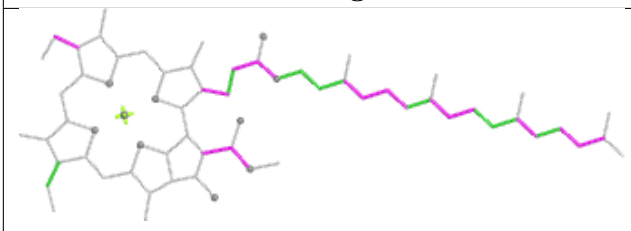
Ligand CLA 9 603



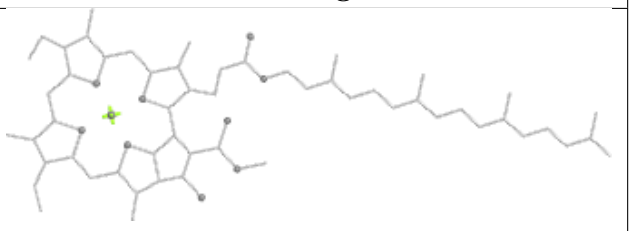
Bond lengths



Bond angles

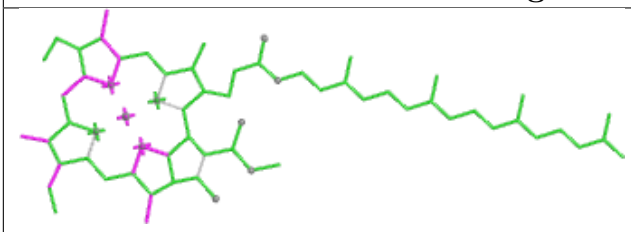


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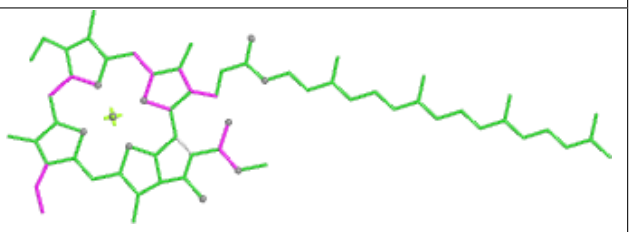


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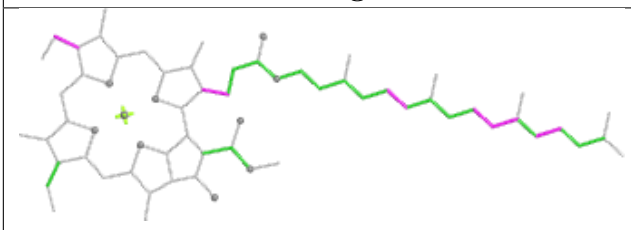
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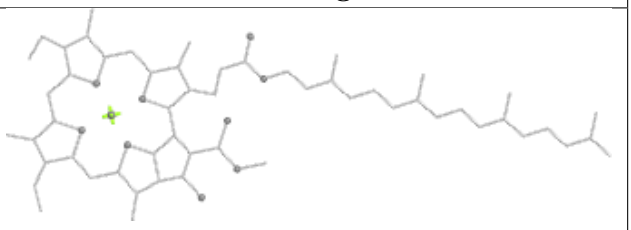
Bond lengths



Bond angles

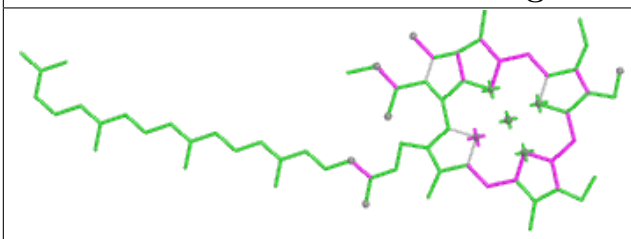


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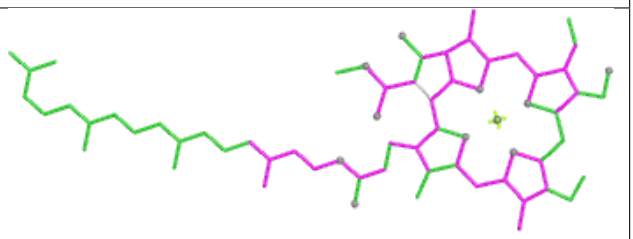


Rings

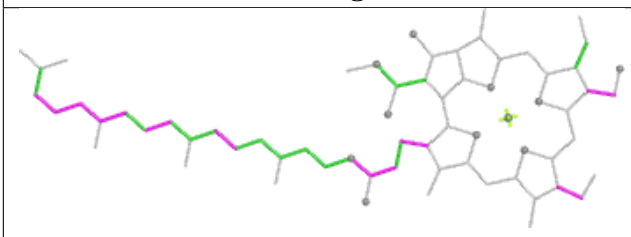
Ligand CHL n 607



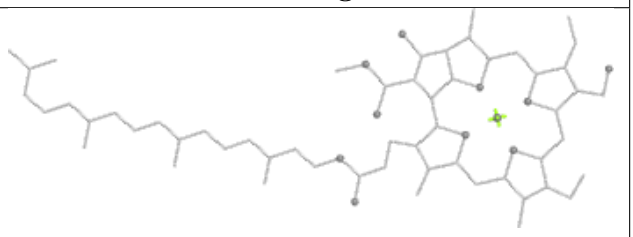
Bond lengths



Bond angles

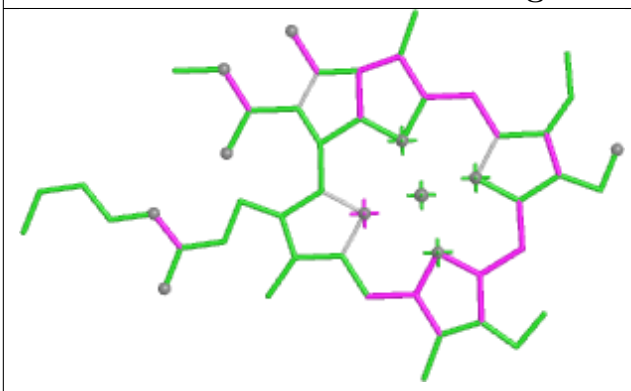


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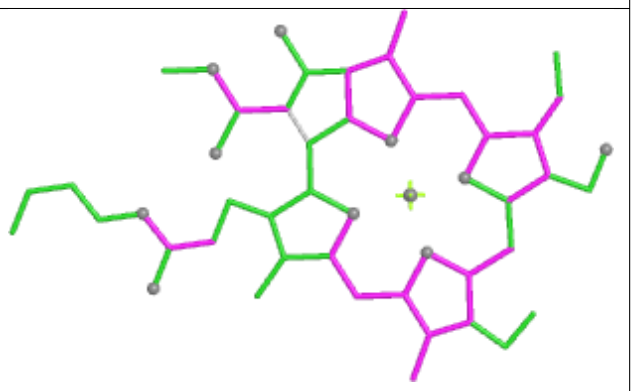


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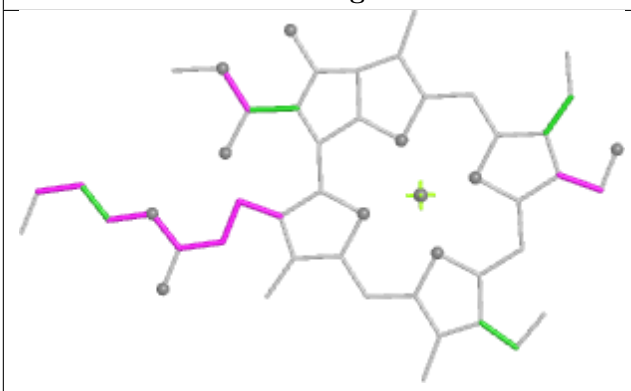
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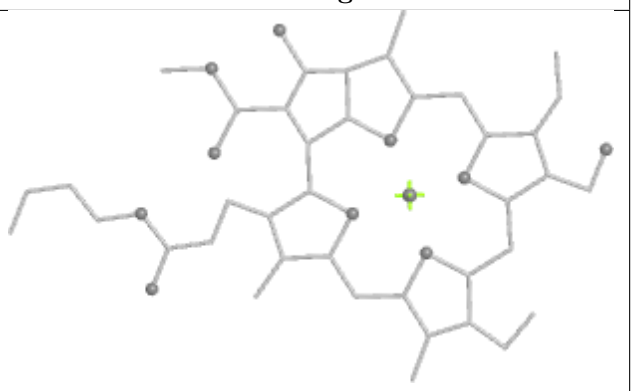
Bond lengths



Bond angles

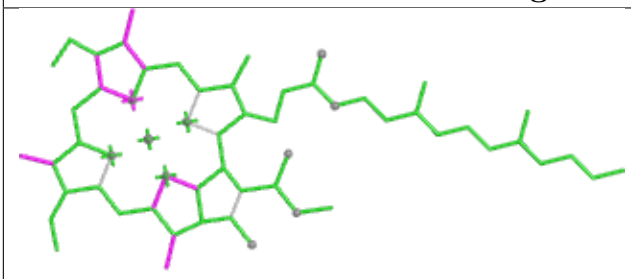


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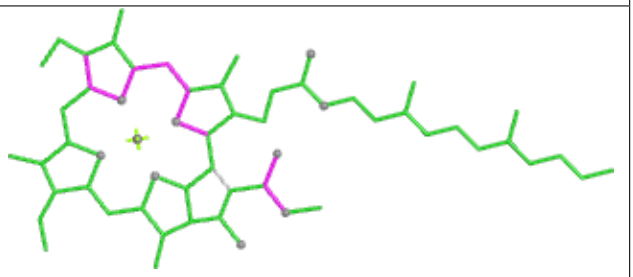


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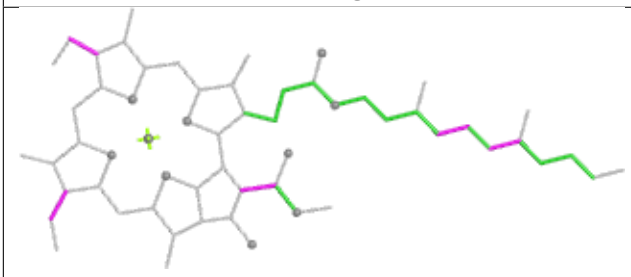
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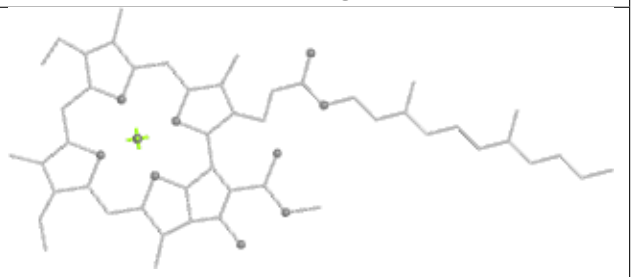
Bond lengths



Bond angles

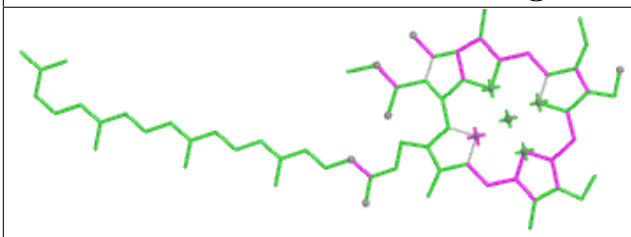


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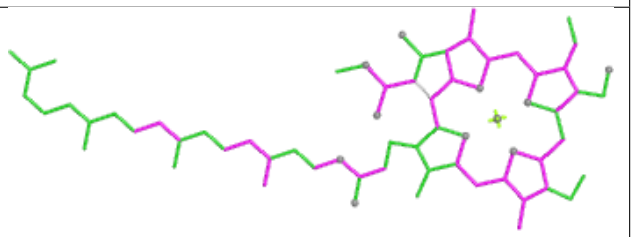


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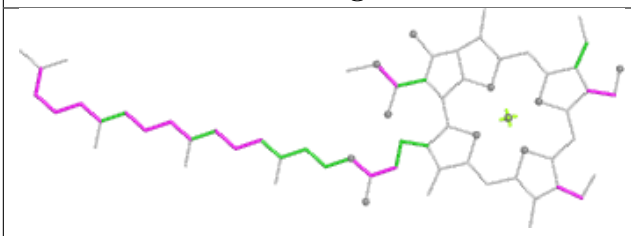
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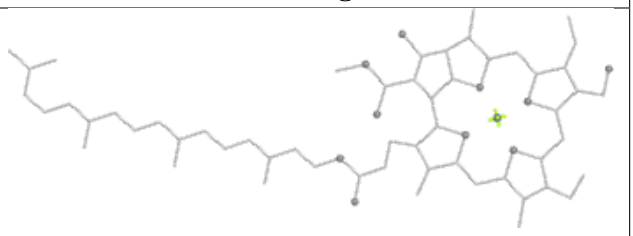
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Bond angles

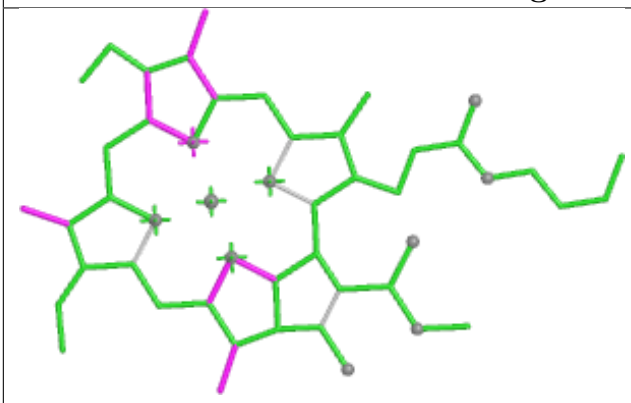


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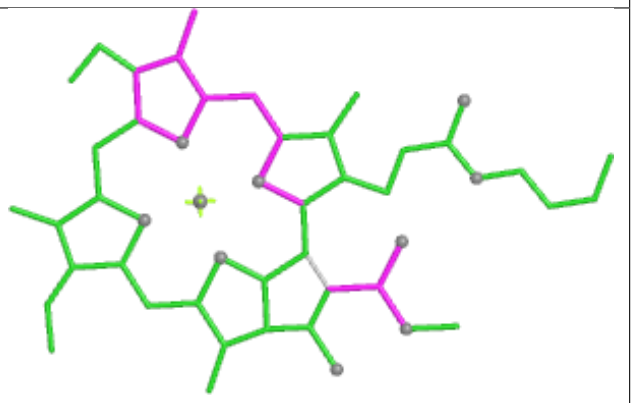


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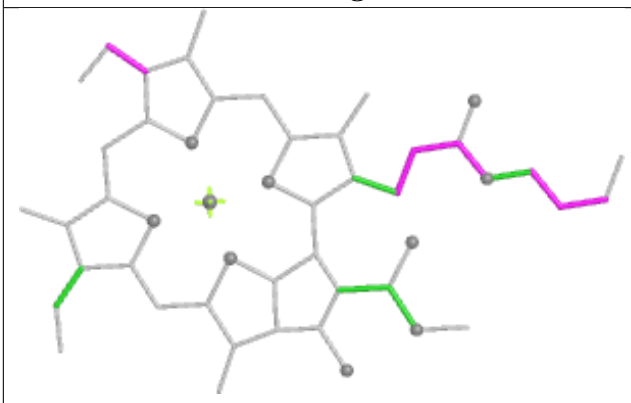
Ligand CLA s 602



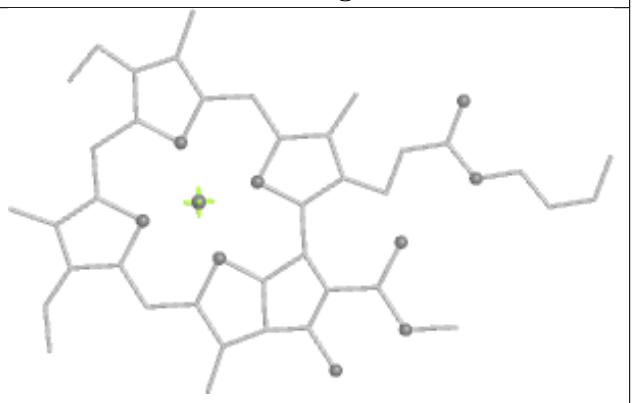
Bond lengths



Bond angles

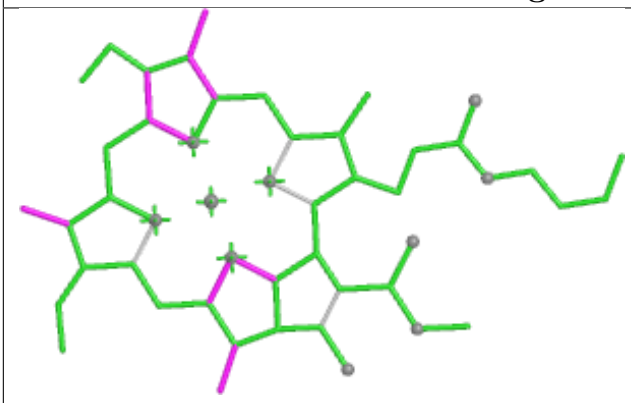


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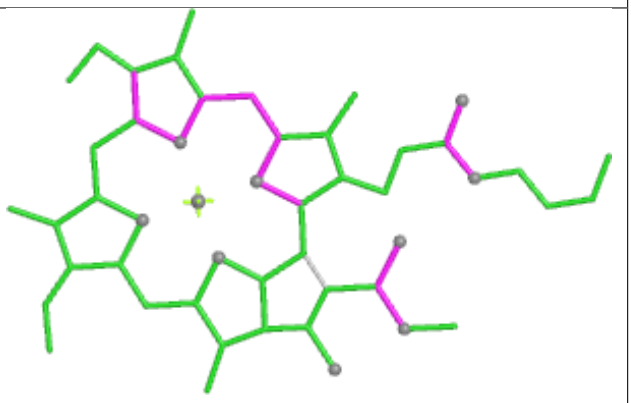


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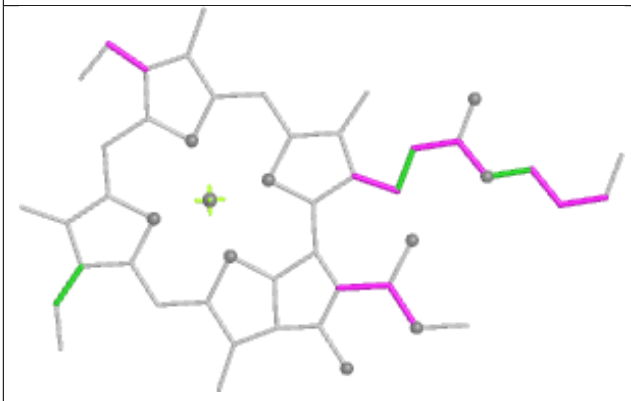
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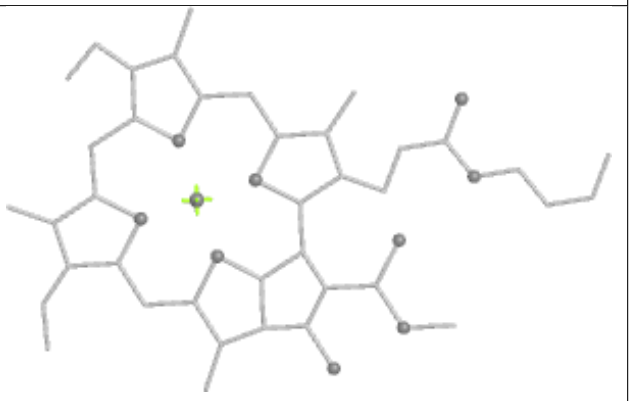
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Bond angles

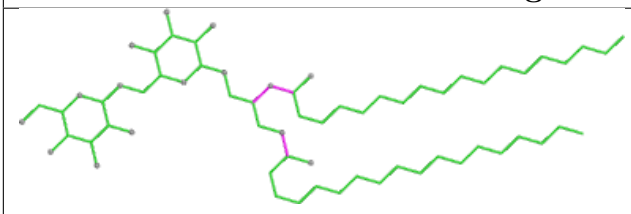


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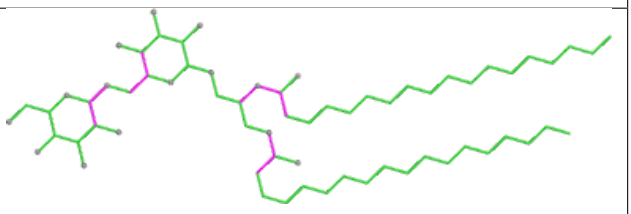


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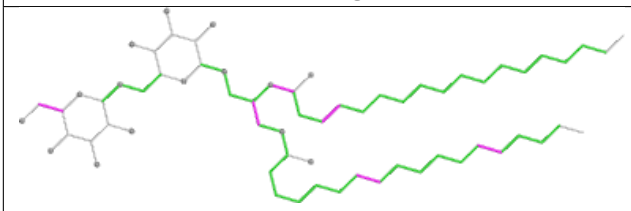
Ligand DGD c 524



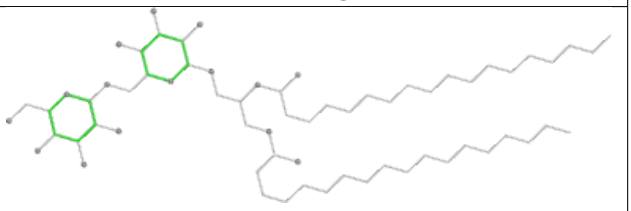
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Bond angles

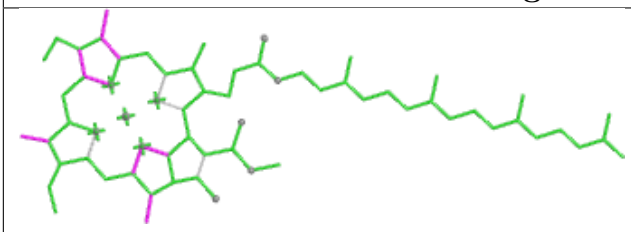


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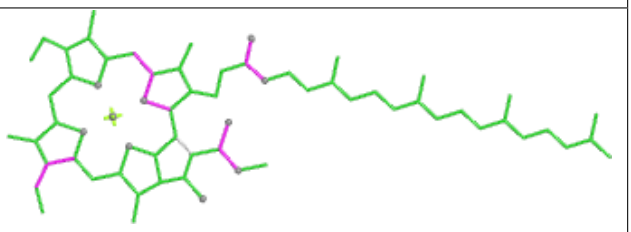


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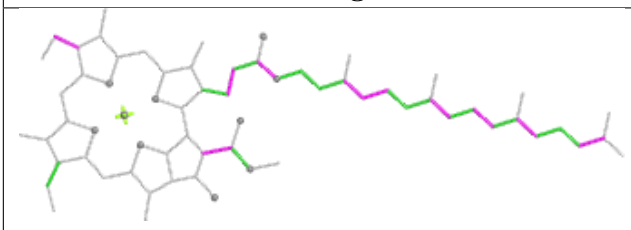
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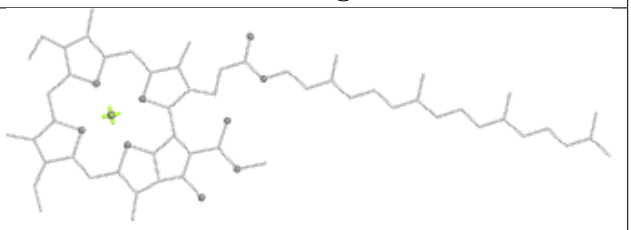
Bond lengths



Bond angles

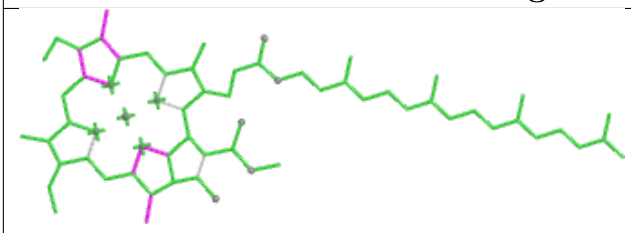


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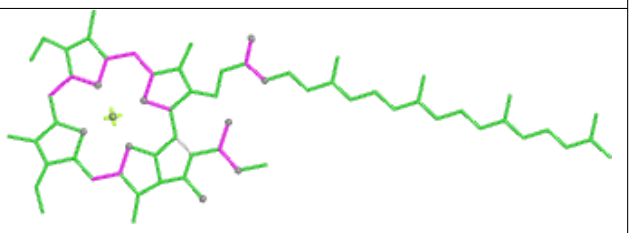


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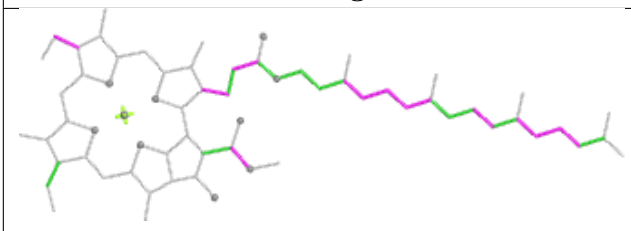
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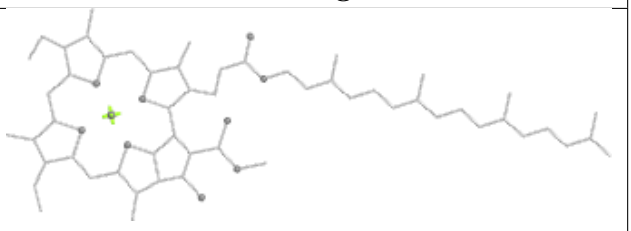
Bond lengths



Bond angles

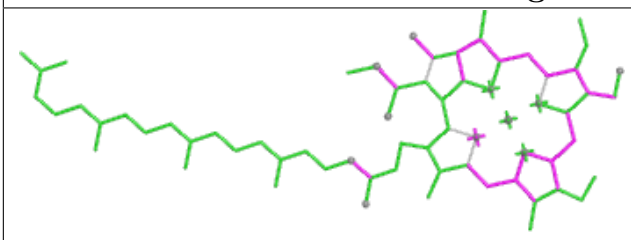


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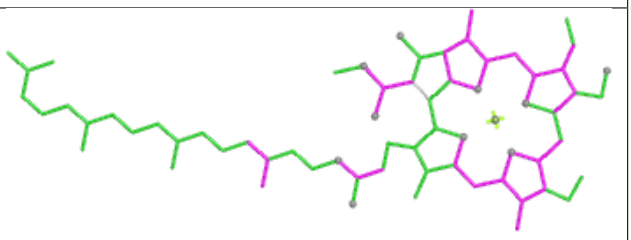


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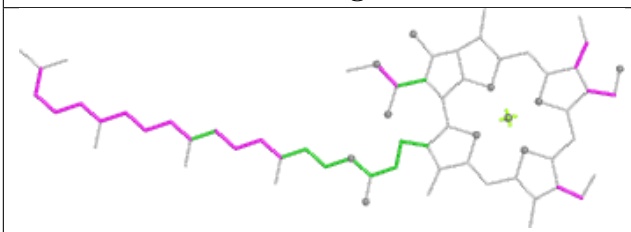
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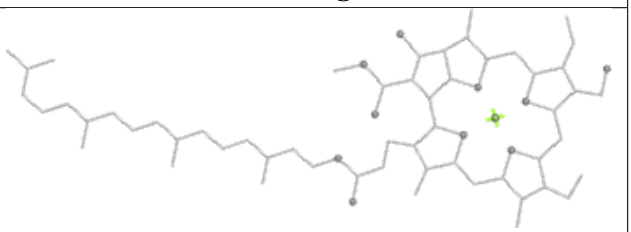
Bond lengths



Bond angles

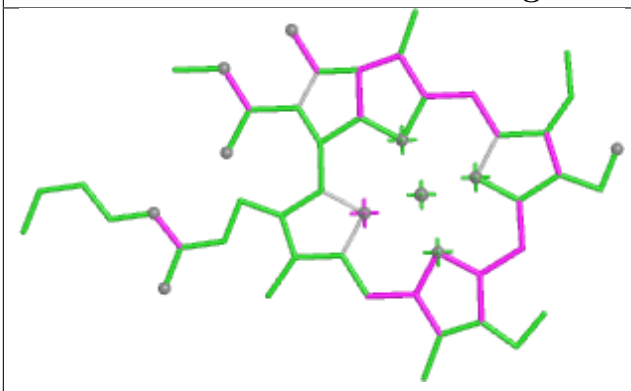


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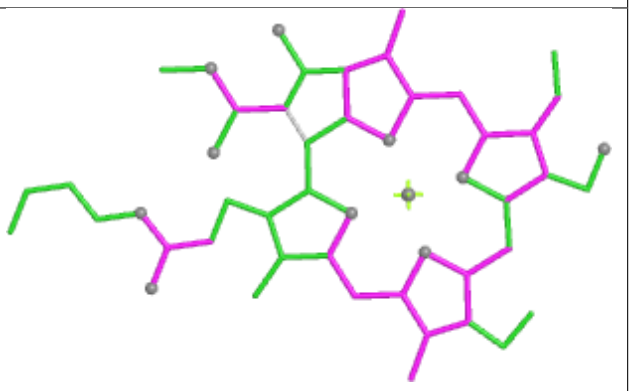


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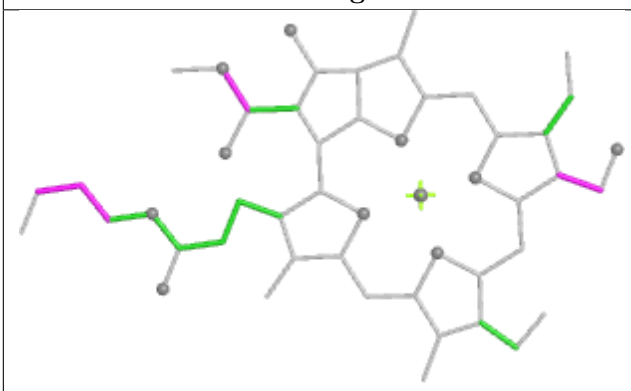
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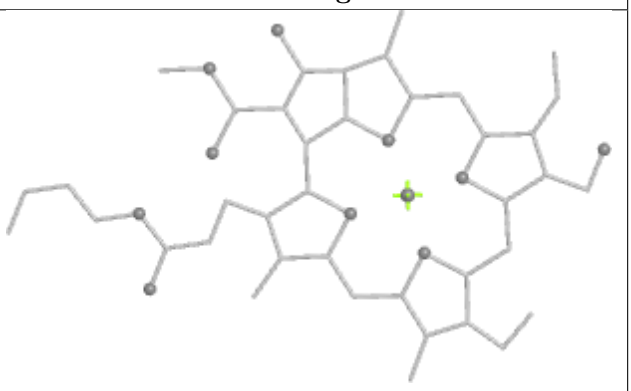
Bond lengths



Bond angles

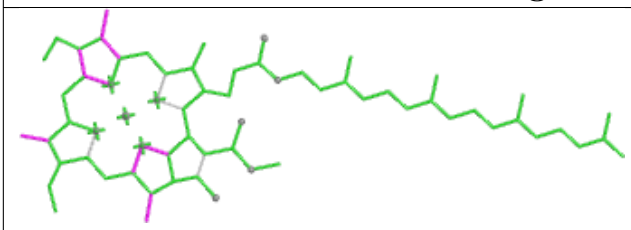


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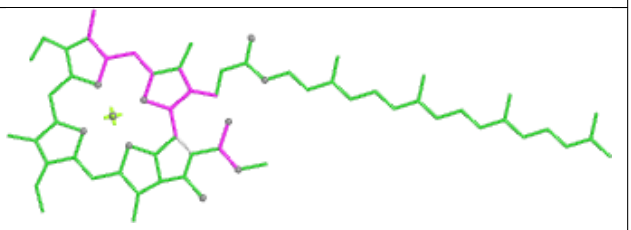


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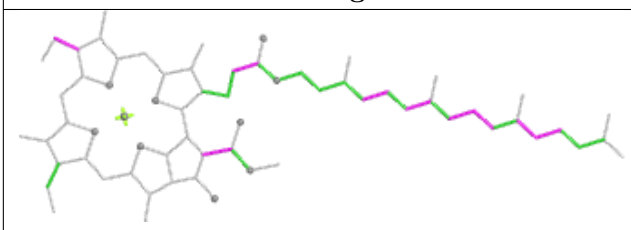
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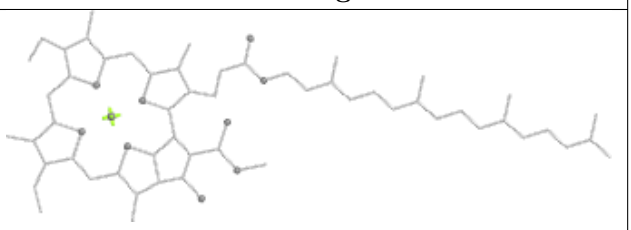
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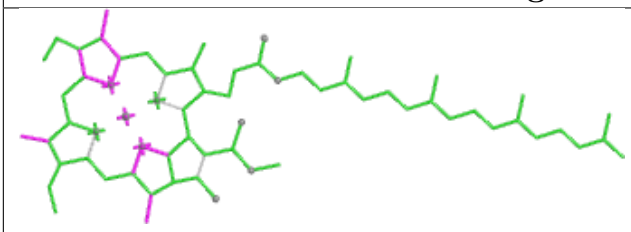


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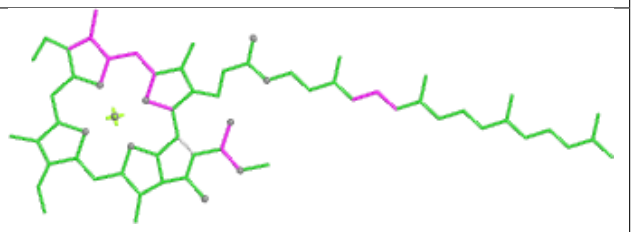


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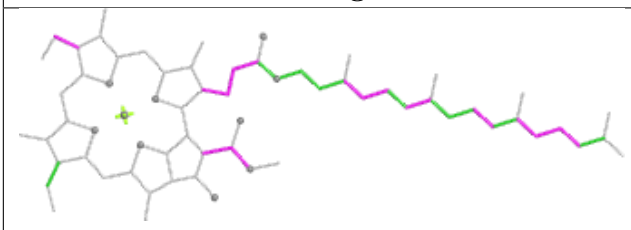
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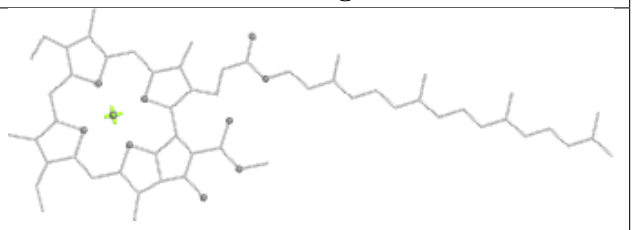
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Bond angles



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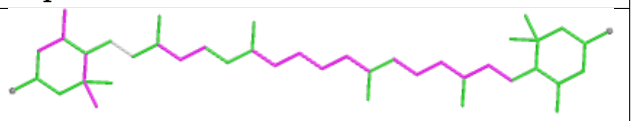


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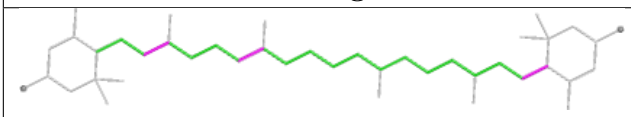
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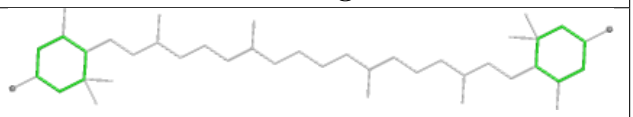
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Bond angles

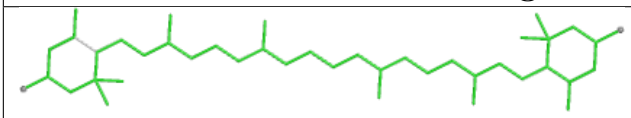


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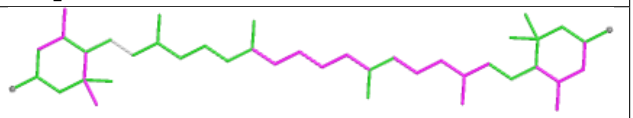


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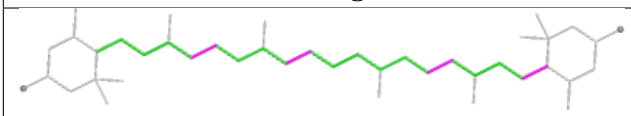
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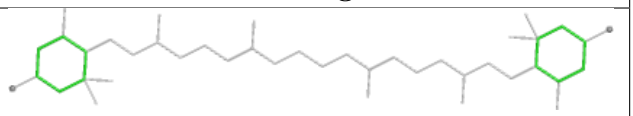
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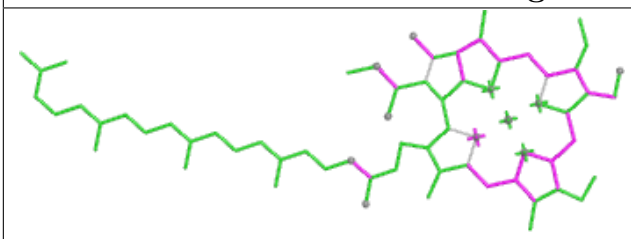


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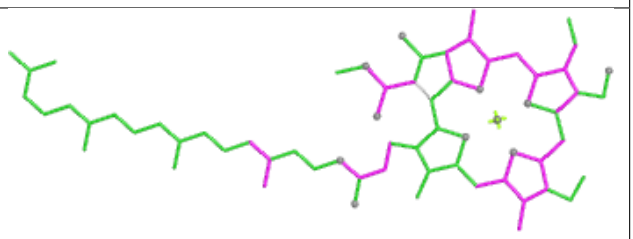


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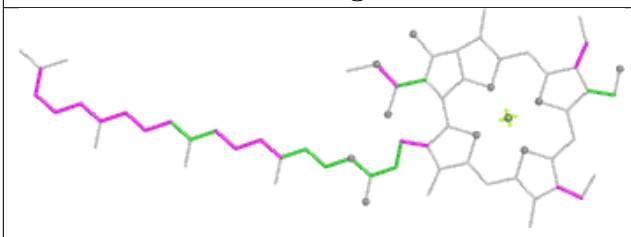
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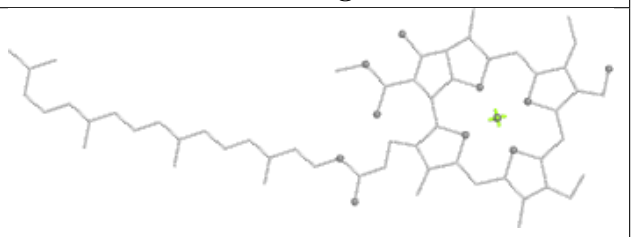
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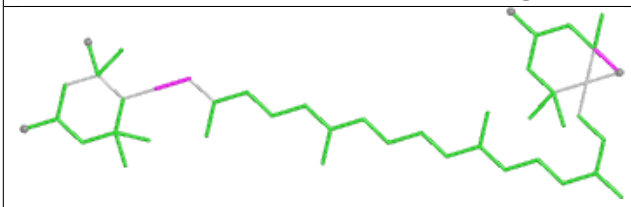


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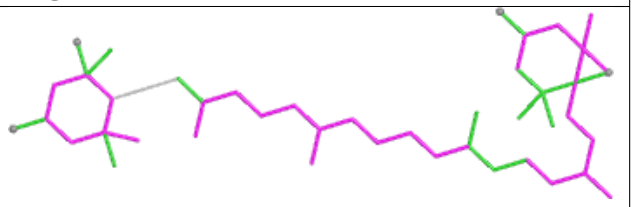


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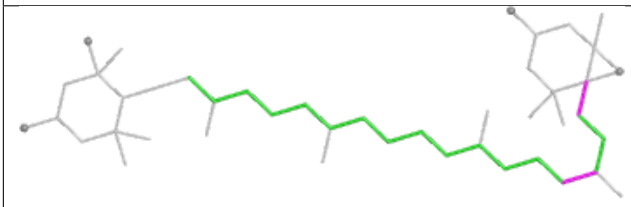
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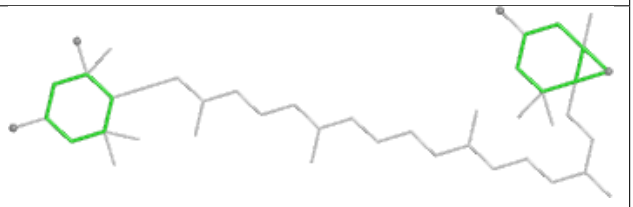
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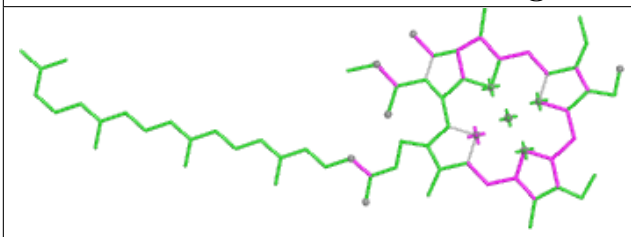


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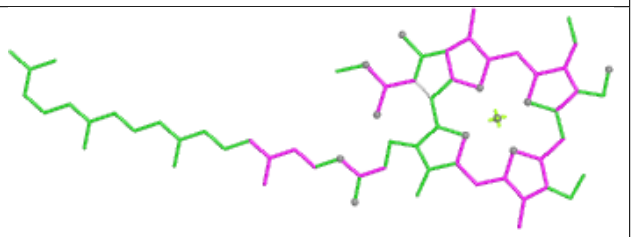


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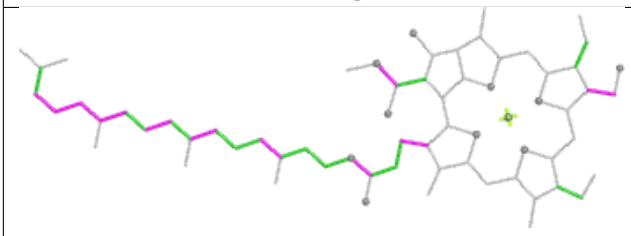
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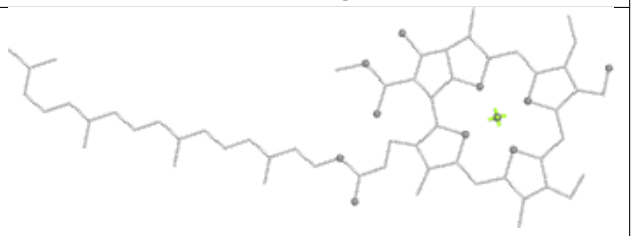
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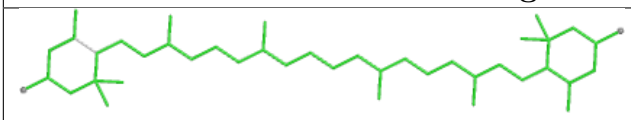


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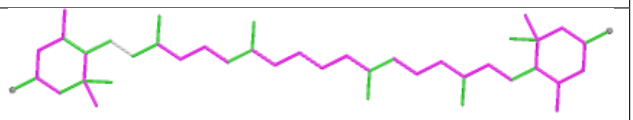


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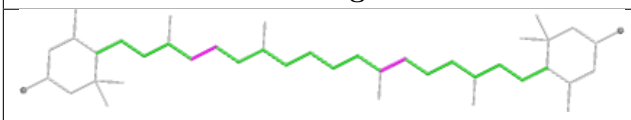
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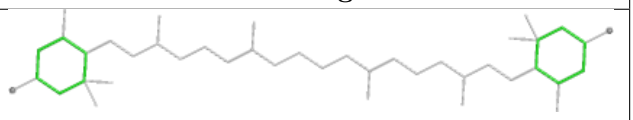
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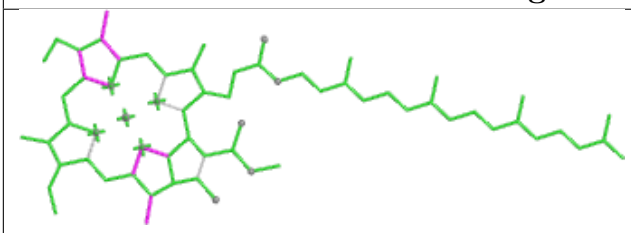


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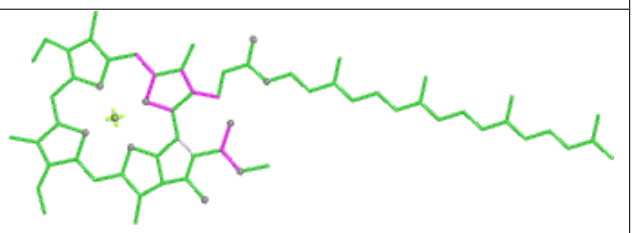


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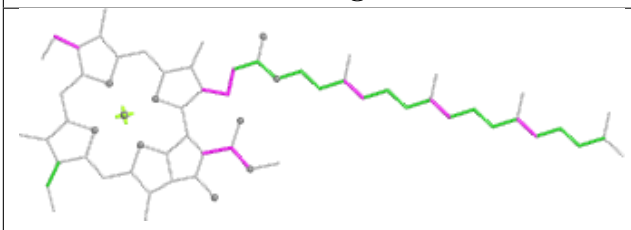
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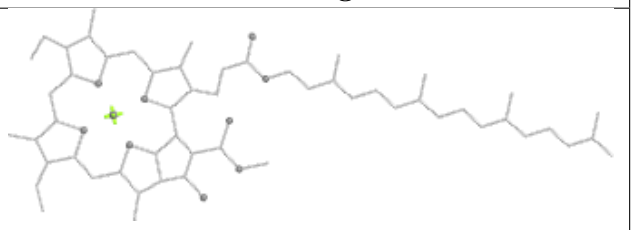
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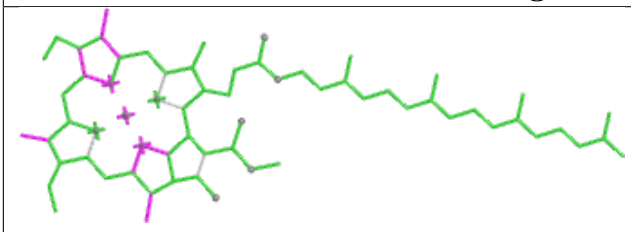


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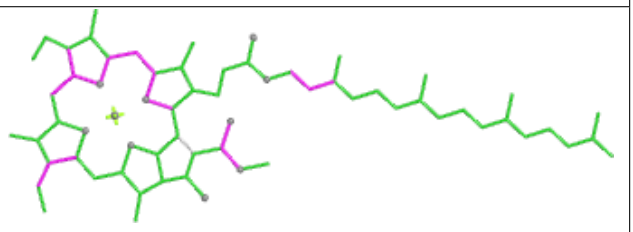


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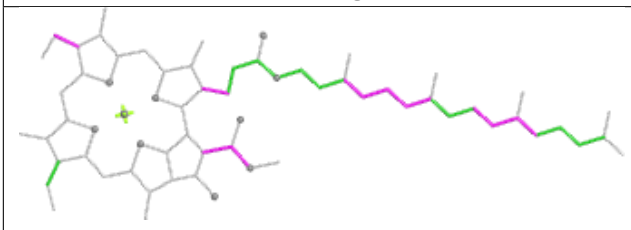
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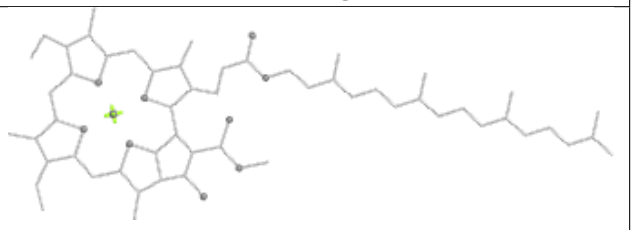
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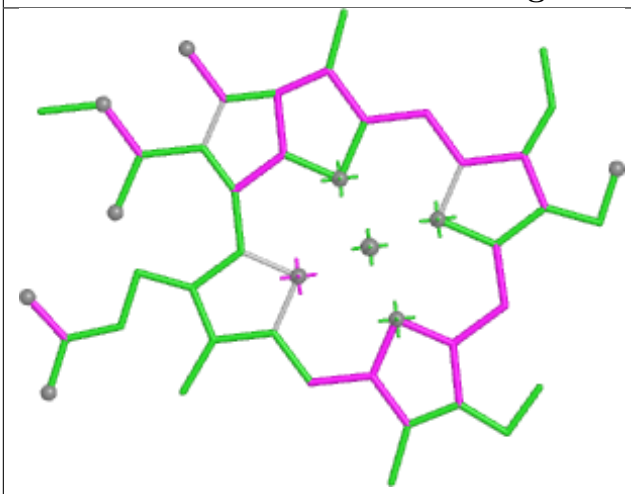


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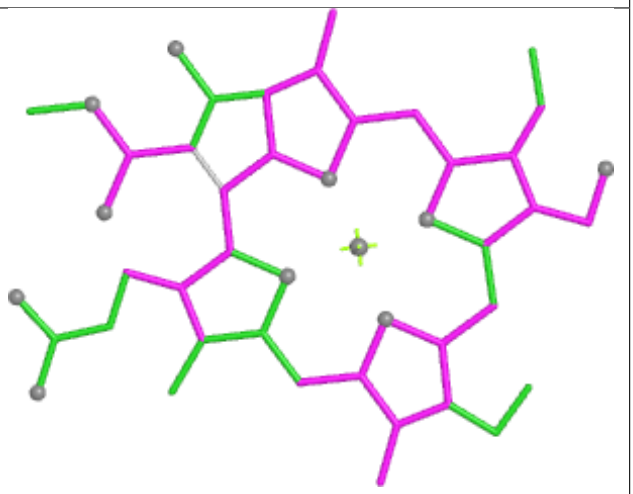


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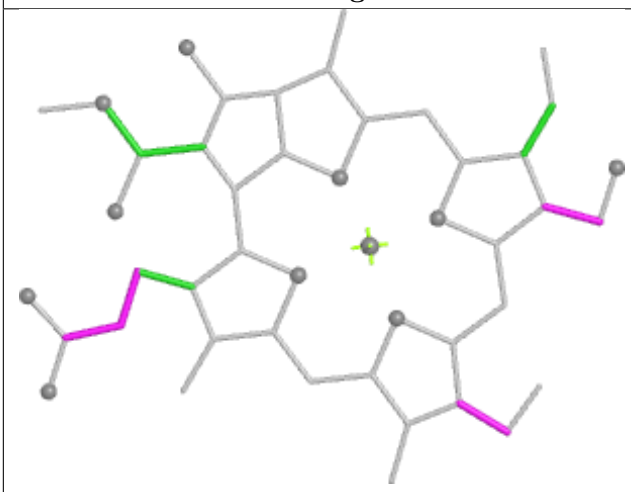
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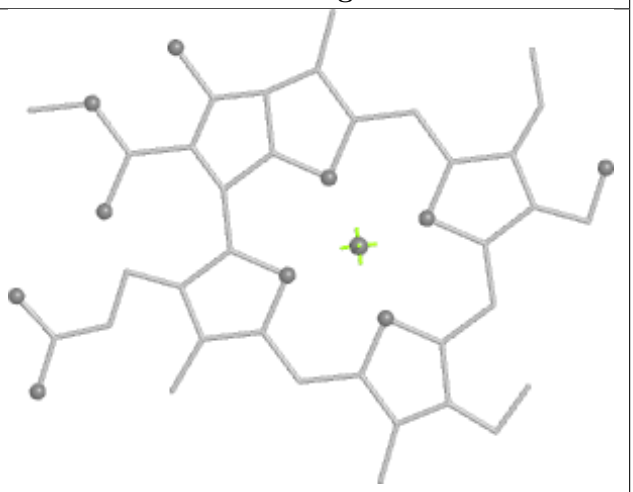
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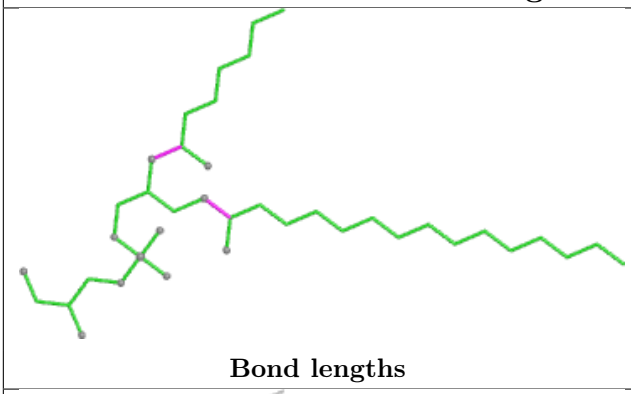


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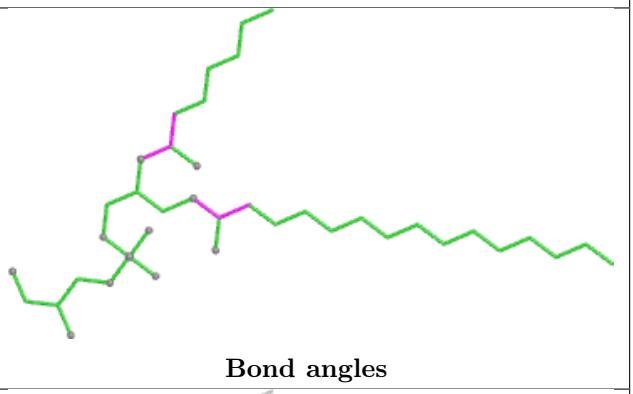


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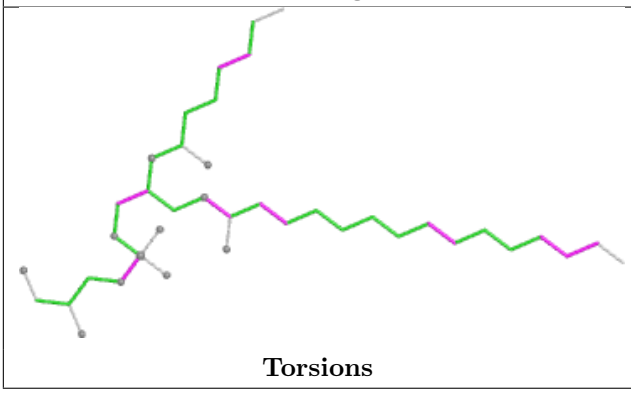
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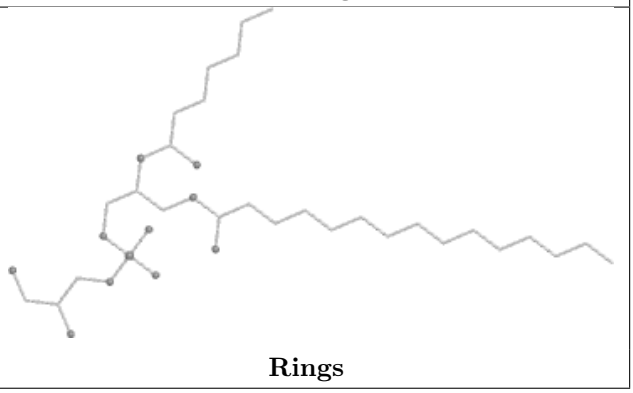
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Bond angles

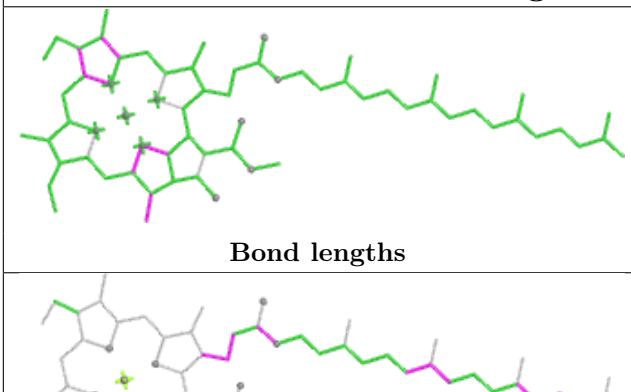


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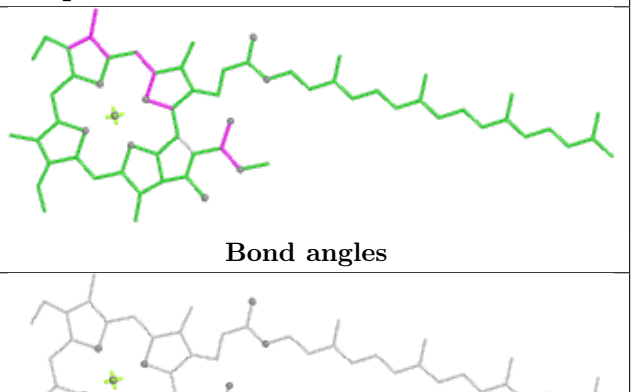


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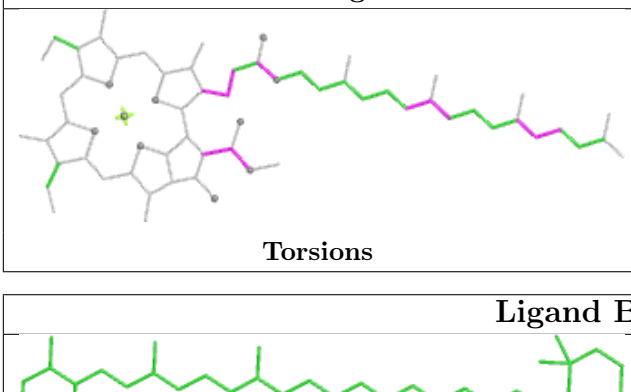
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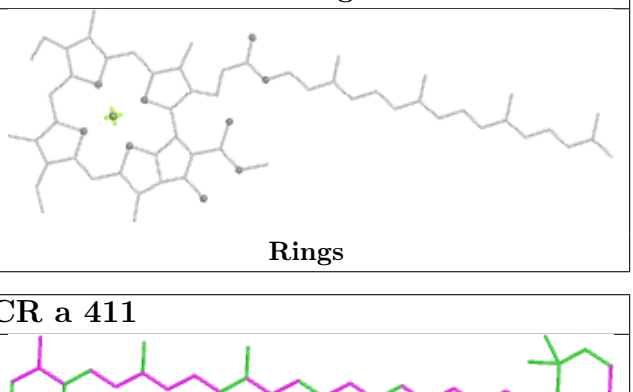
Bond lengths



Bond angles

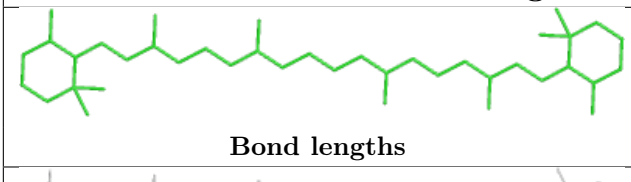


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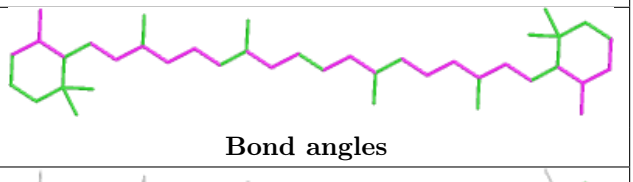


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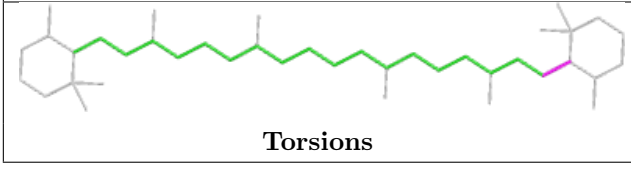
Ligand BCR a 411



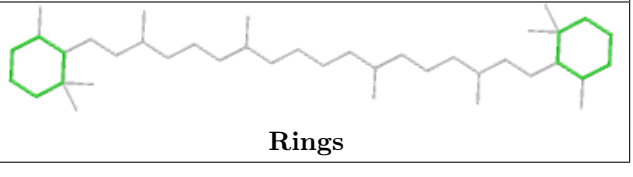
Bond lengths



Bond angles

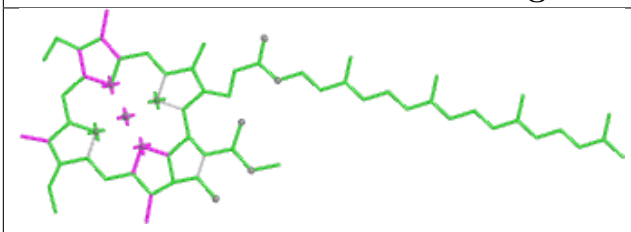


Torsions

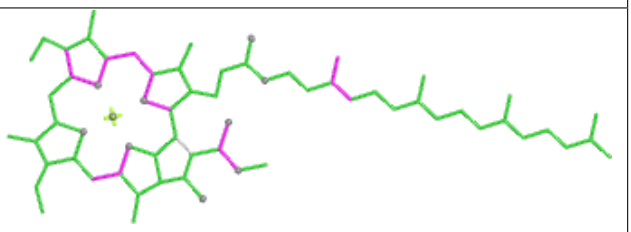


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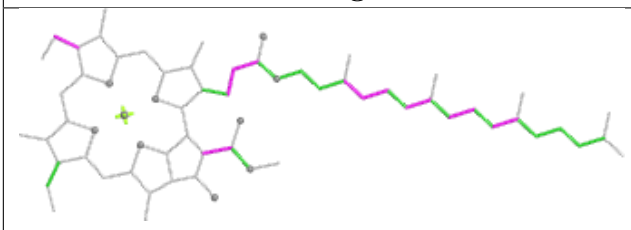
Ligand CLA 7 602



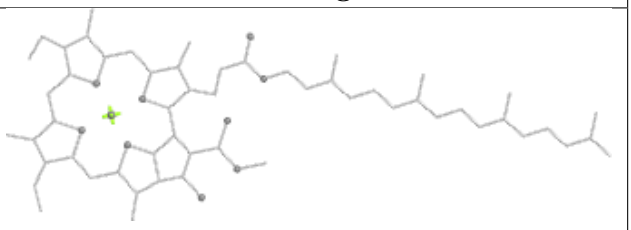
Bond lengths



Bond angles

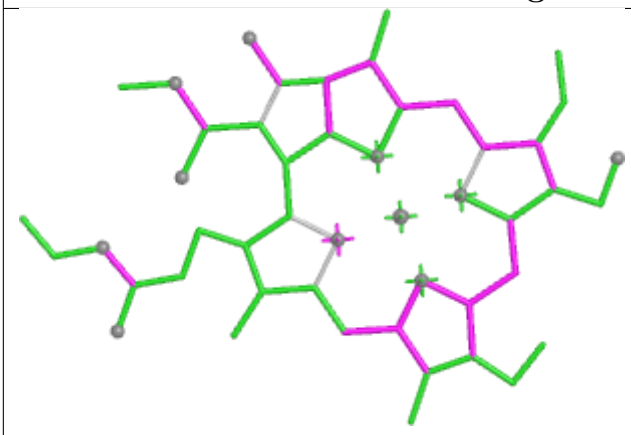


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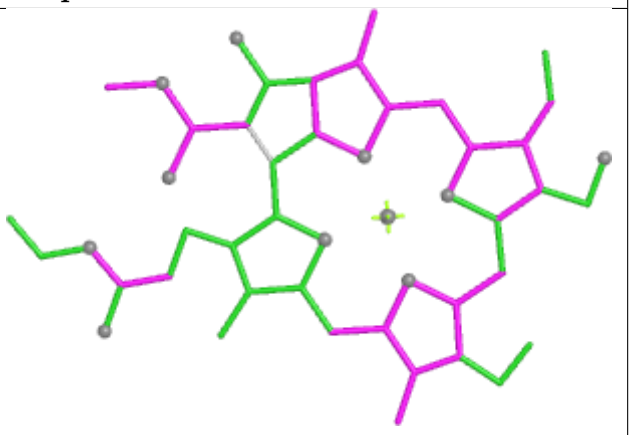


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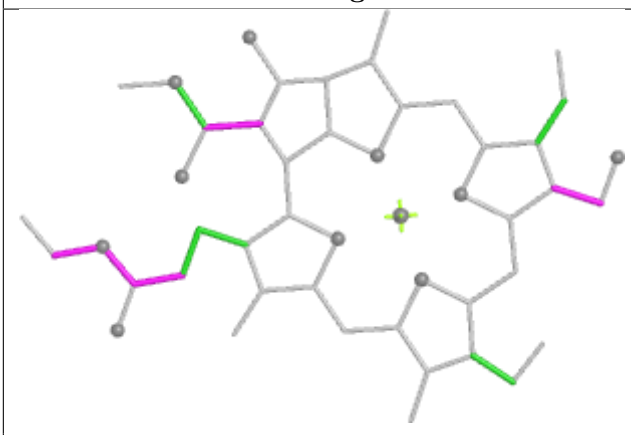
Ligand CHL q 605



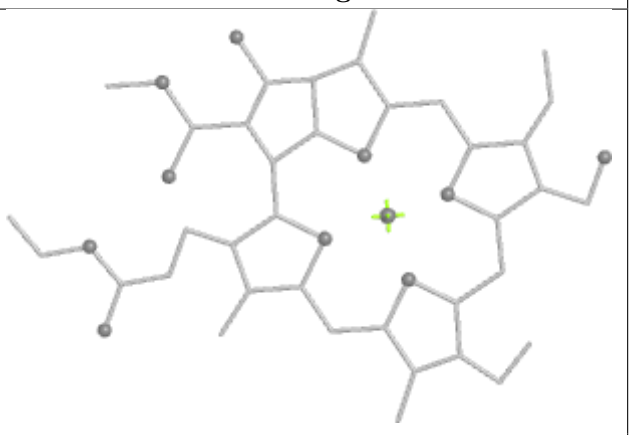
Bond lengths



Bond angles

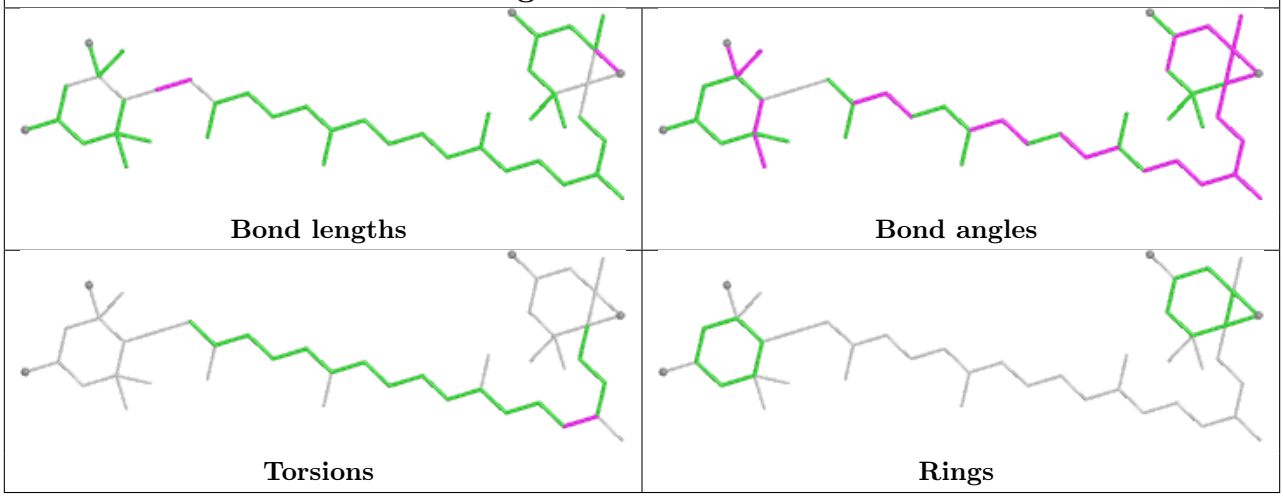


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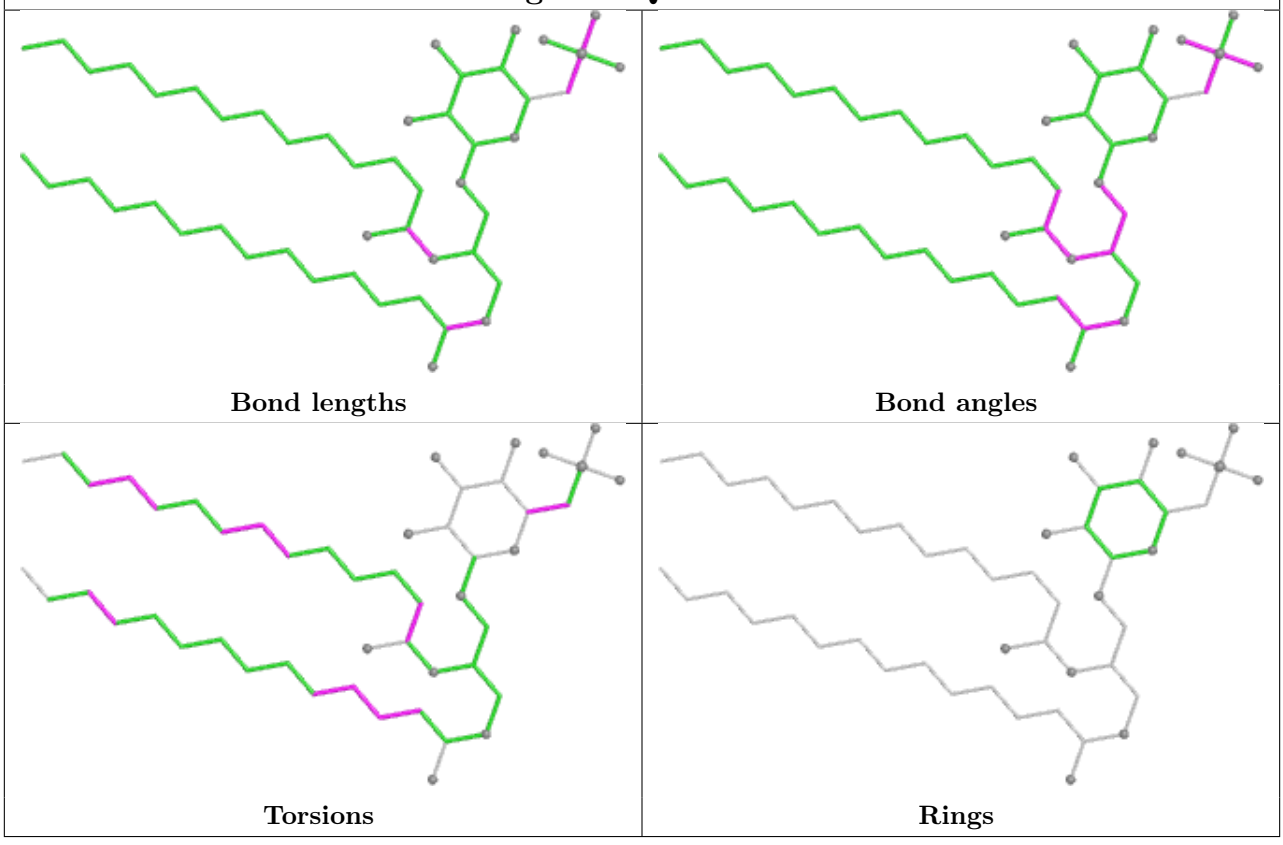


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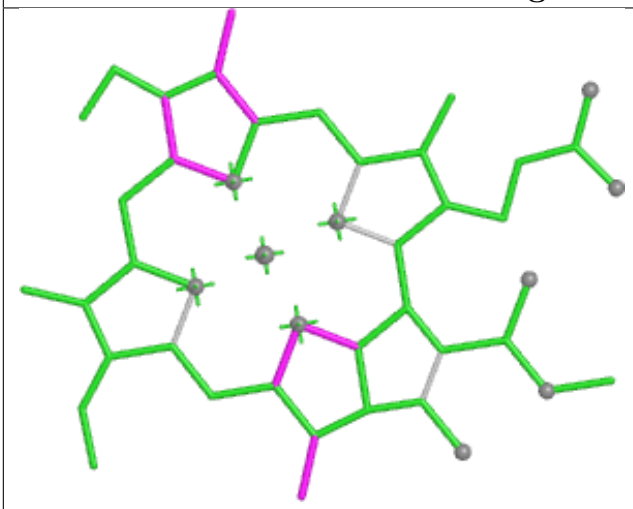
Ligand NEX n 1623



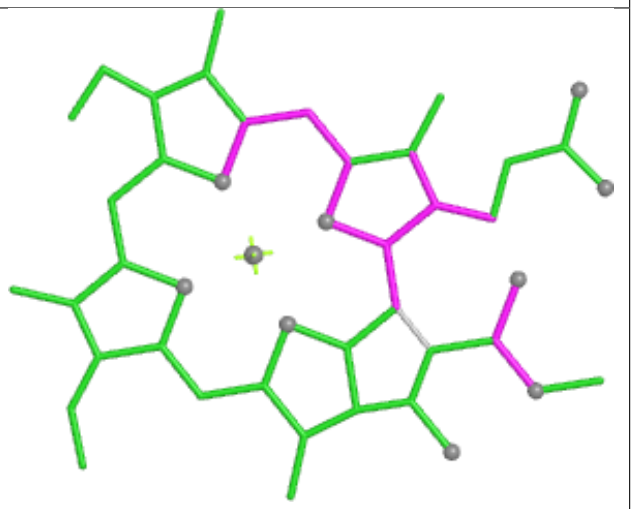
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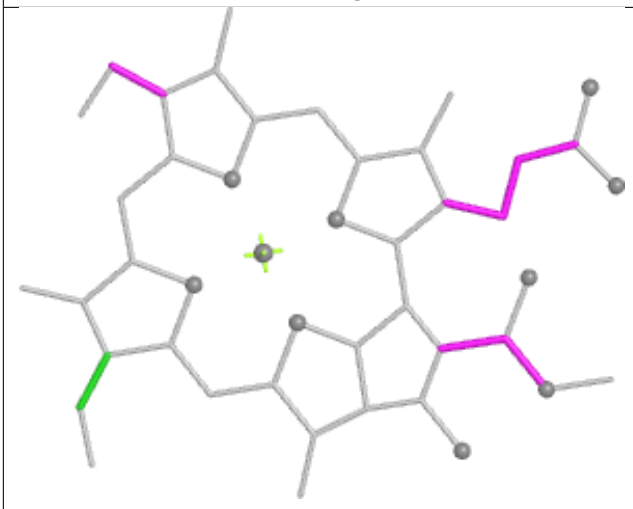
Ligand CLA 3 612



Bond lengths



Bond angles

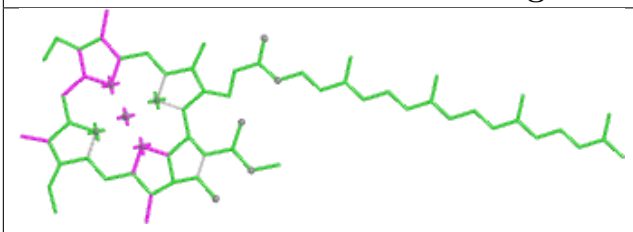


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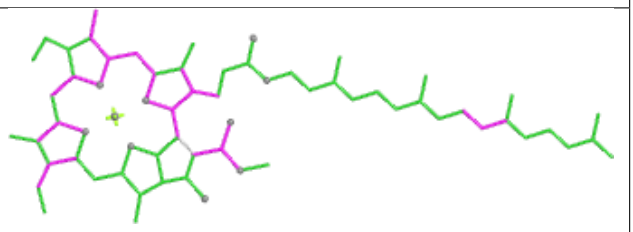


Rings

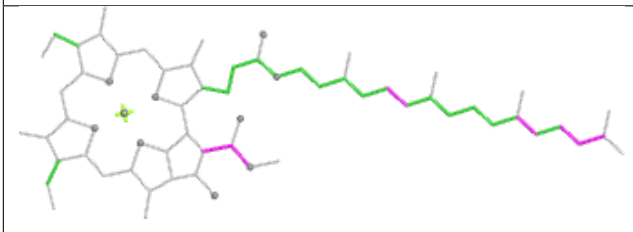
Ligand CLA b 616



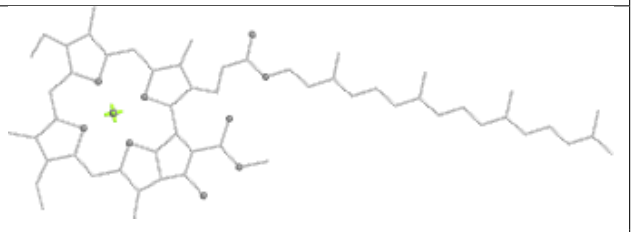
Bond lengths



Bond angles

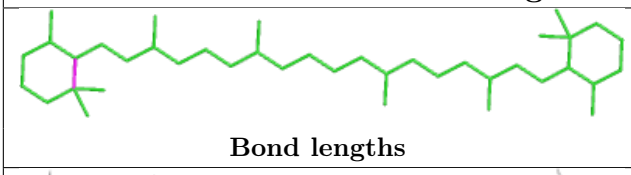


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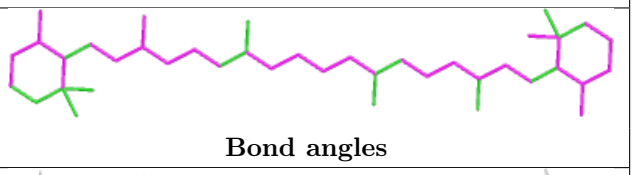


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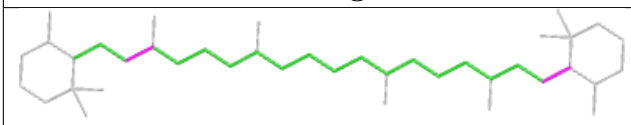
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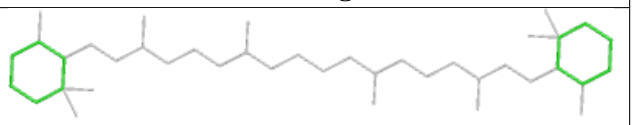
Bond lengths



Bond angles

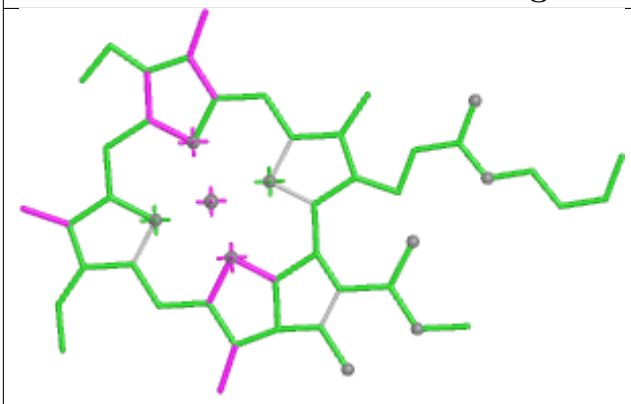


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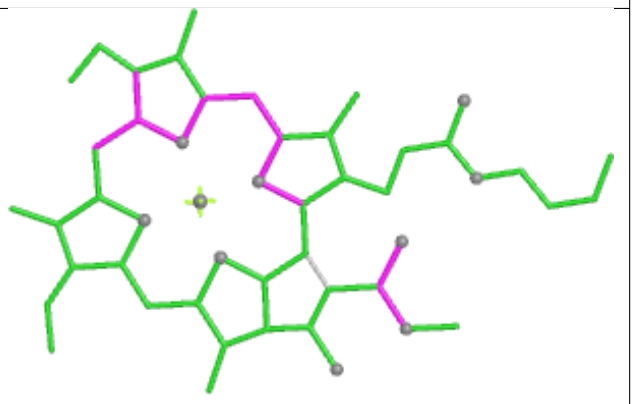


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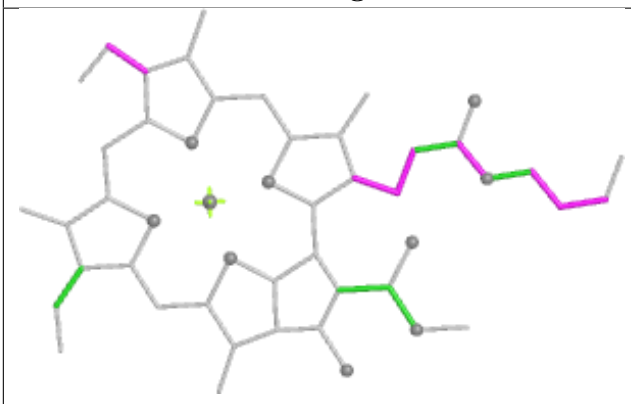
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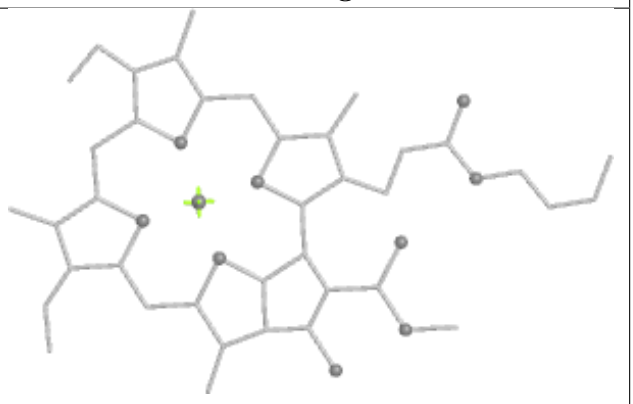
Bond lengths



Bond angles

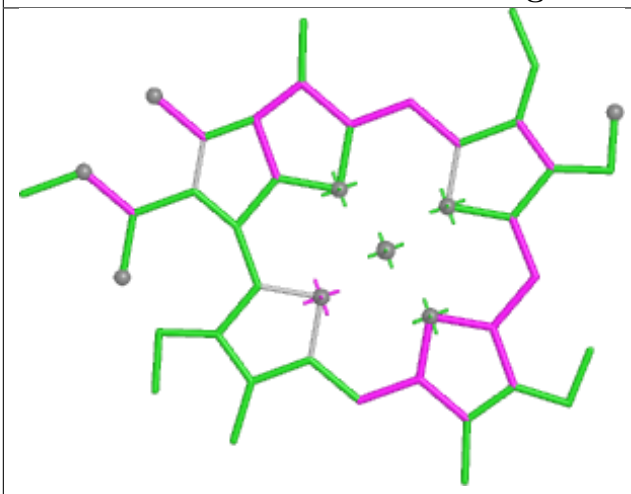


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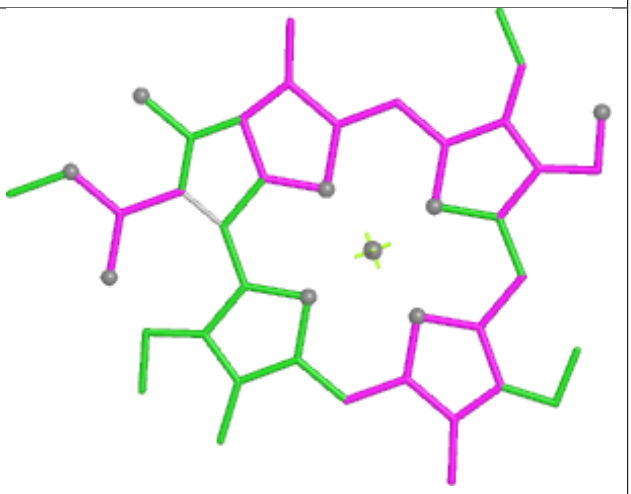


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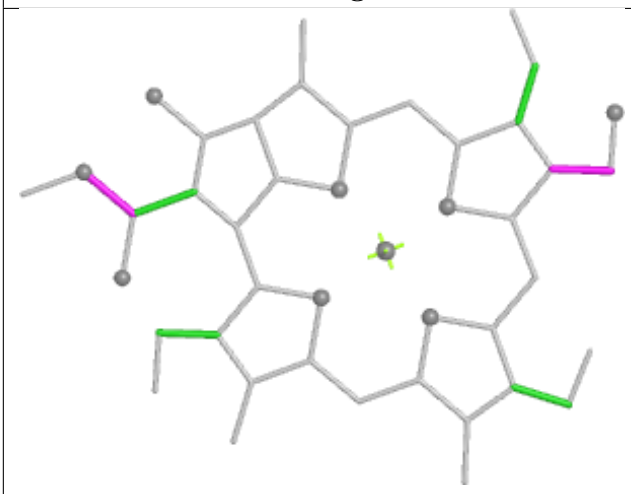
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Bond lengths



Bond angles

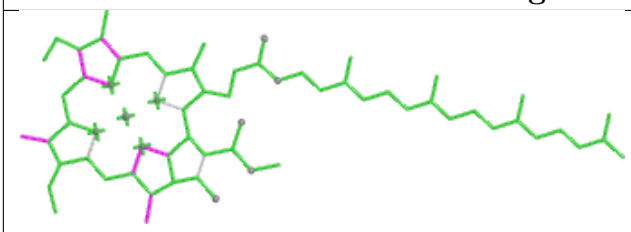


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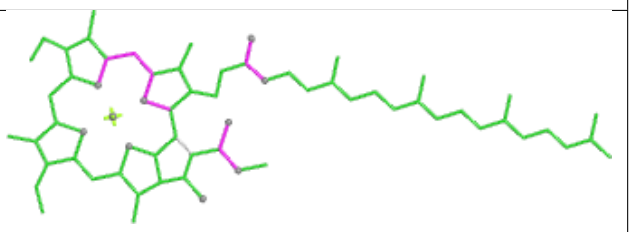


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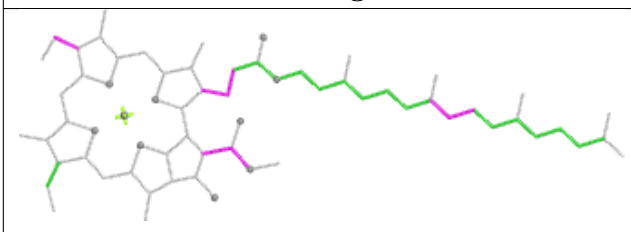
Ligand CLA 5 610



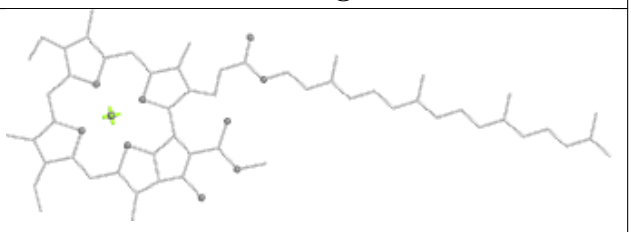
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Bond angles

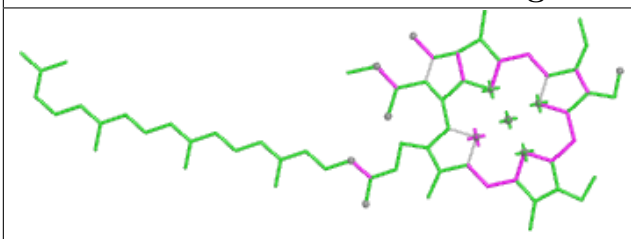


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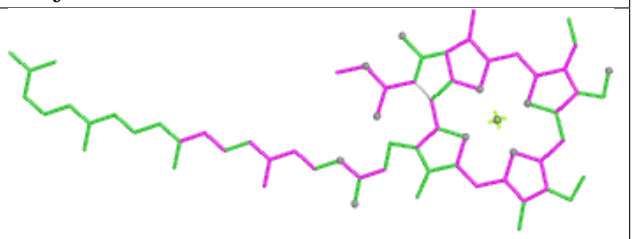


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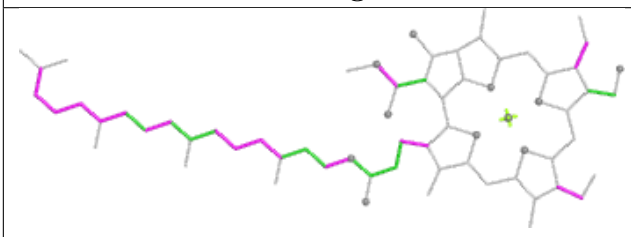
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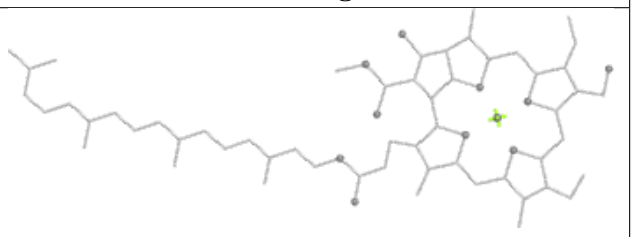
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Bond angles

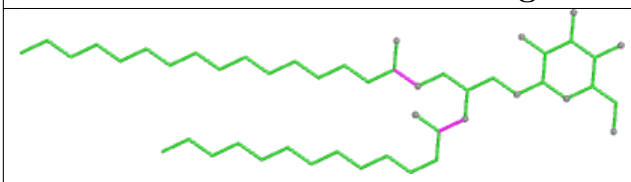


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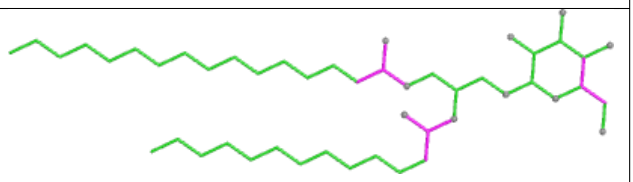


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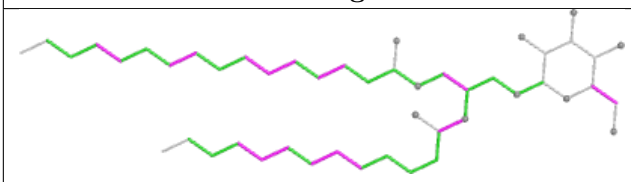
Ligand LMG H 102



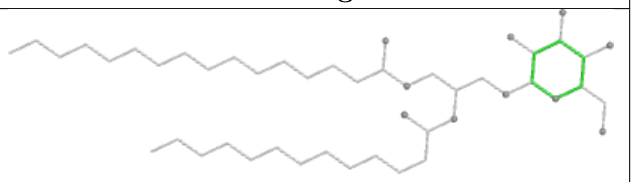
Bond lengths



Bond angles

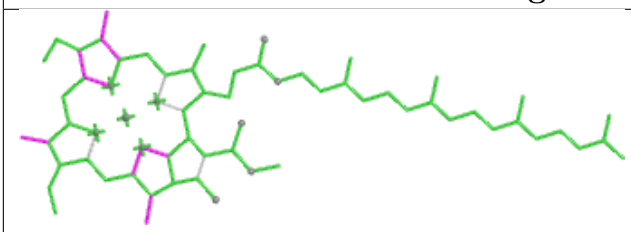


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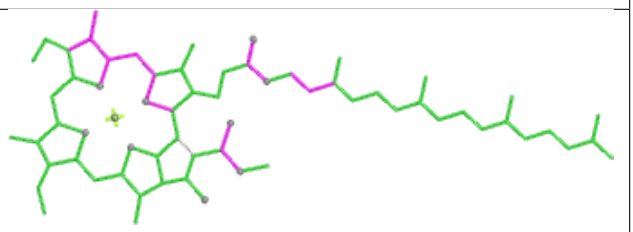


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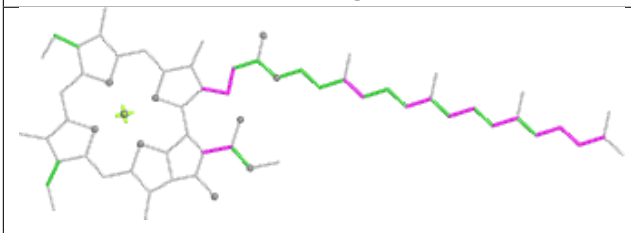
Ligand CLA 1 610



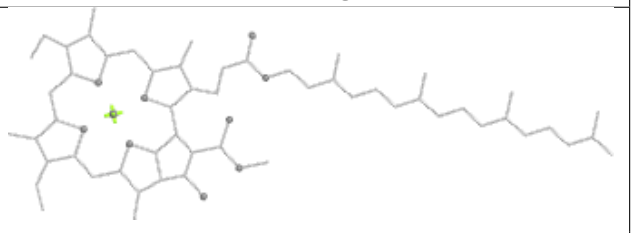
Bond lengths



Bond angles

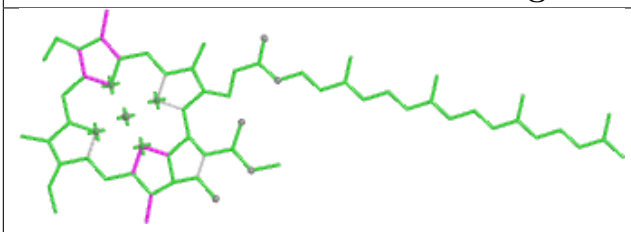


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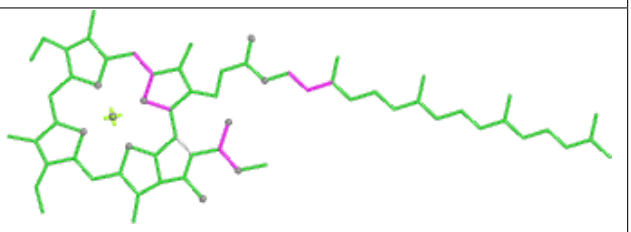


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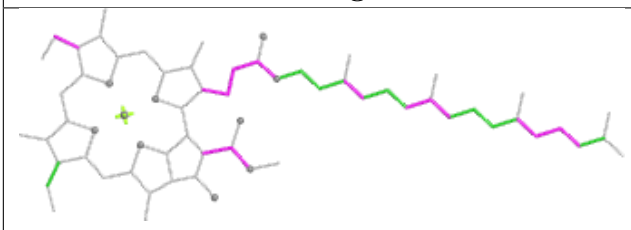
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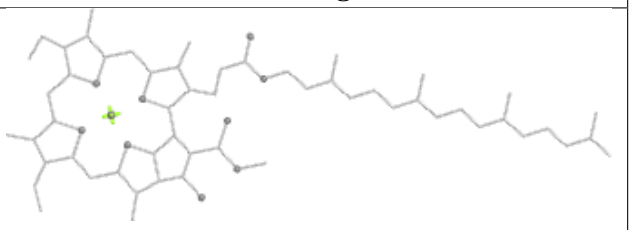
Bond lengths



Bond angles



Torsions

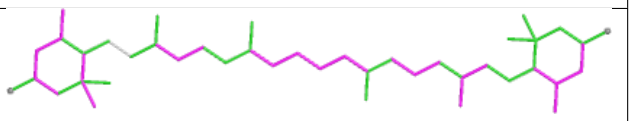


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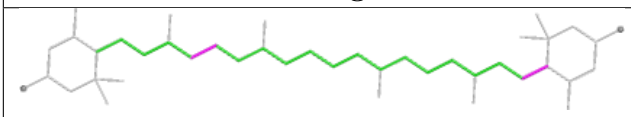
Ligand LUT 7 1621



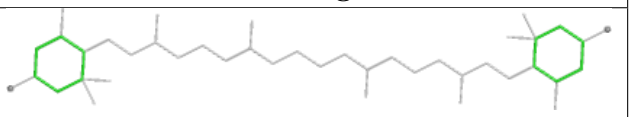
Bond lengths



Bond angles

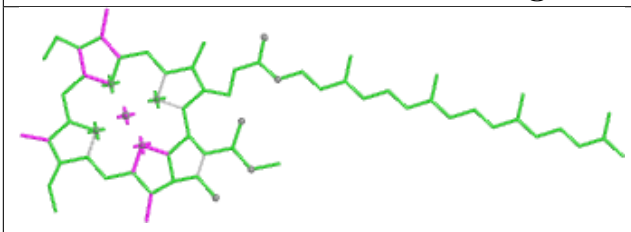


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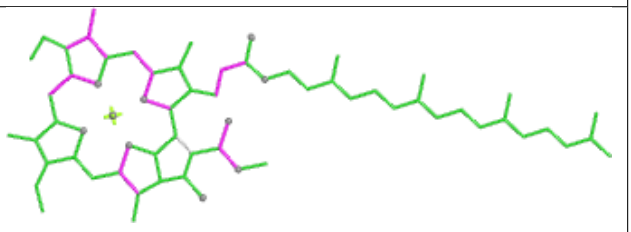


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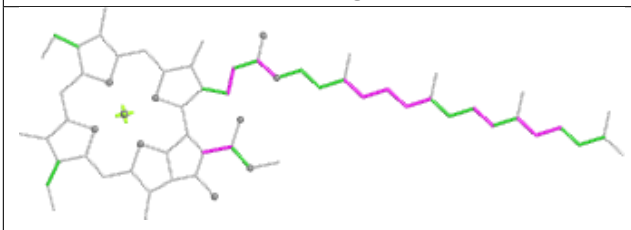
Ligand CLA 7 613



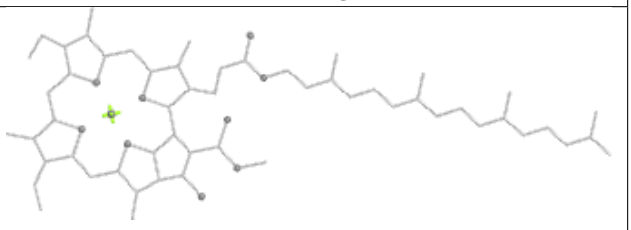
Bond lengths



Bond angles

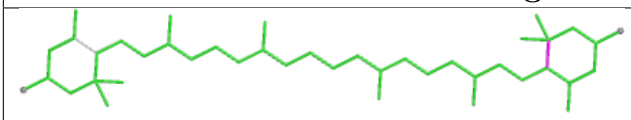


Torsions

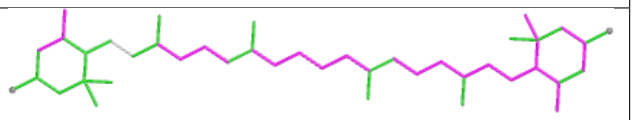


Rings

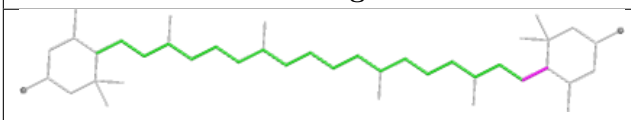
Ligand LUT R 620



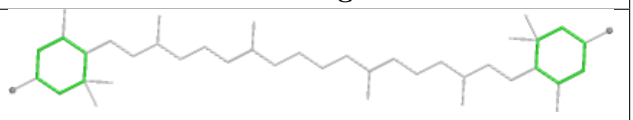
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Bond angles

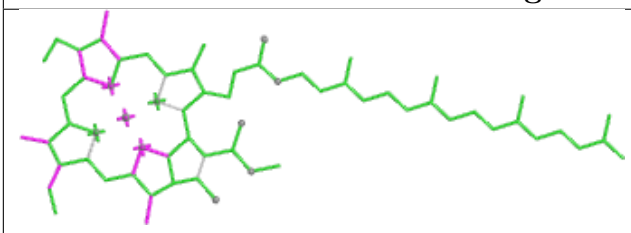


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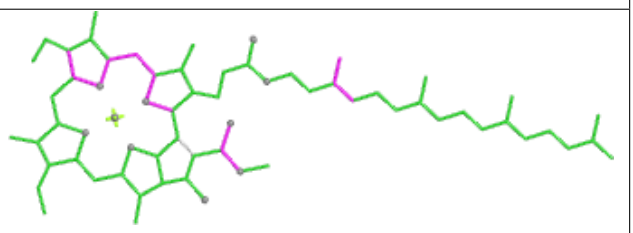


Rings

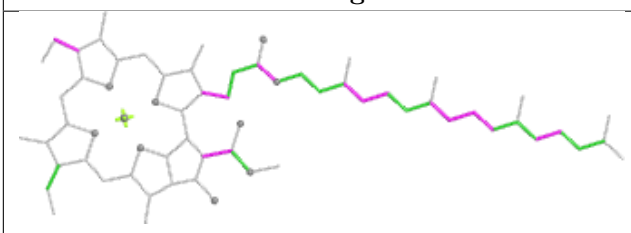
Ligand CLA C 504



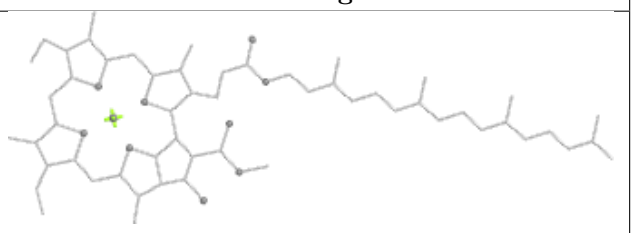
Bond lengths



Bond angles

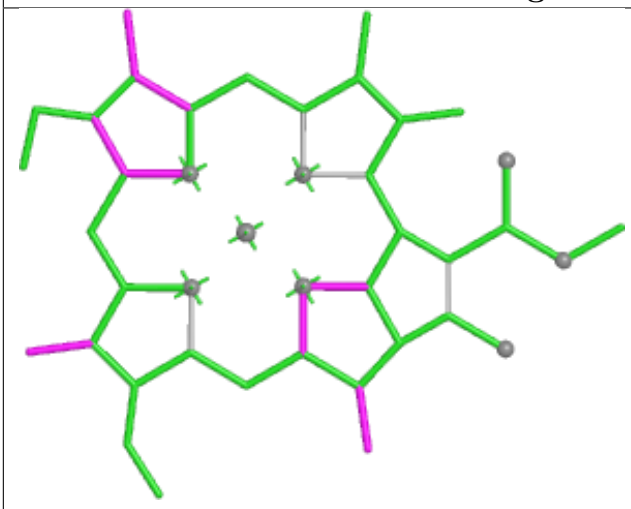


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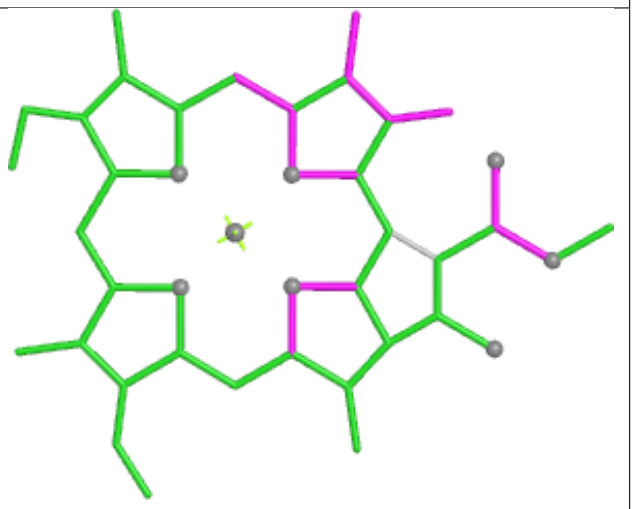


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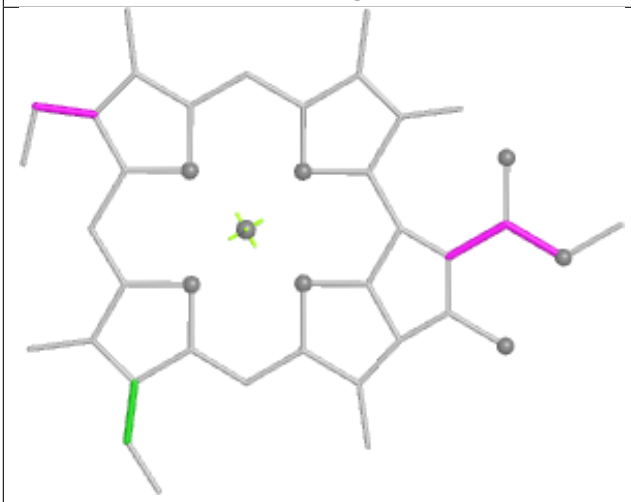
Ligand CLA S 609



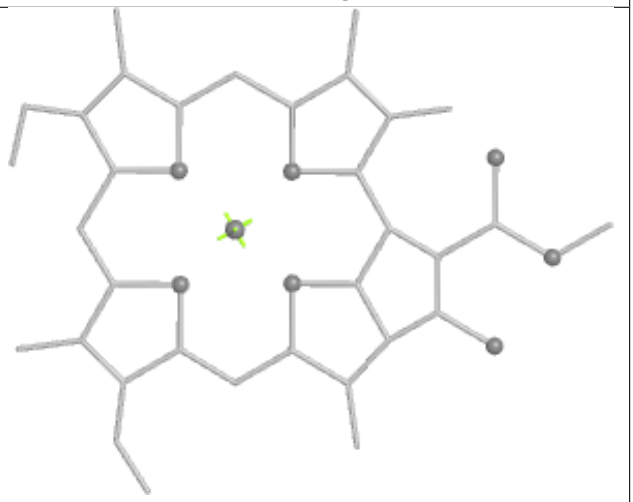
Bond lengths



Bond angles

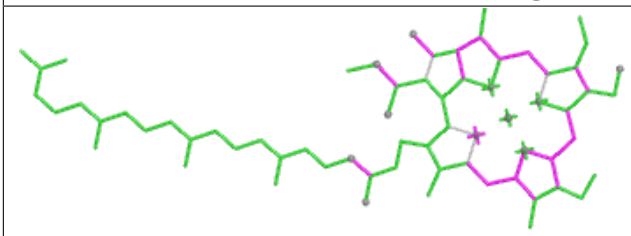


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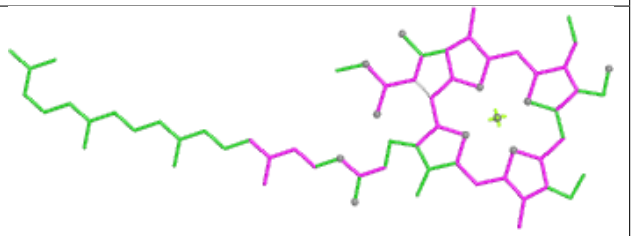


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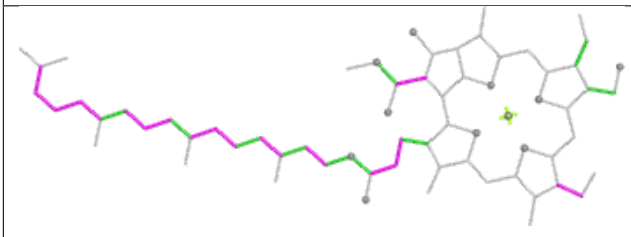
Ligand CHL 7 601



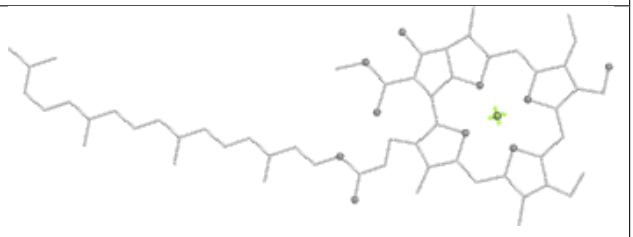
Bond lengths



Bond angles

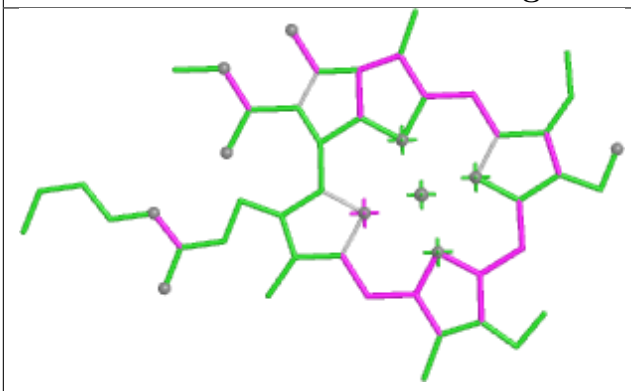


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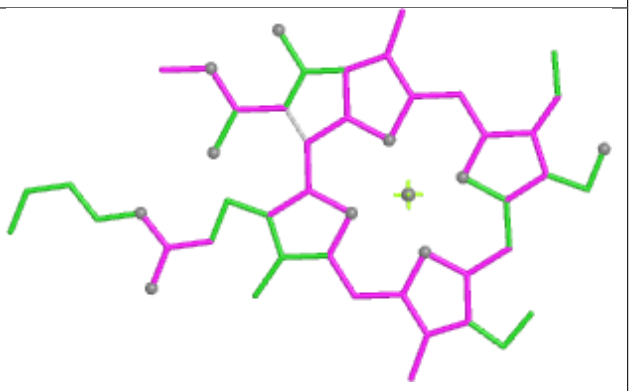


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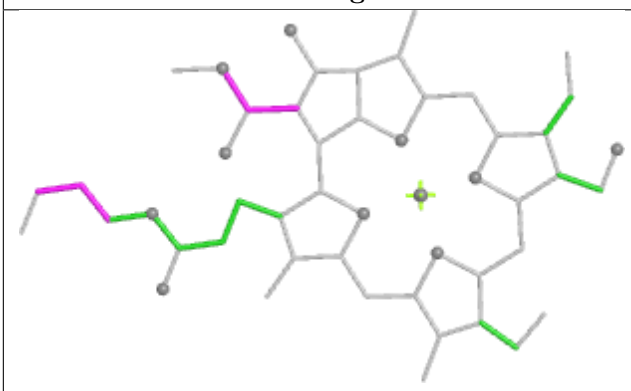
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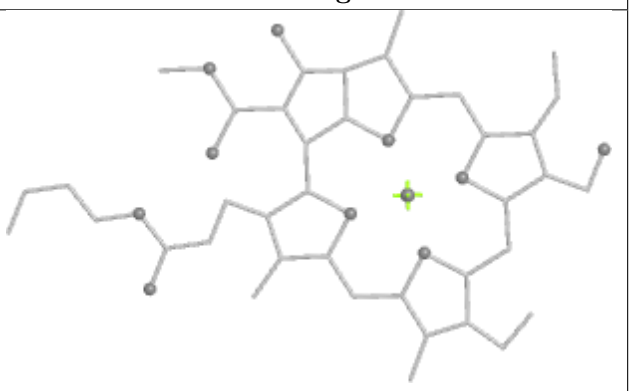
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Bond angles

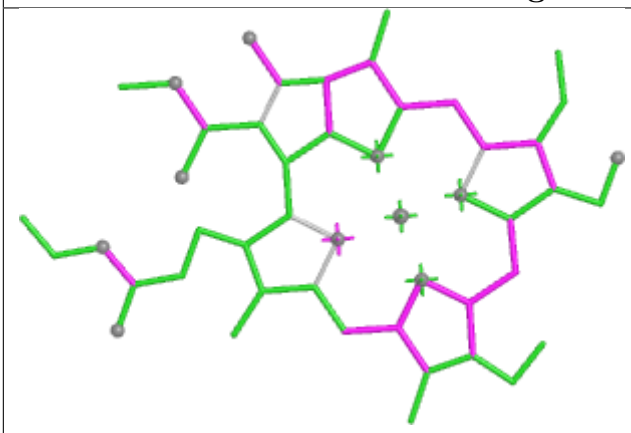


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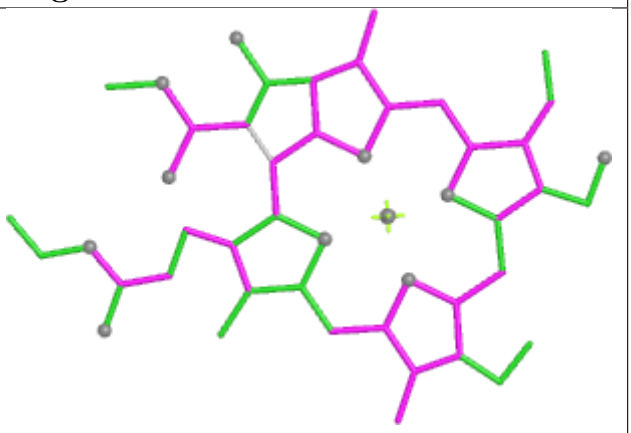


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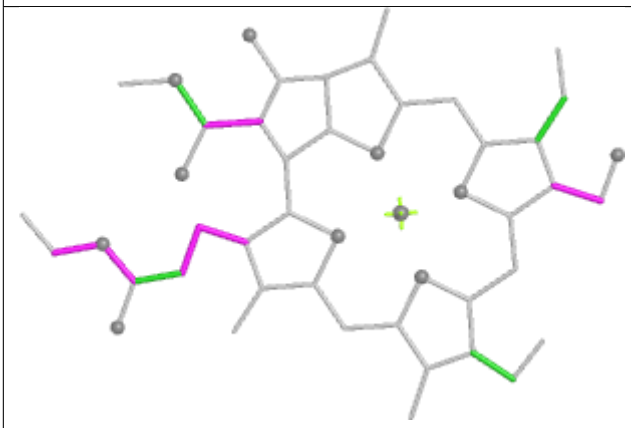
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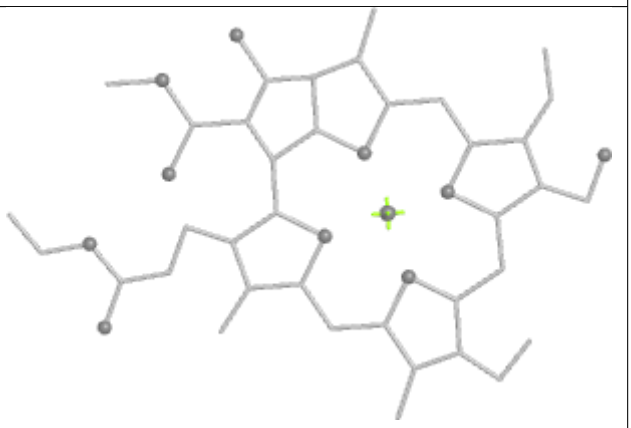
Bond lengths



Bond angles

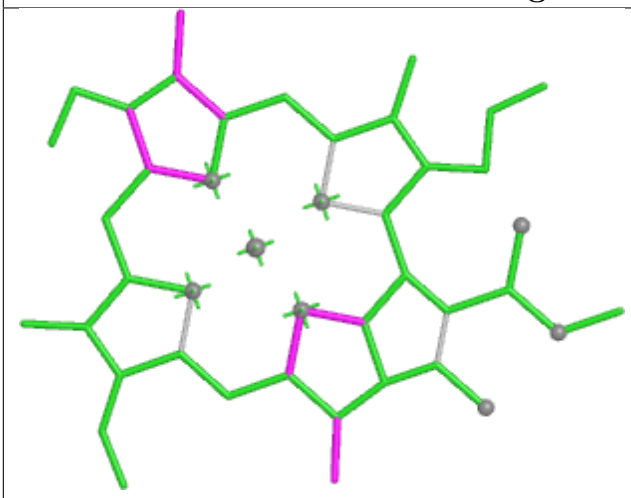


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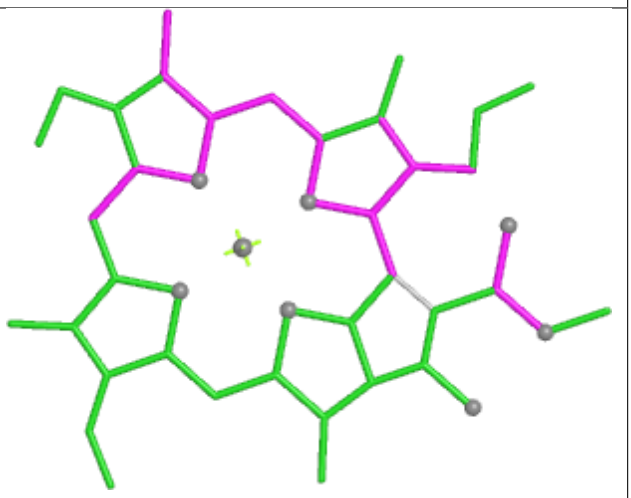


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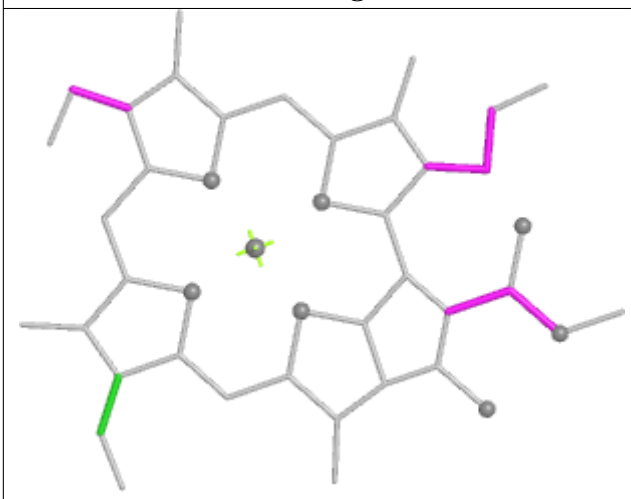
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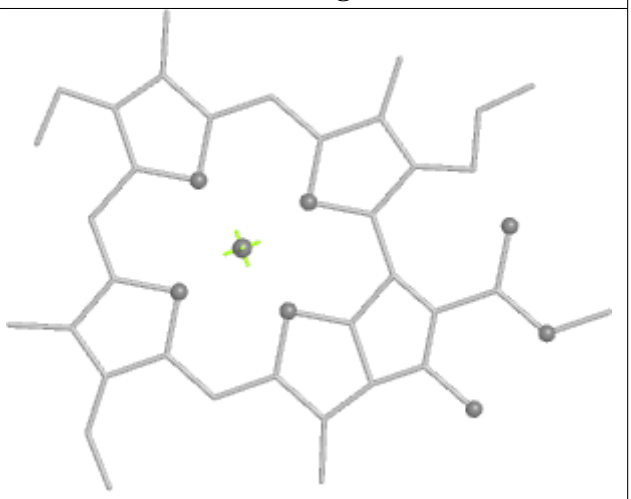
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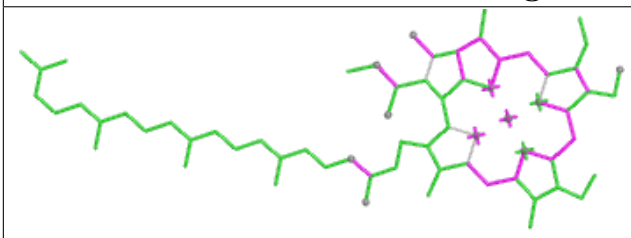


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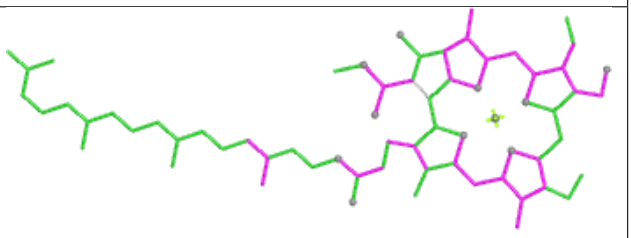


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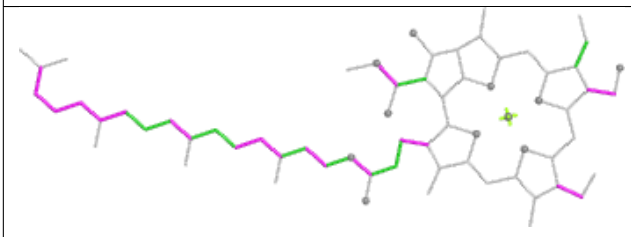
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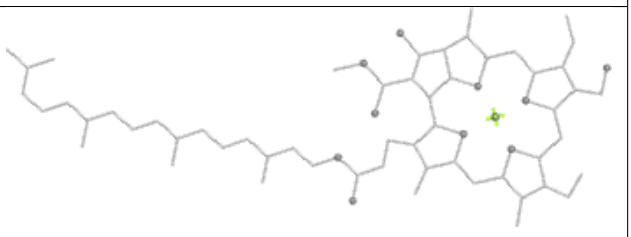
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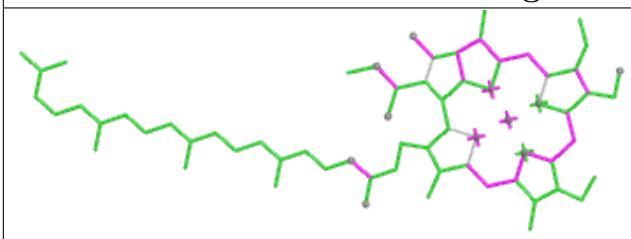


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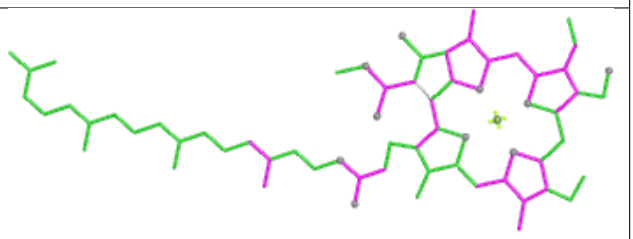


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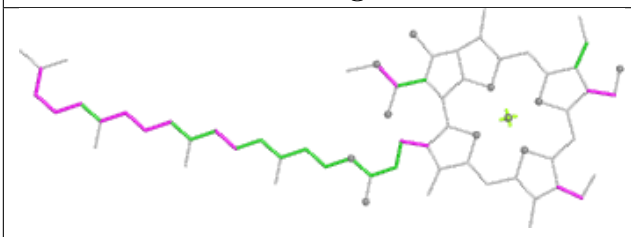
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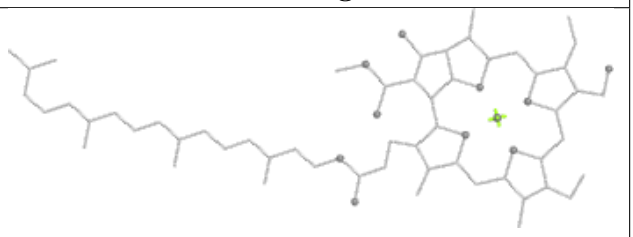
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Bond angles

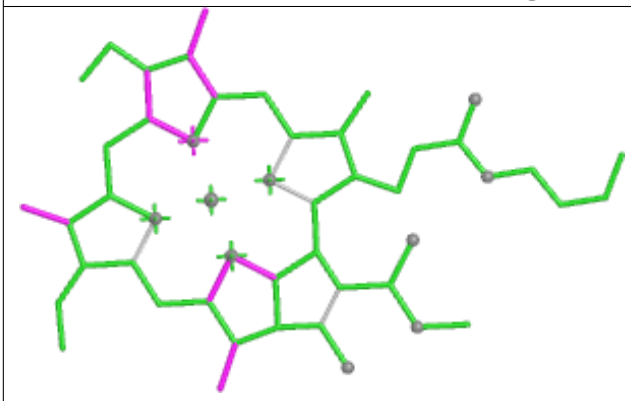


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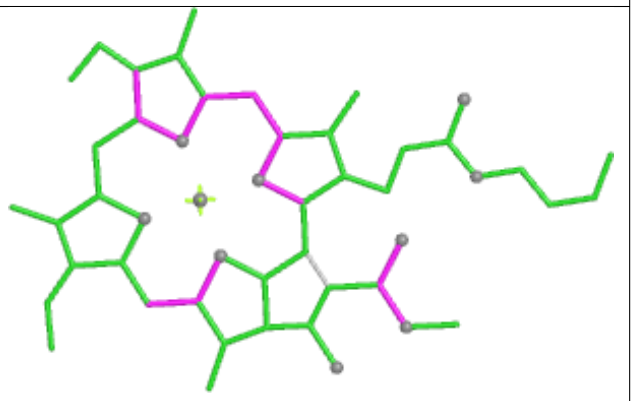


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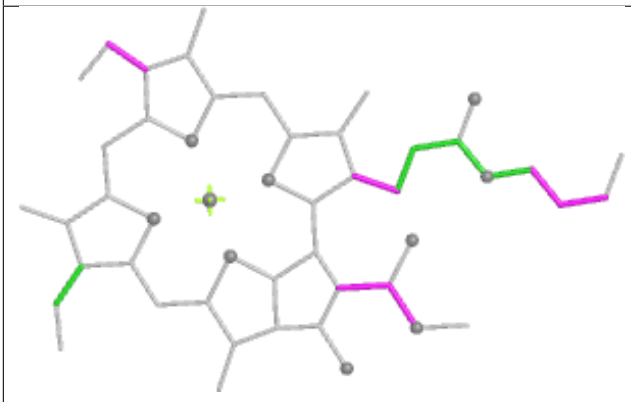
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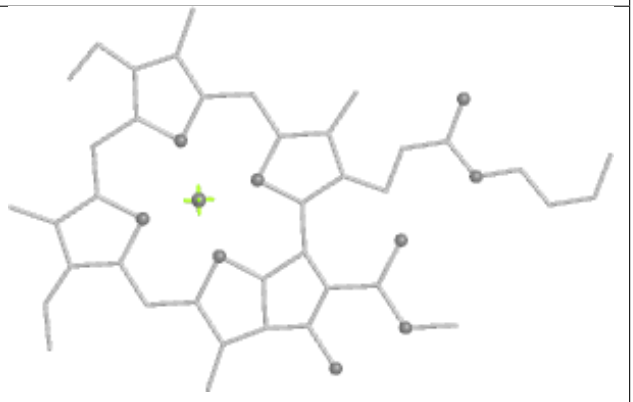
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Bond angles

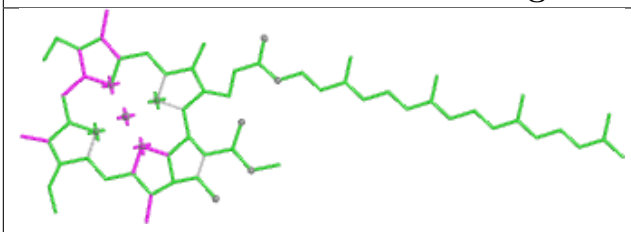


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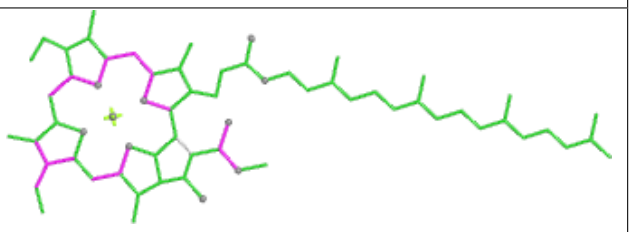


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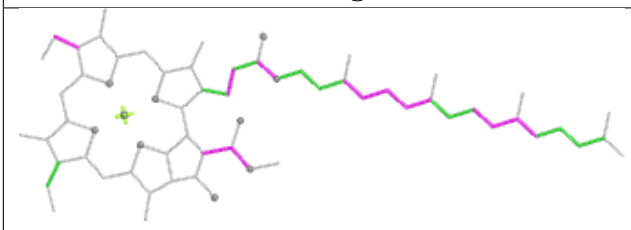
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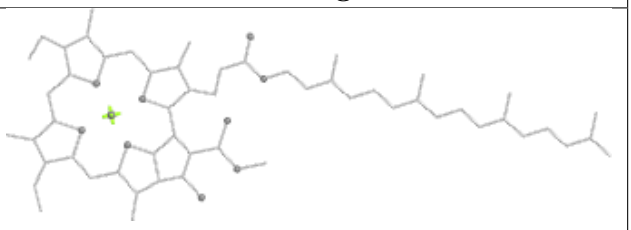
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Bond angles

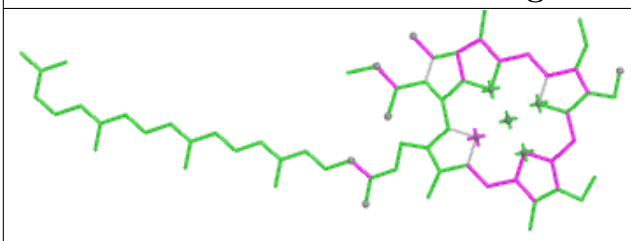


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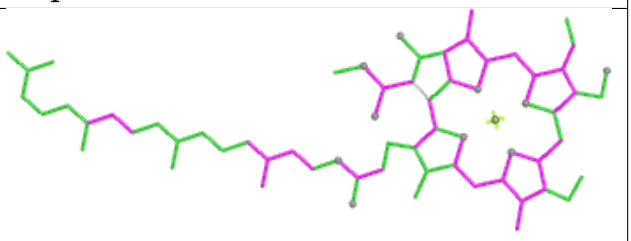


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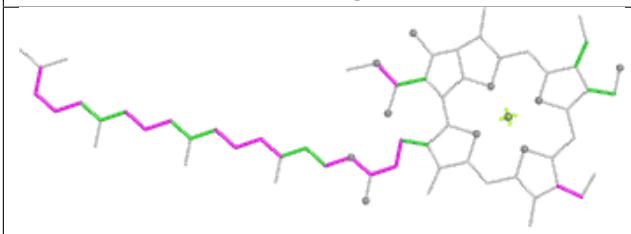
Ligand CHL p 601



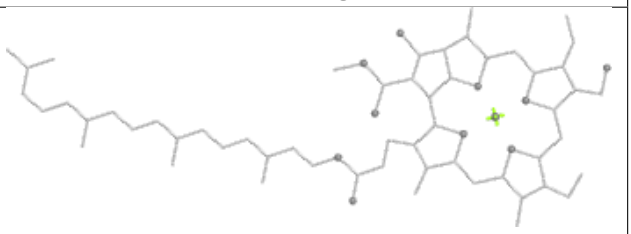
Bond lengths



Bond angles

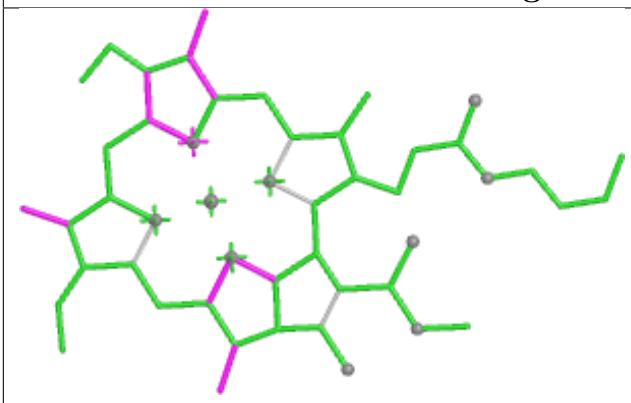


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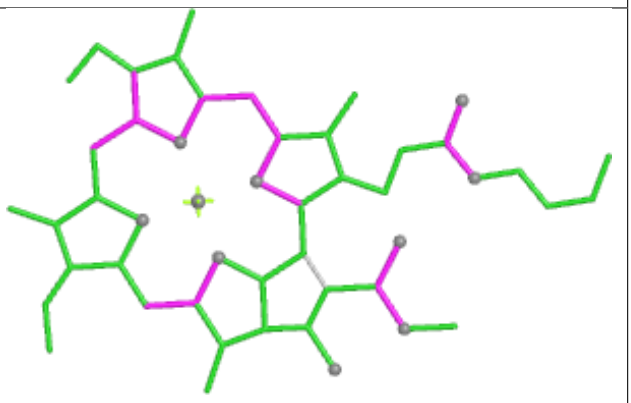


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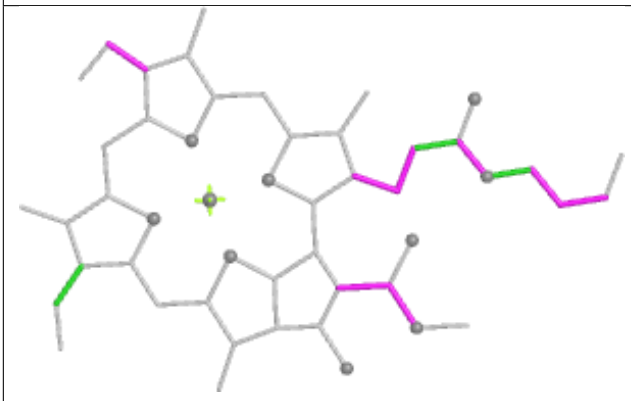
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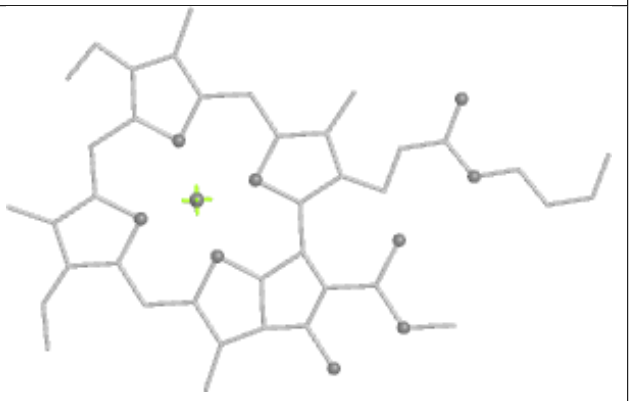
Bond lengths



Bond angles

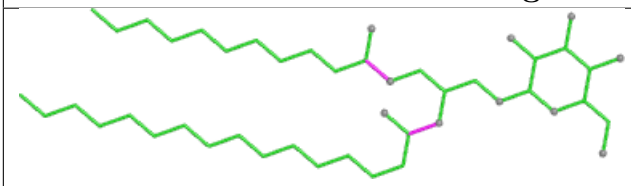


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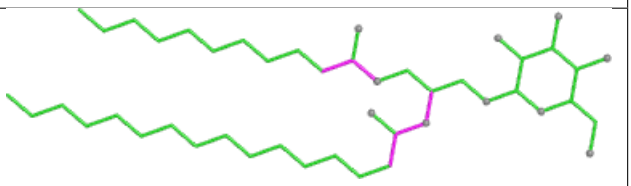


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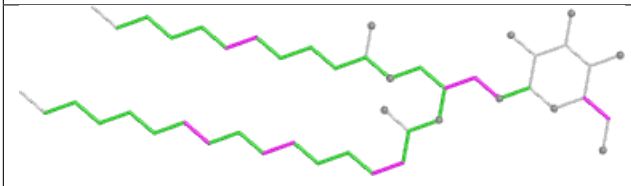
Ligand LMG d 411



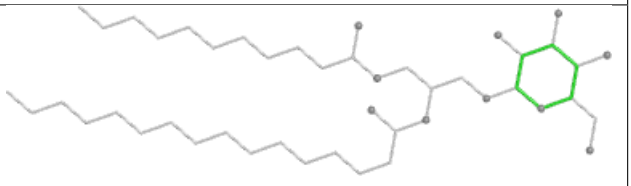
Bond lengths



Bond angles

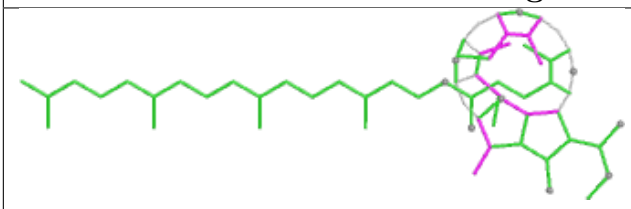


Torsions

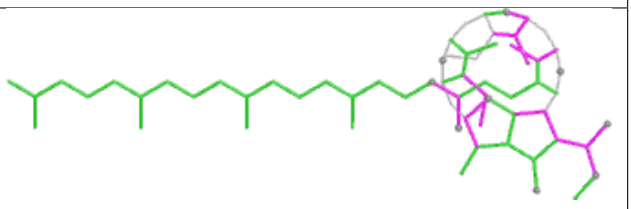


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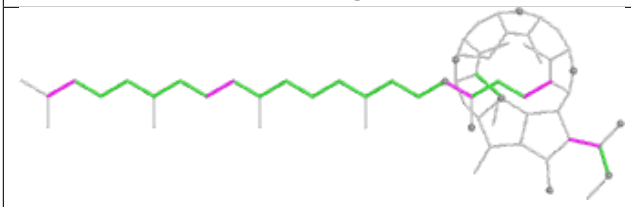
Ligand PHO a 409



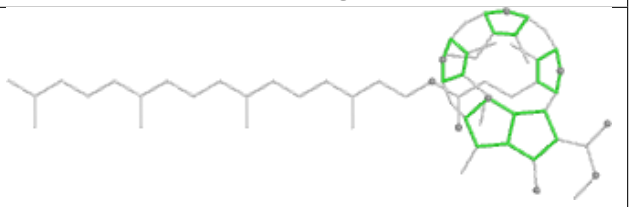
Bond lengths



Bond angles

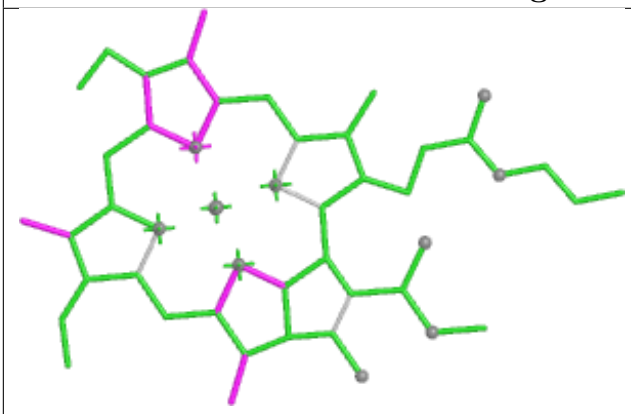


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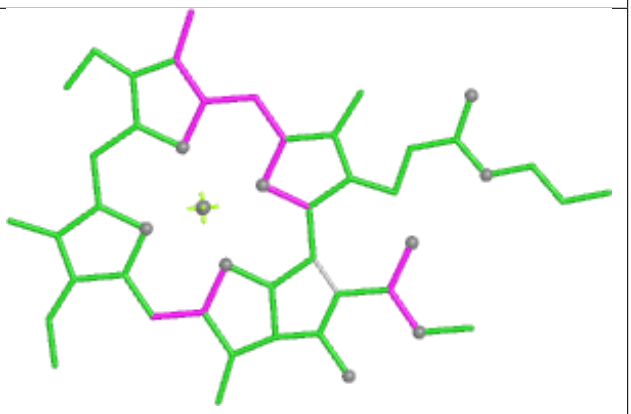


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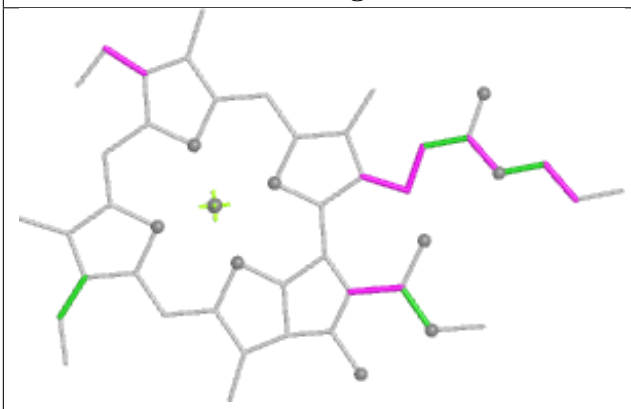
Ligand CLA r 604



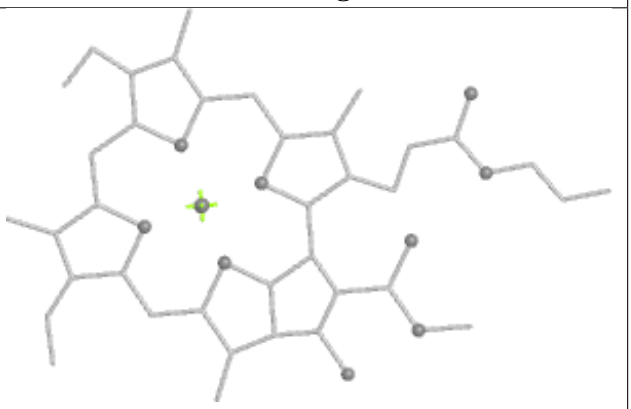
Bond lengths



Bond angles

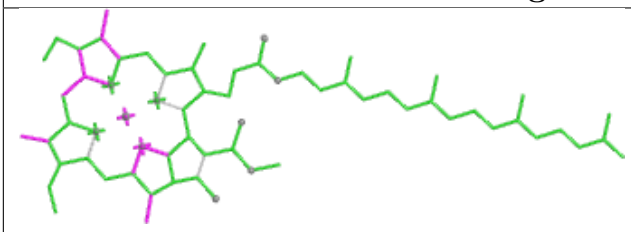


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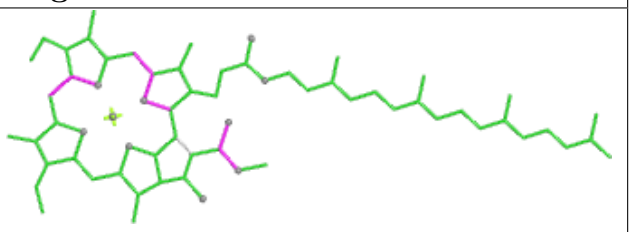


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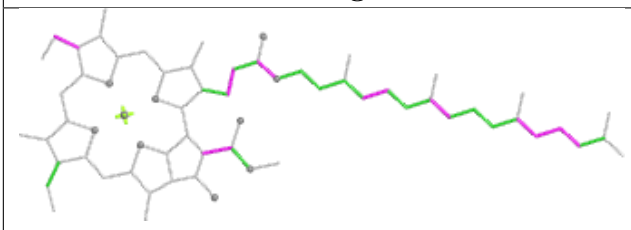
Ligand CLA g 613



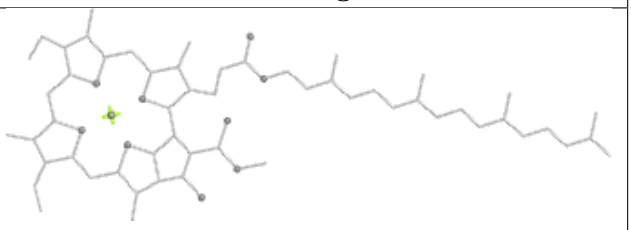
Bond lengths



Bond angles

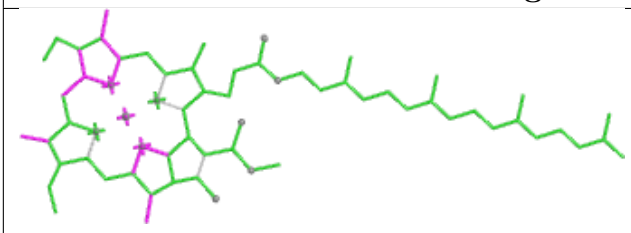


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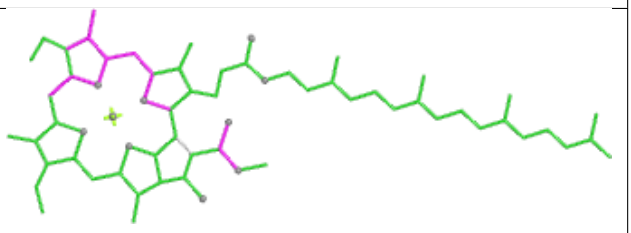


Rings

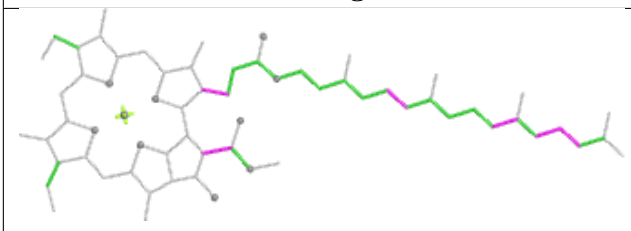
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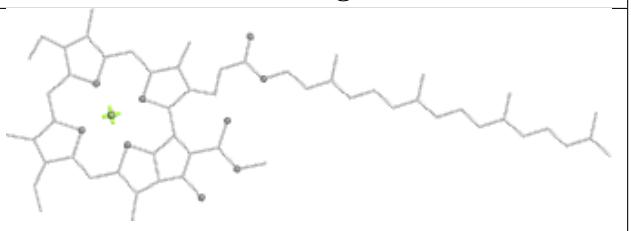
Bond lengths



Bond angles

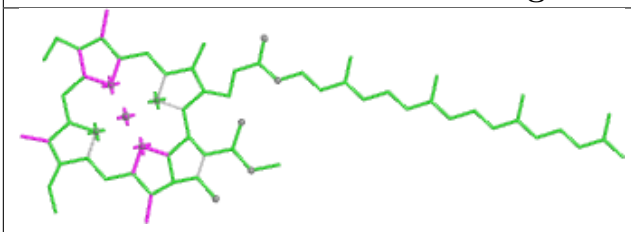


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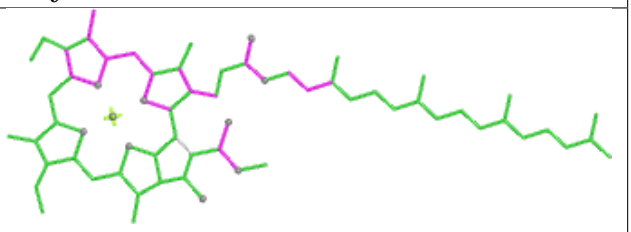


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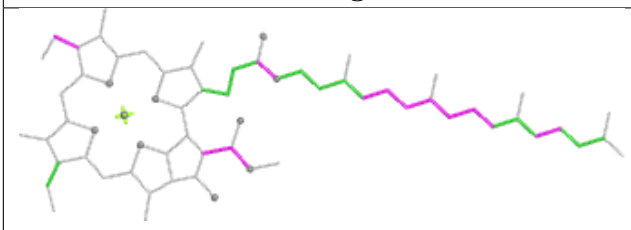
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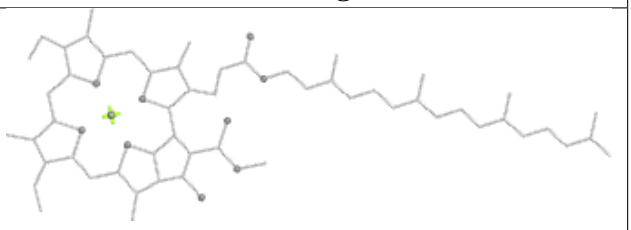
Bond lengths



Bond angles

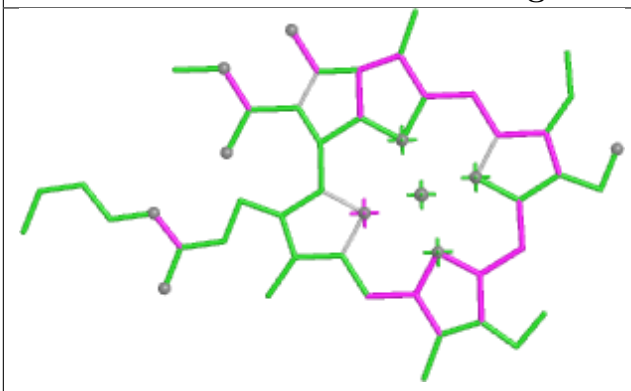


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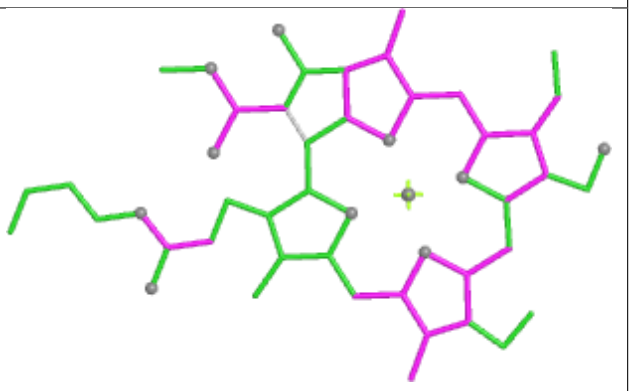


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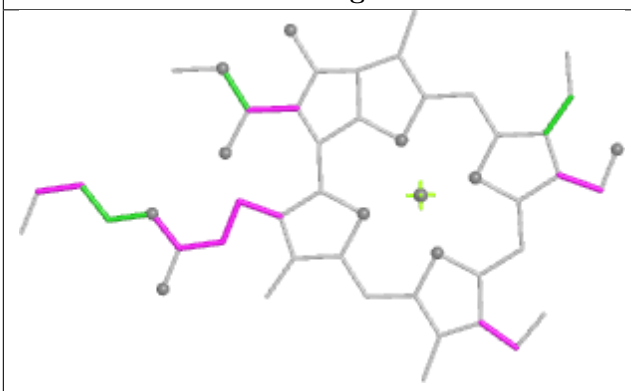
Ligand CHL 9 607



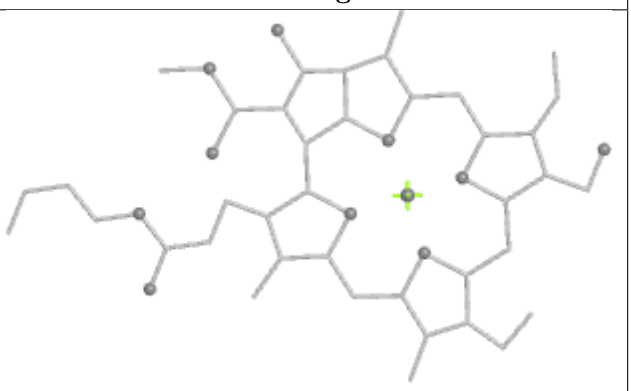
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Bond angles

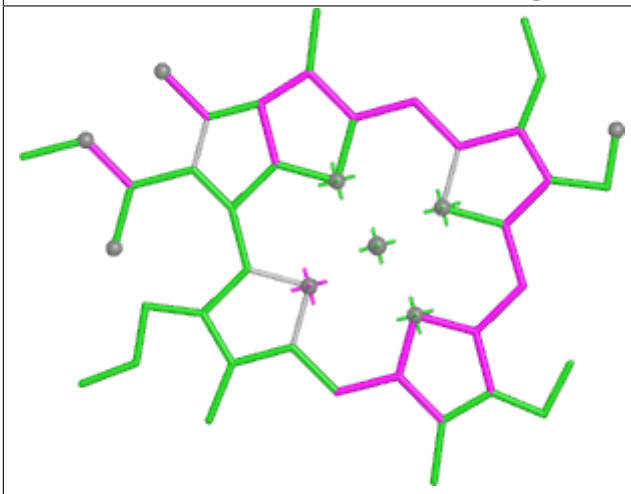


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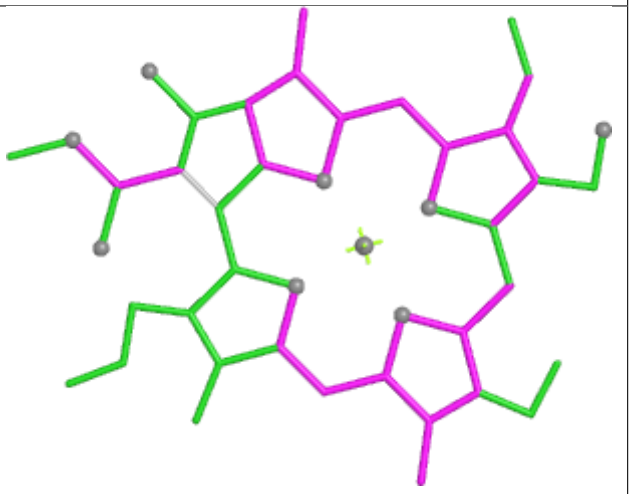


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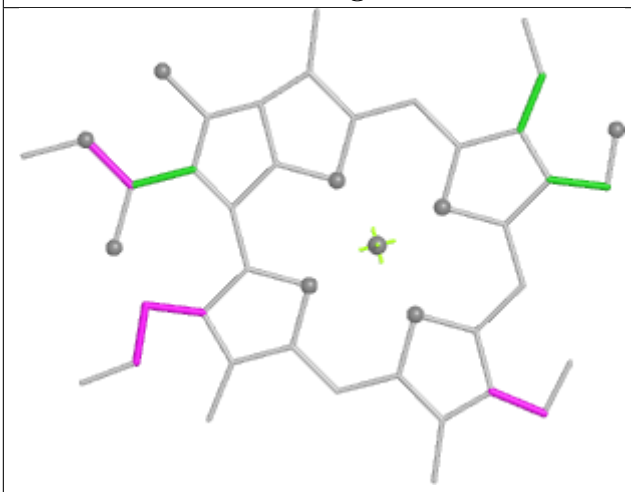
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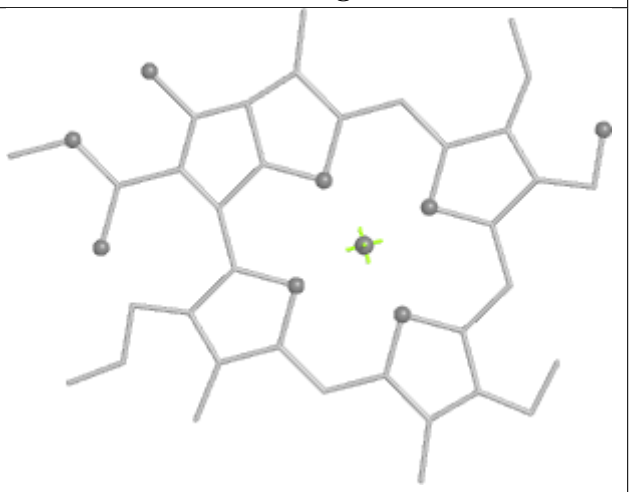
Bond lengths



Bond angles

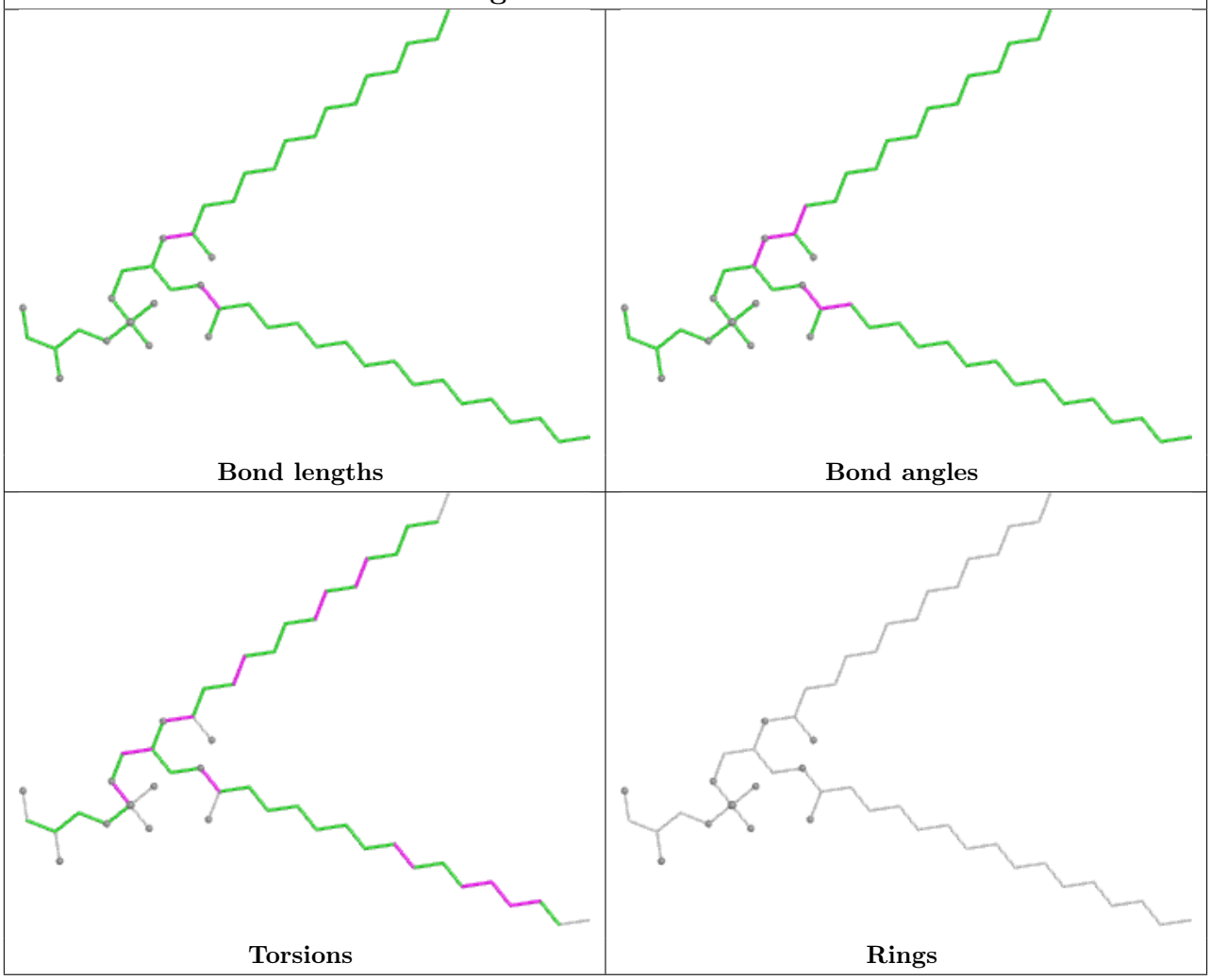


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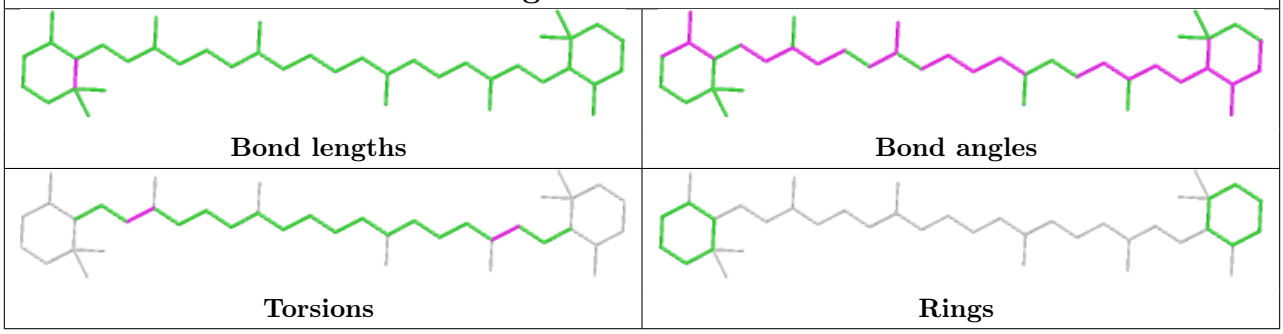


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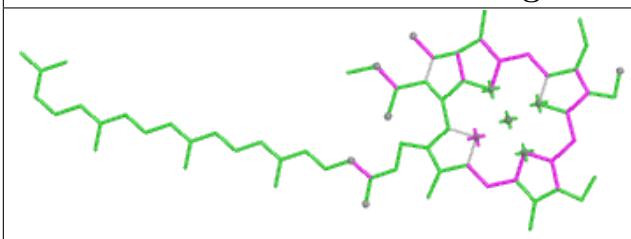
Ligand LHG c 2630



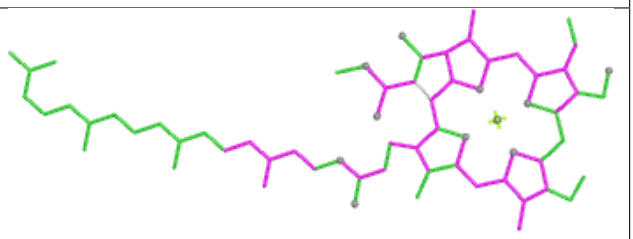
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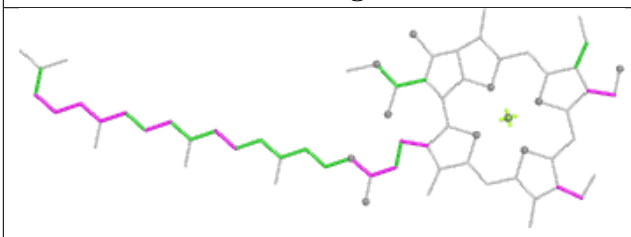
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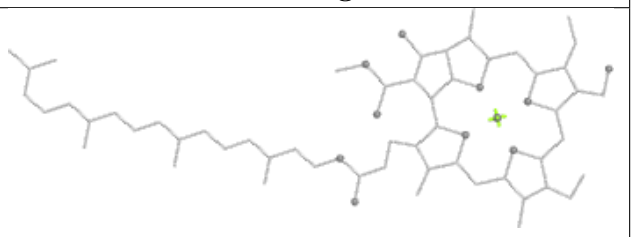
Bond lengths



Bond angles

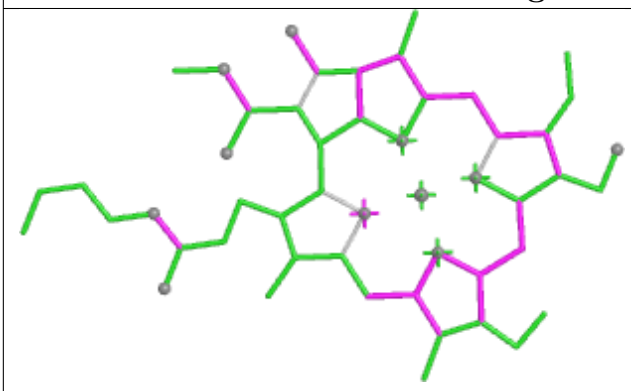


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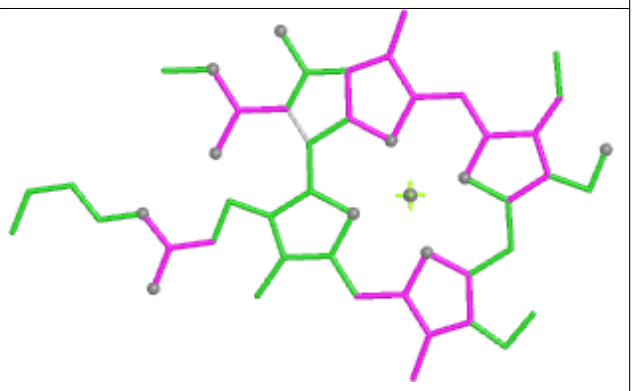


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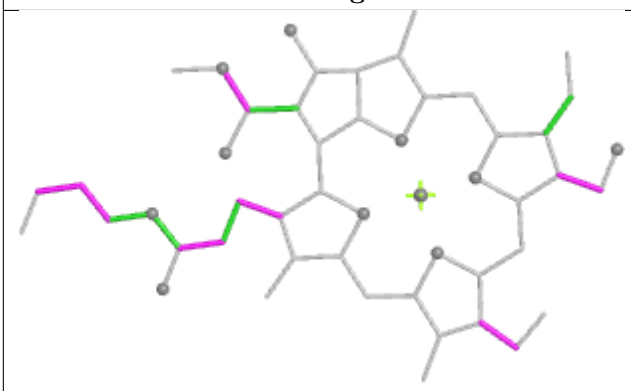
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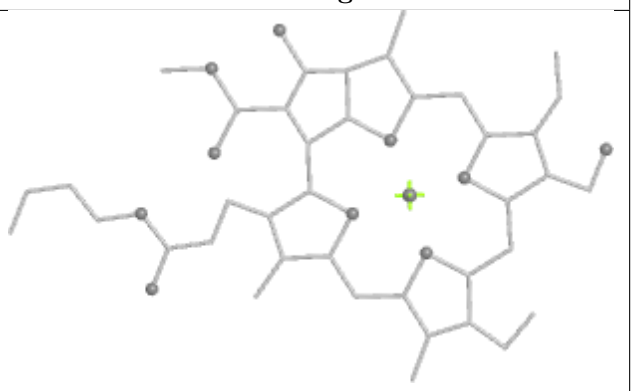
Bond lengths



Bond angles

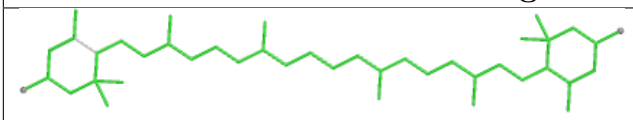


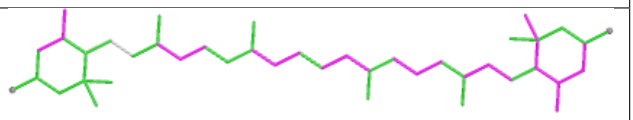
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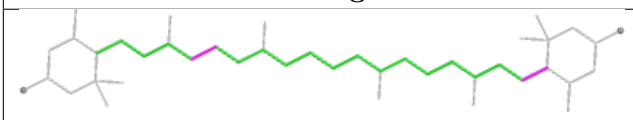


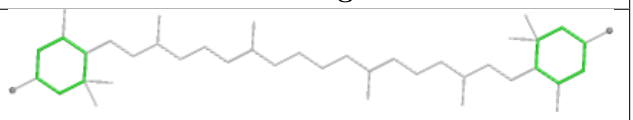
Rings

Ligand LUT 0 1621


Bond lengths

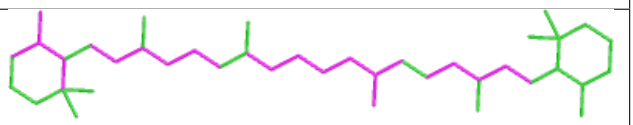

Bond angles

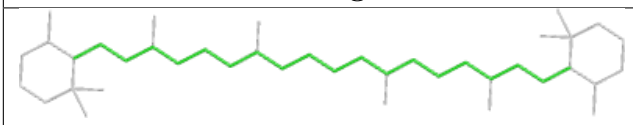

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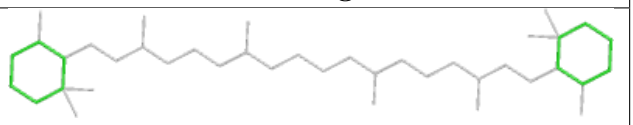

Rings

Ligand BCR c 517

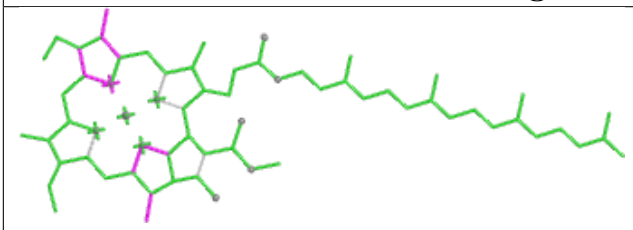

Bond lengths

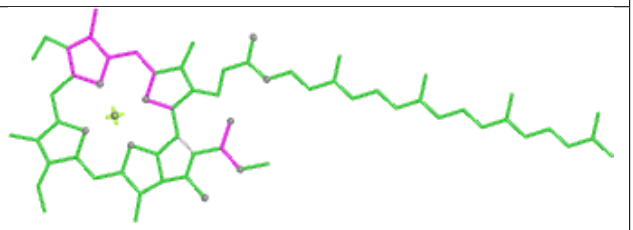

Bond angles

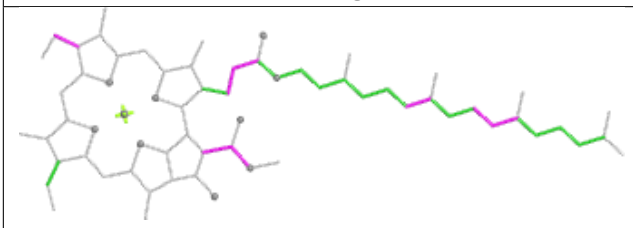

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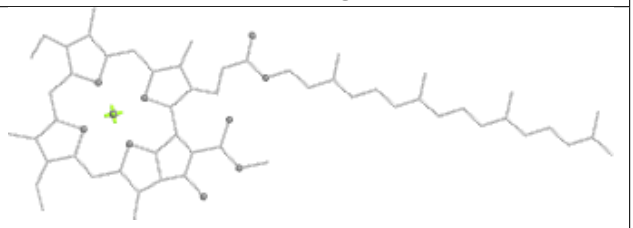

Rings

Ligand CLA 3 602

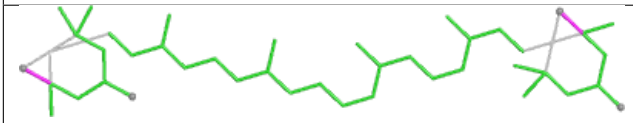

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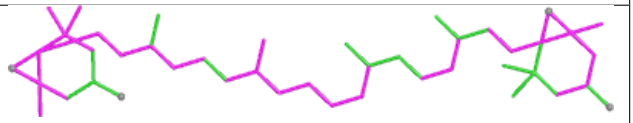

Bond angles

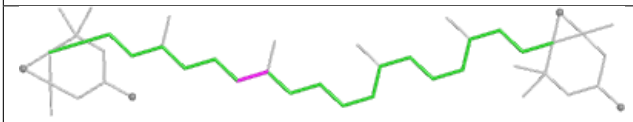

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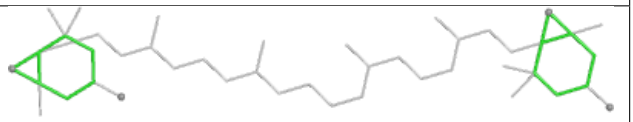

Rings

Ligand XAT 1 1622

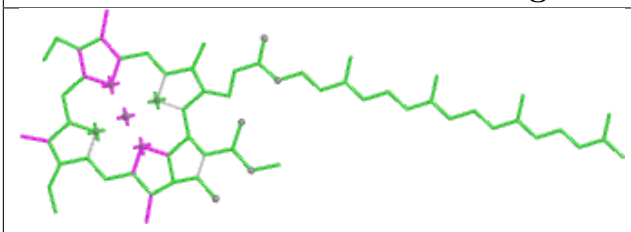

Bond lengths


Bond angles

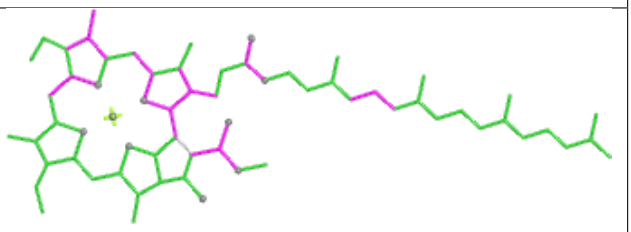

Torsions


Rings

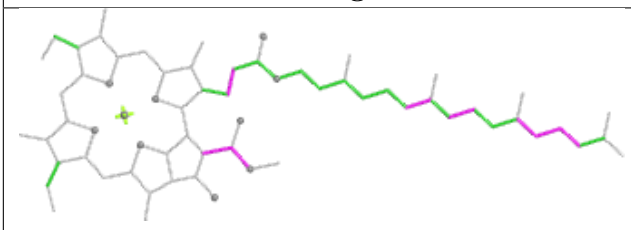
Ligand CLA c 507



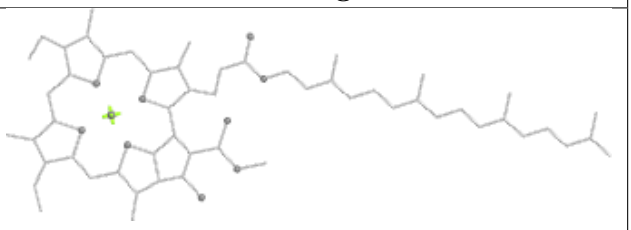
Bond lengths



Bond angles



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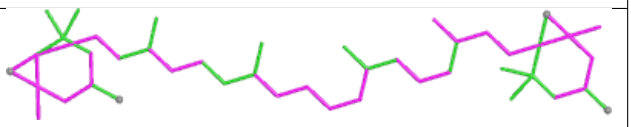


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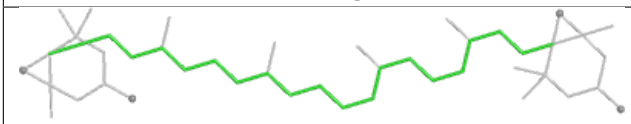
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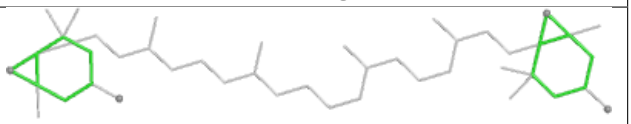
Bond lengths



Bond angles

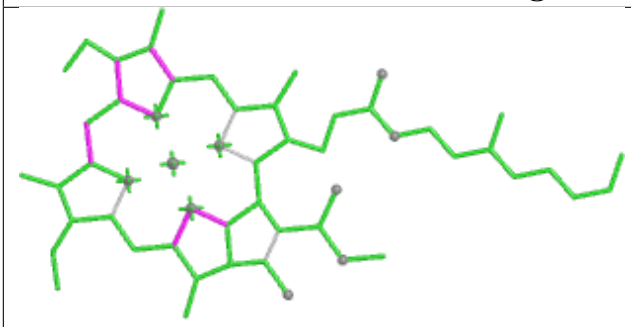


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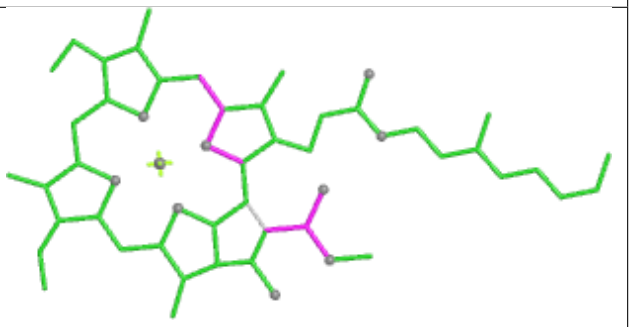


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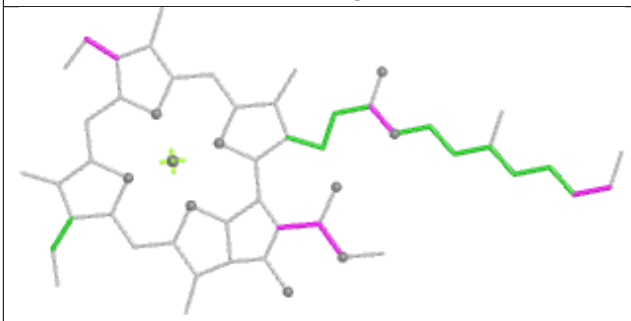
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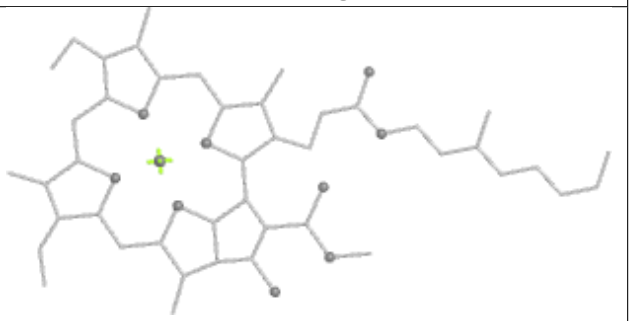
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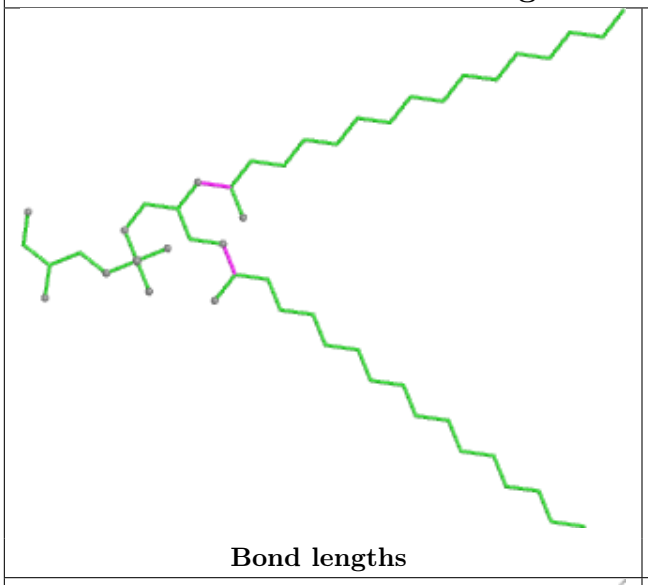


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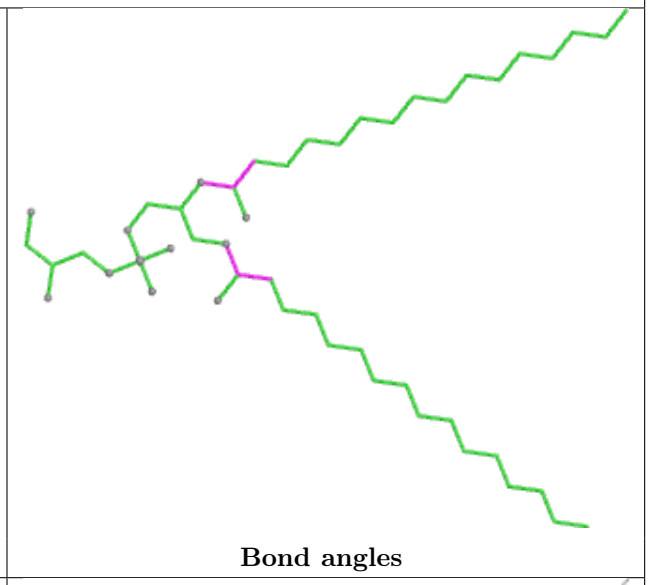


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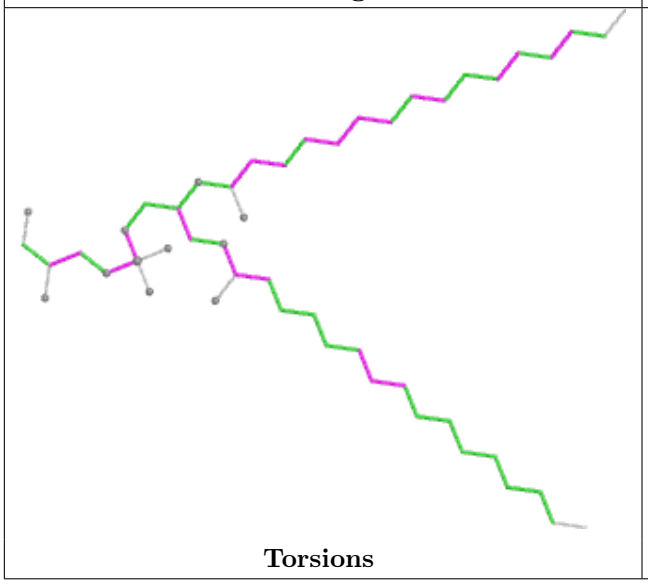
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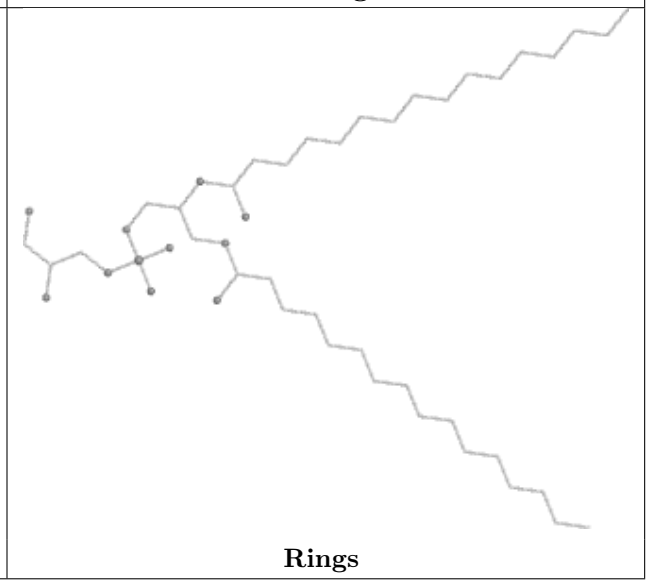
Bond lengths



Bond angles

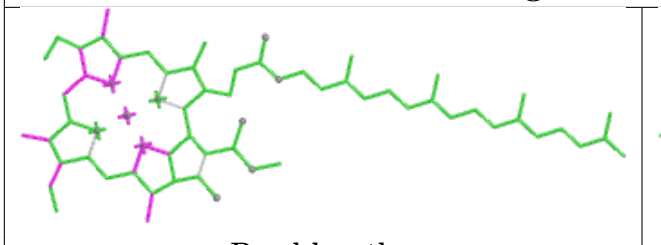


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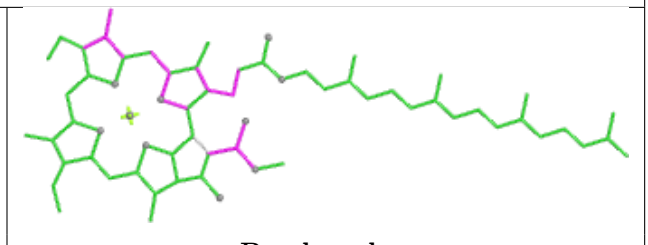


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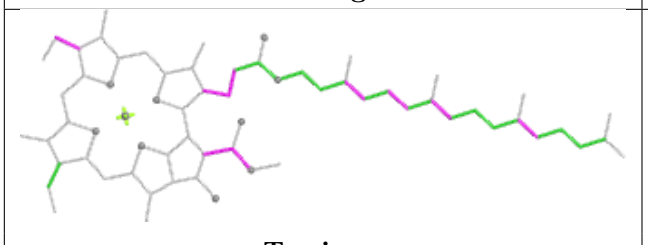
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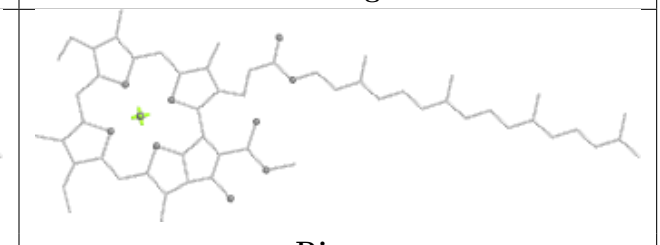
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Bond angles

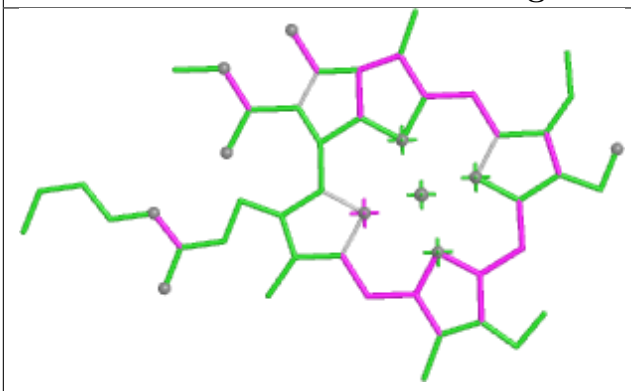


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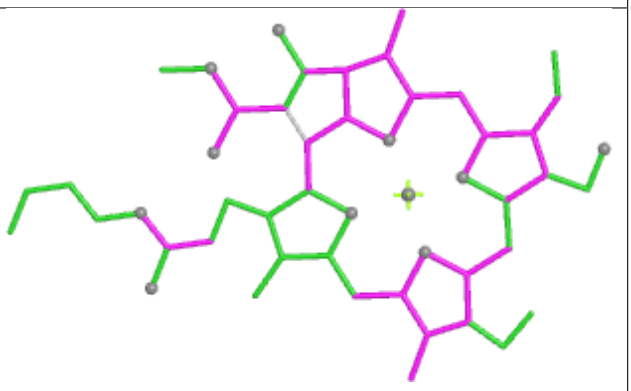


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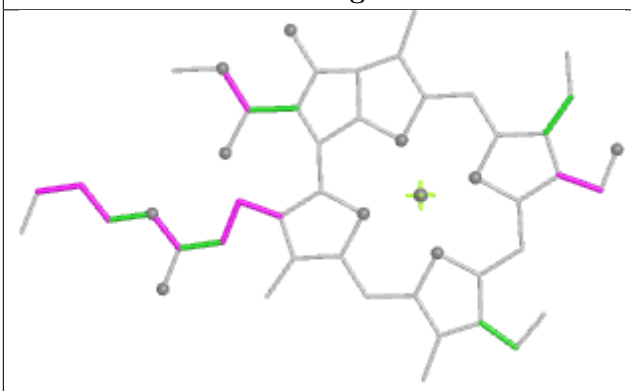
Ligand CHL 3 608



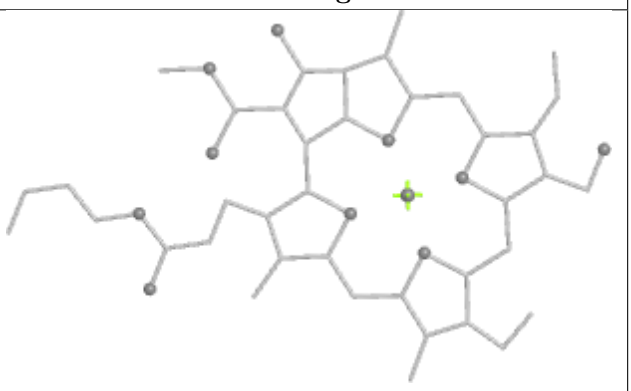
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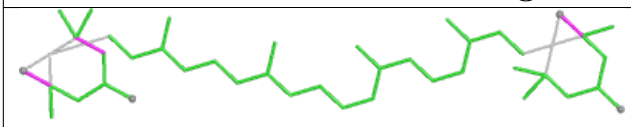


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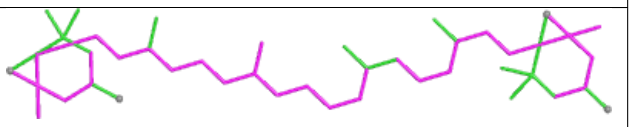


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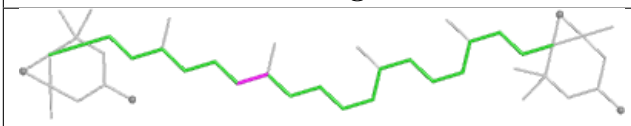
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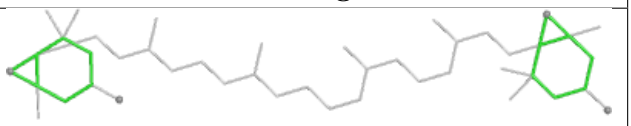
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Bond angles

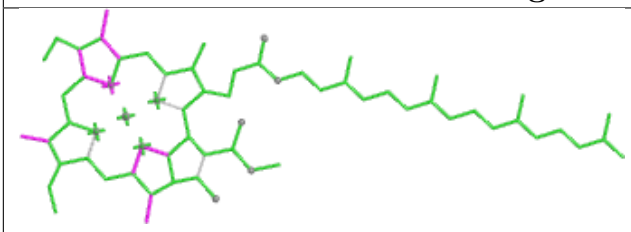


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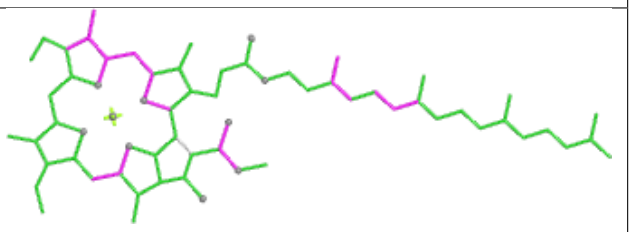


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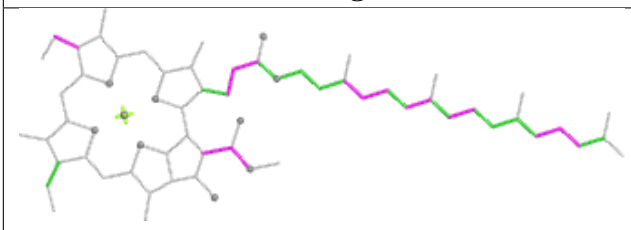
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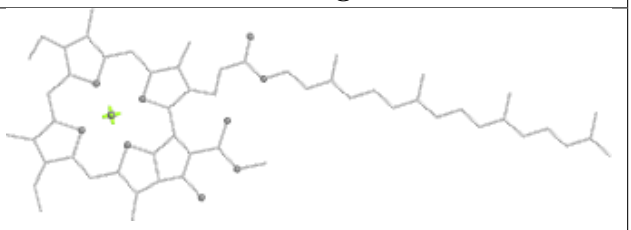
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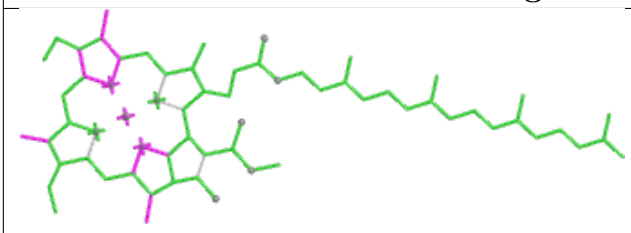


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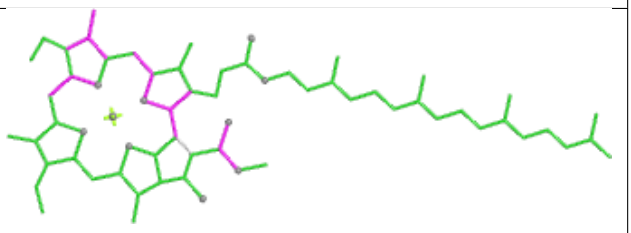


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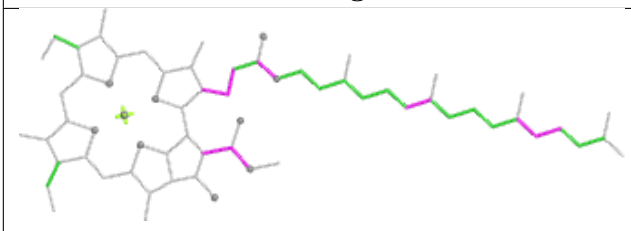
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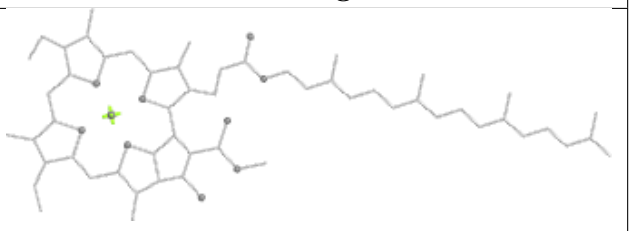
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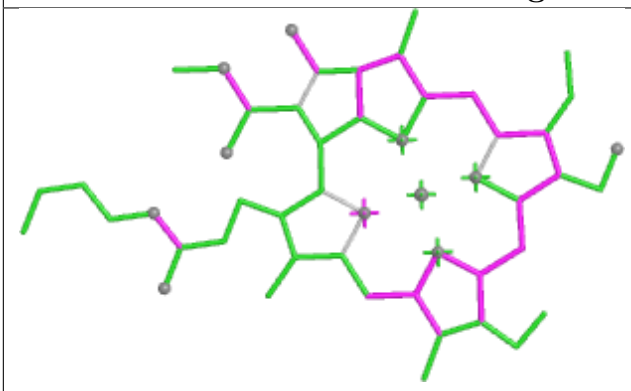


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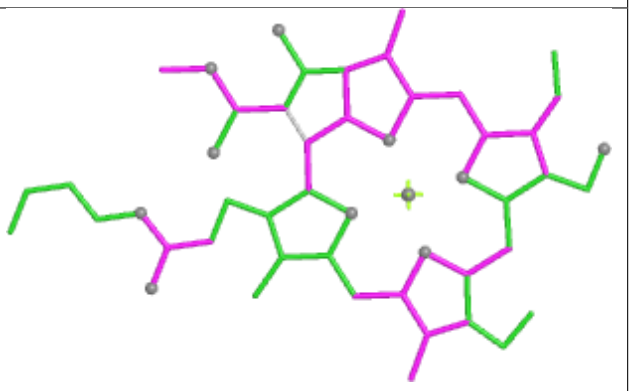


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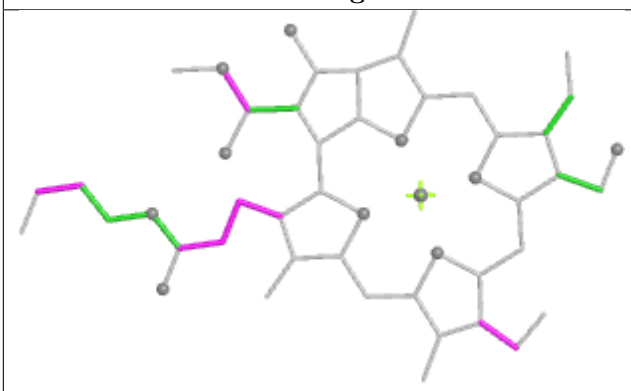
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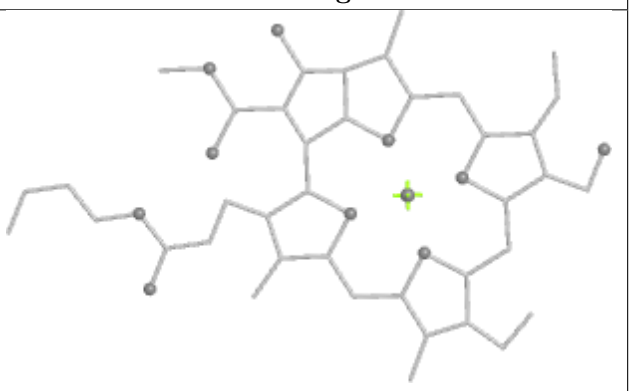
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Bond angles

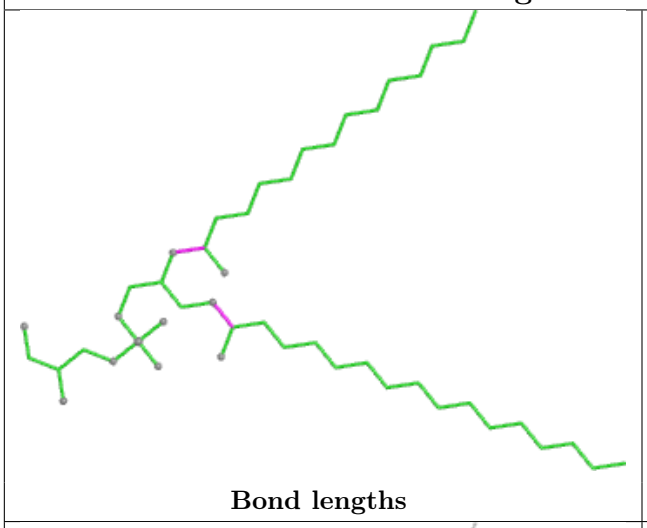


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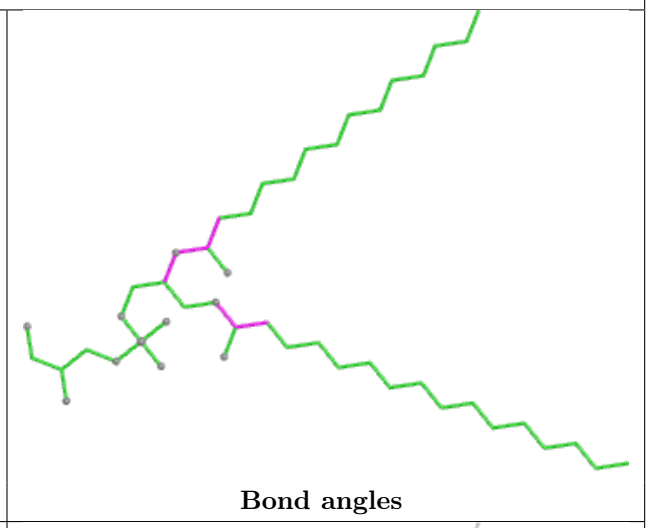


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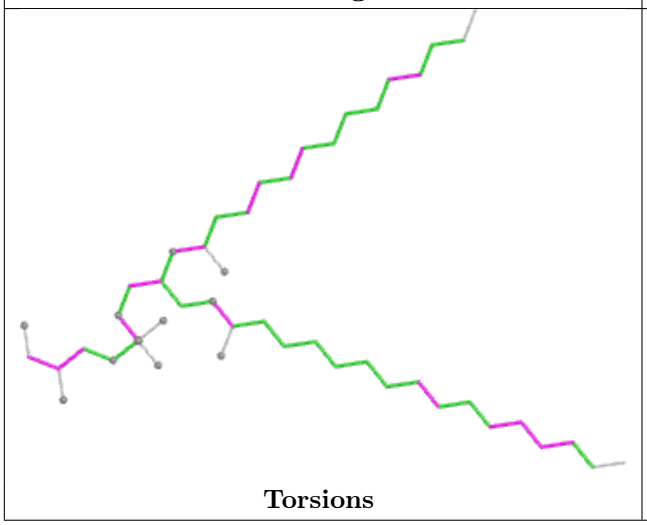
Ligand LHG C 2630



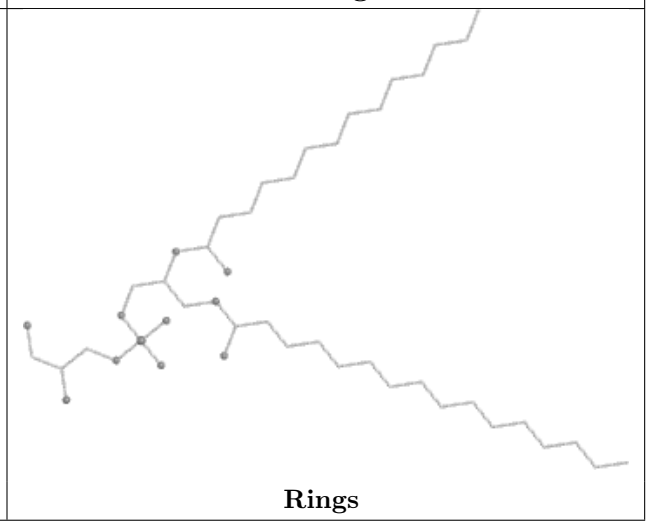
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Bond angles

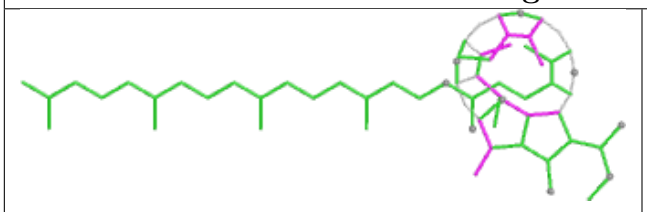


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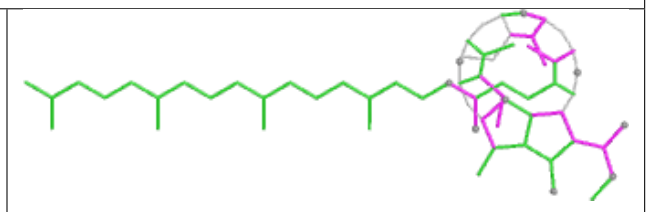


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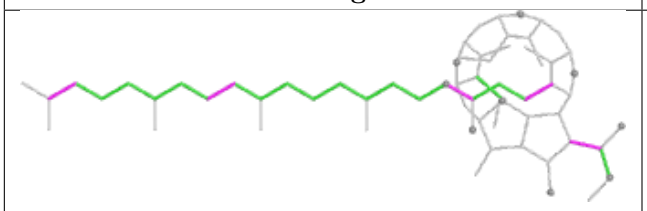
Ligand PHO A 409



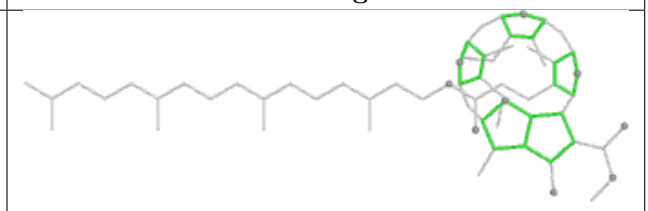
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Bond angles

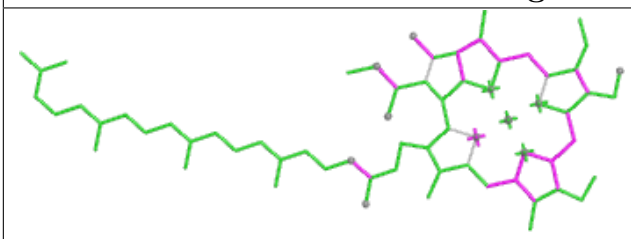


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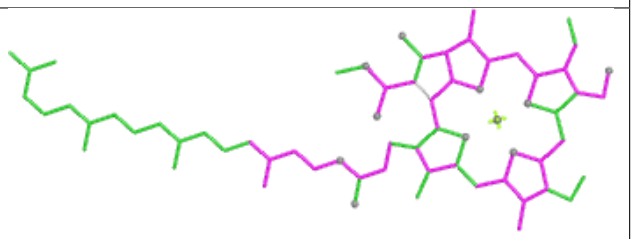


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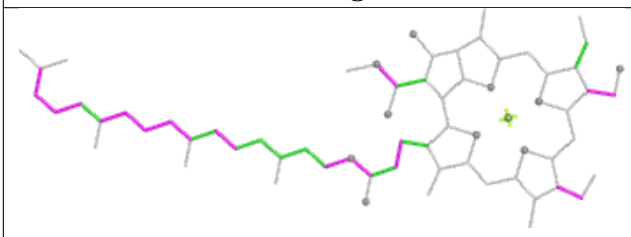
Ligand CHL 7 607



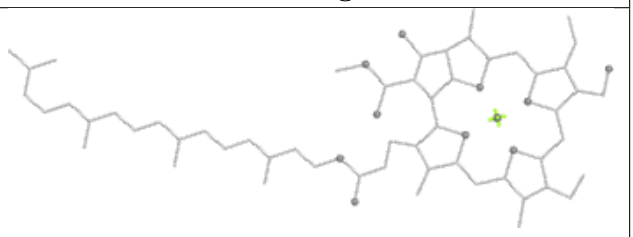
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Bond angles

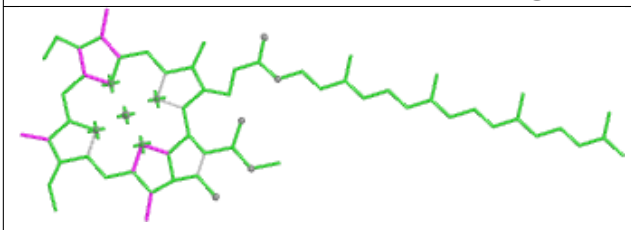


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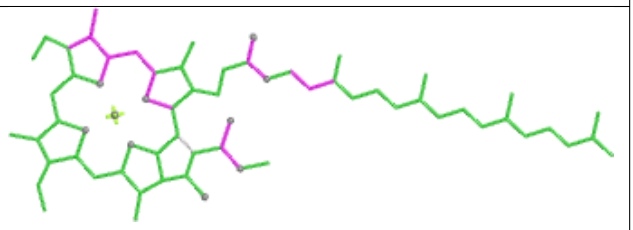


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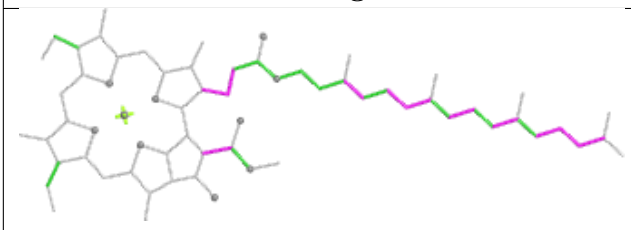
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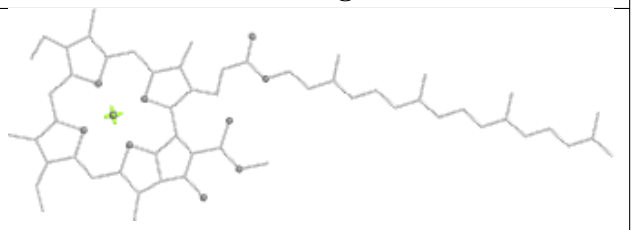
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Bond angles

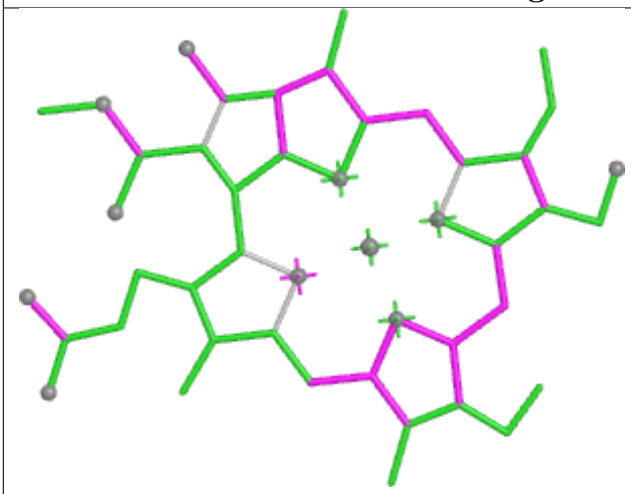


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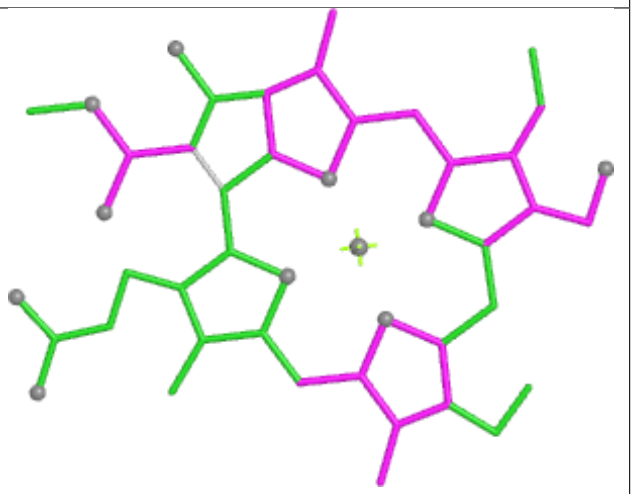


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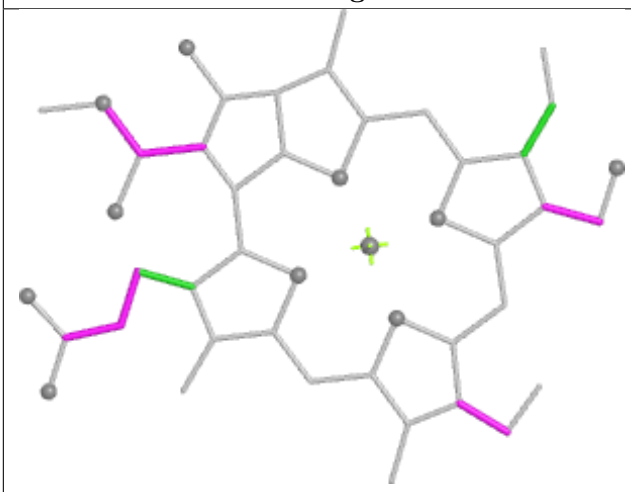
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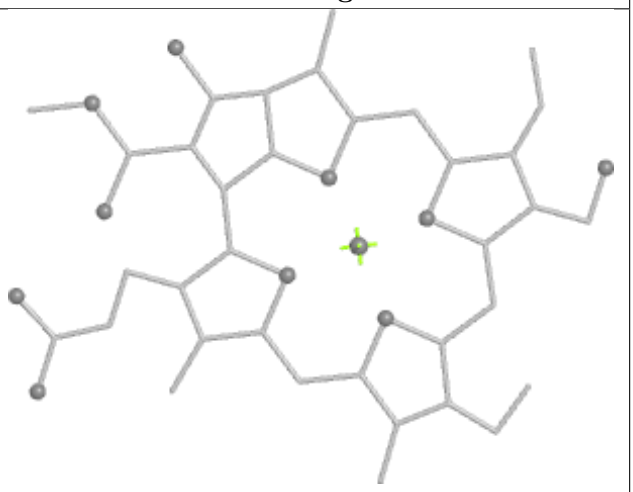
Bond lengths



Bond angles

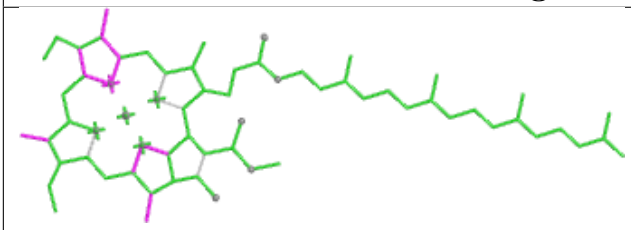


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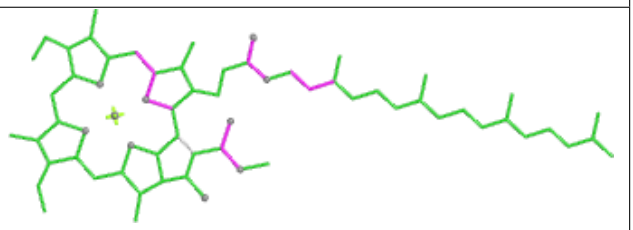


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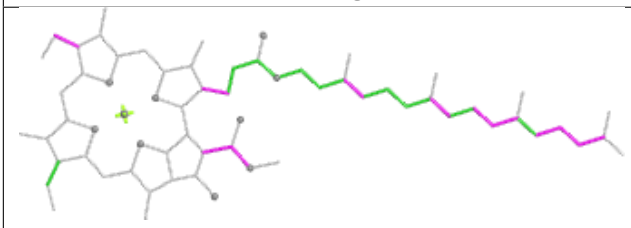
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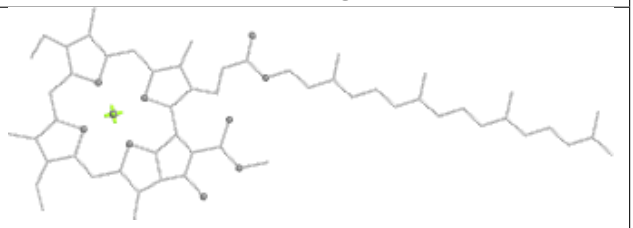
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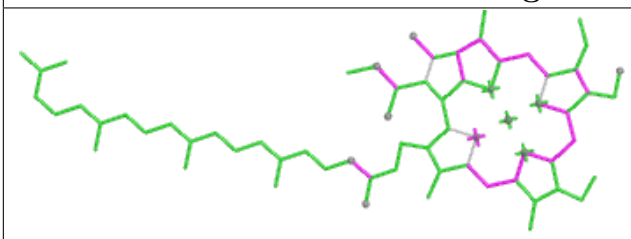


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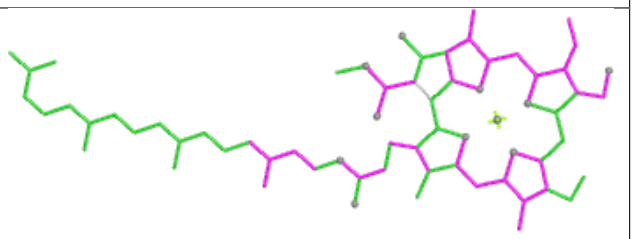


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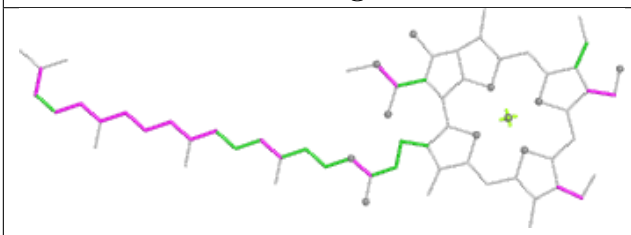
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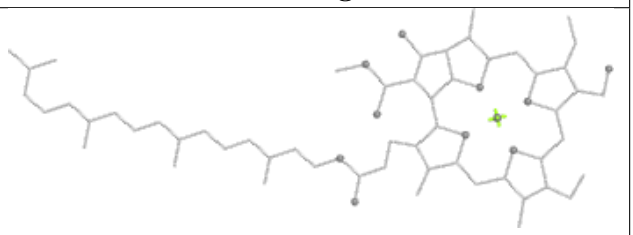
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Bond angles

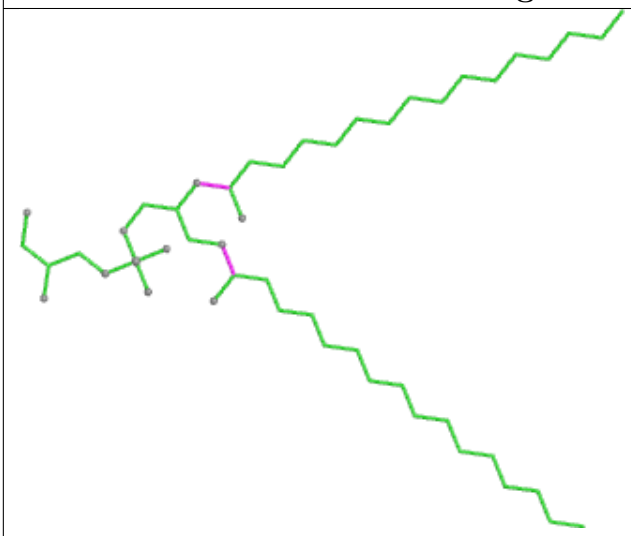


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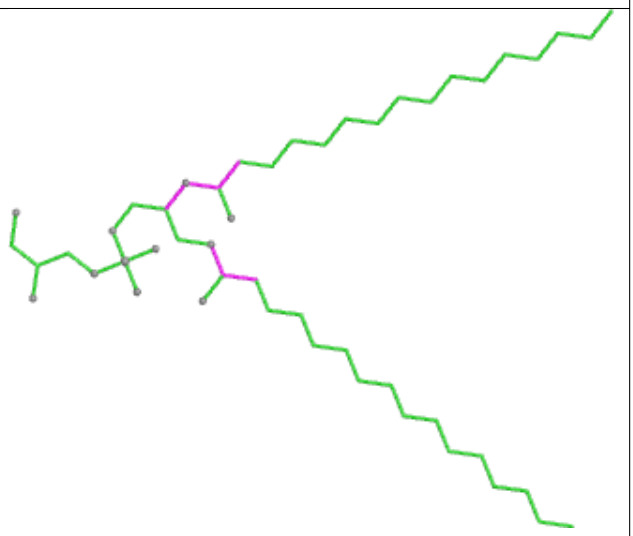


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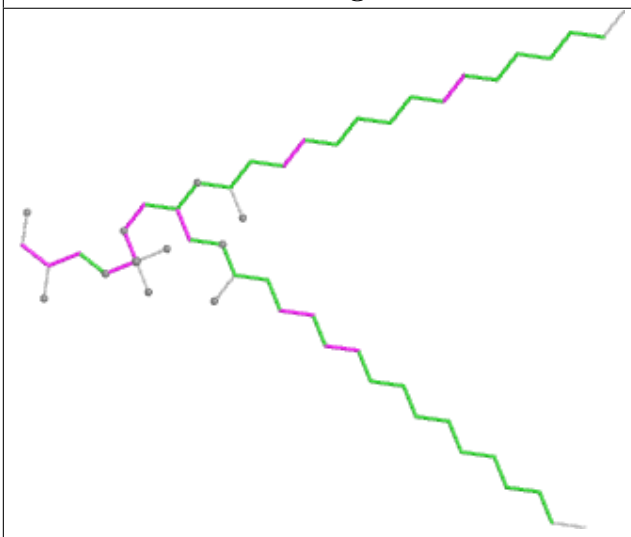
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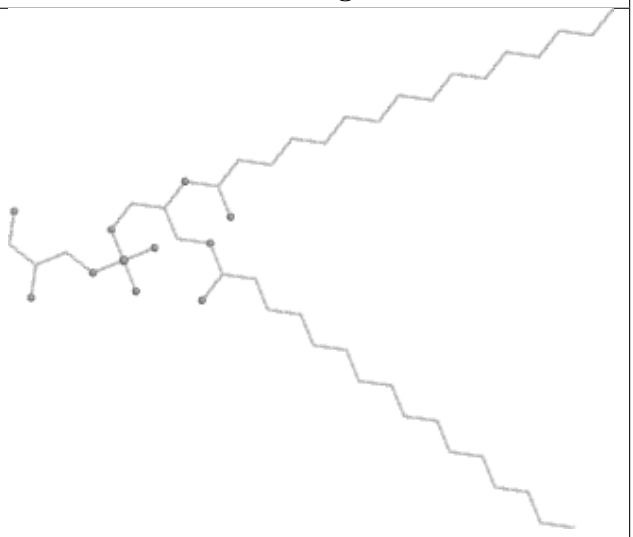
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Bond angles

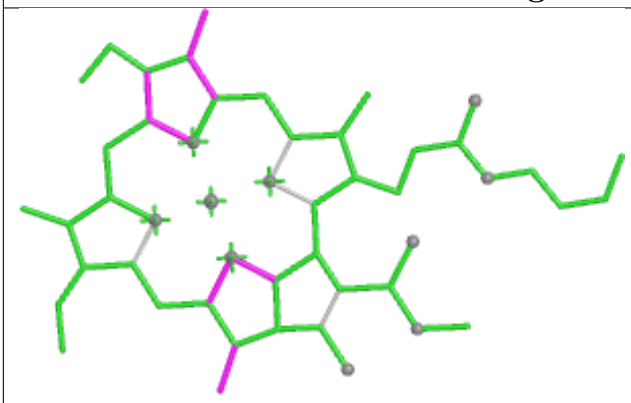


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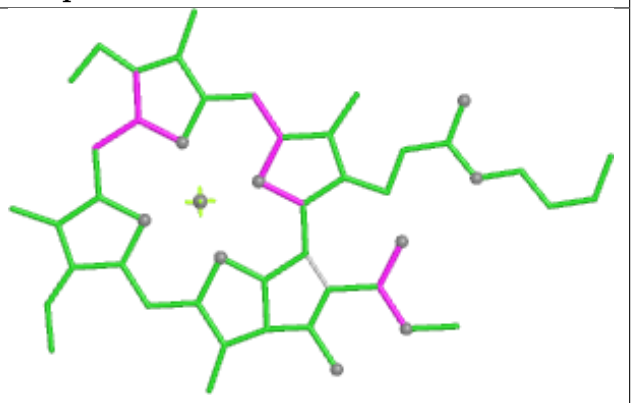


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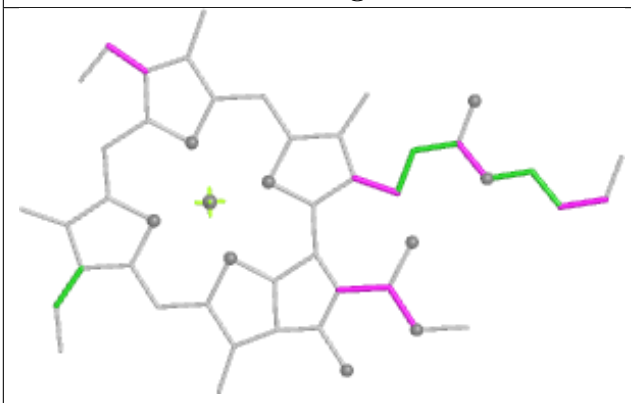
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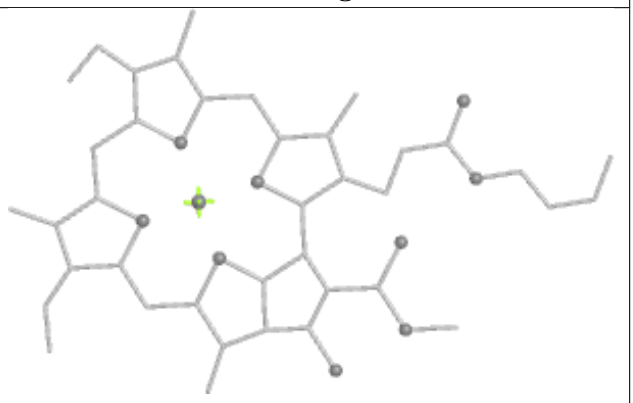
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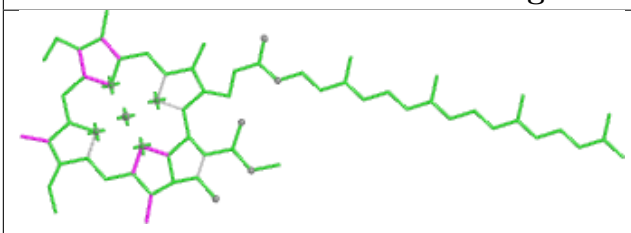


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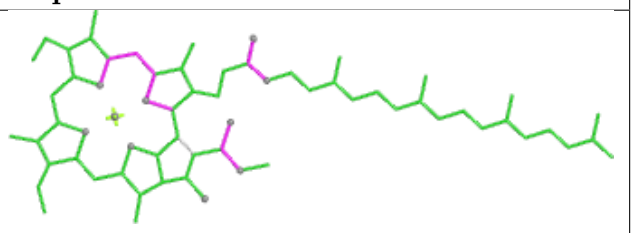


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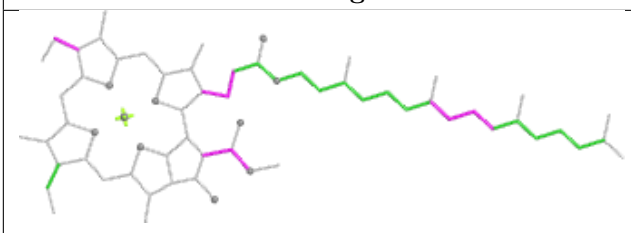
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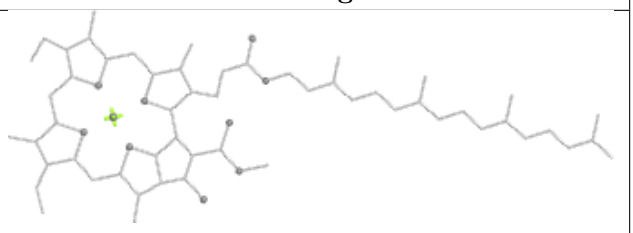
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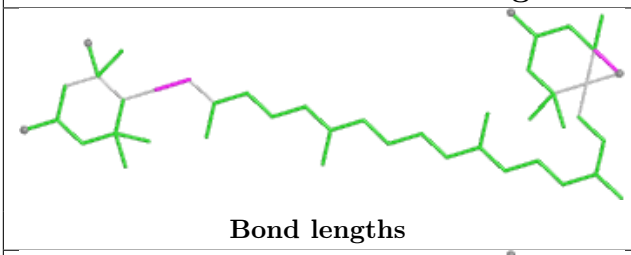


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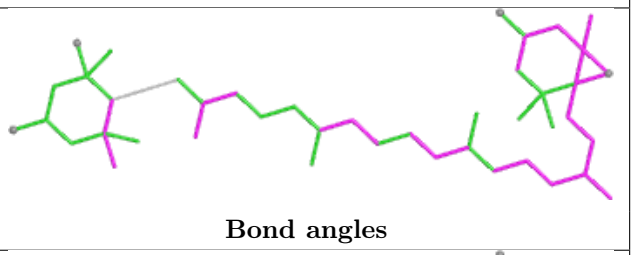


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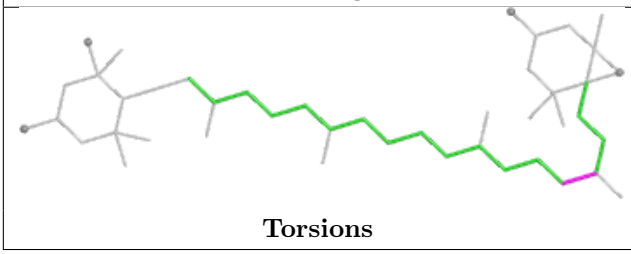
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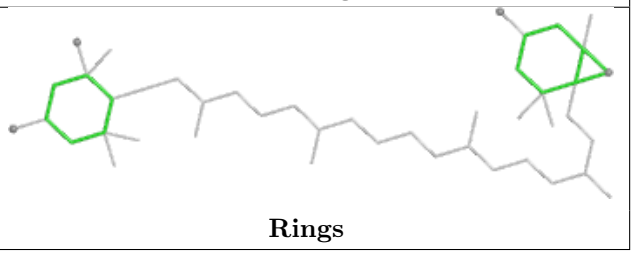
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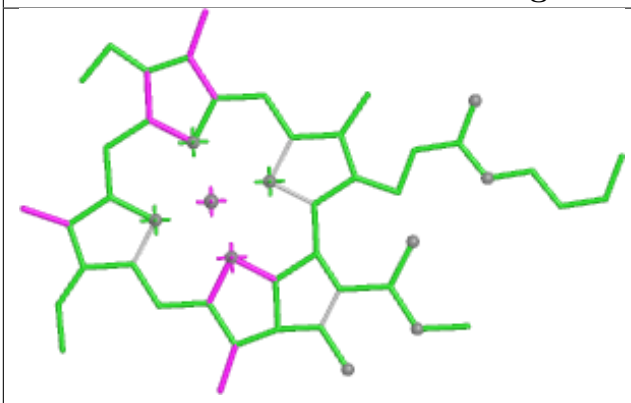


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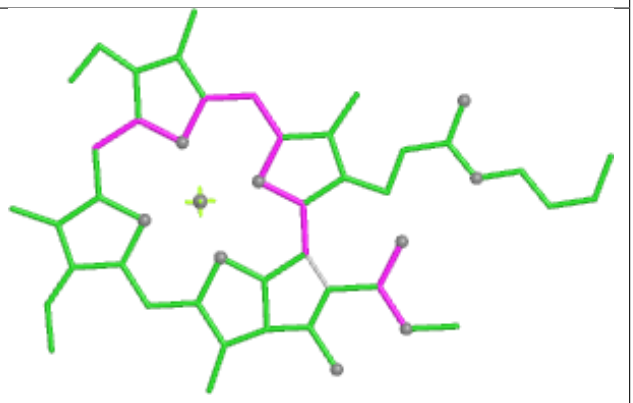


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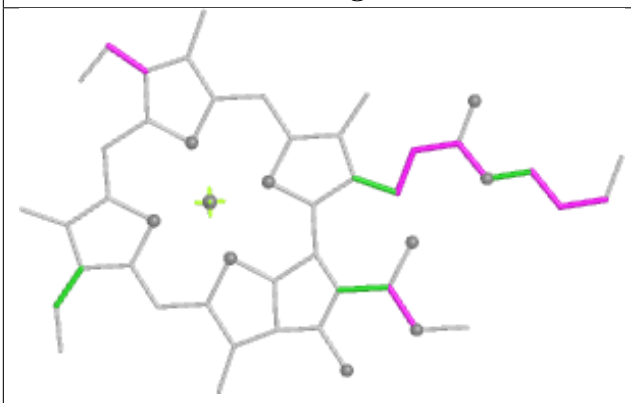
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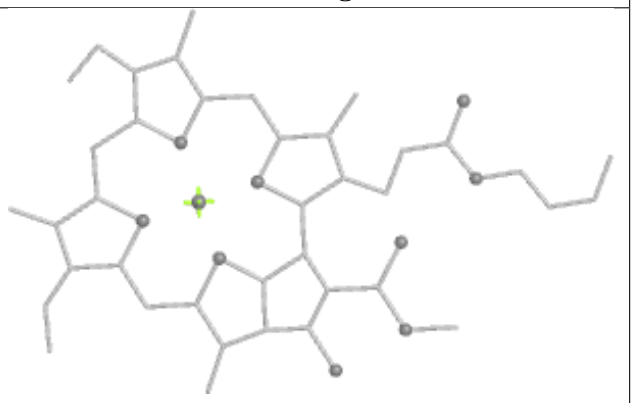
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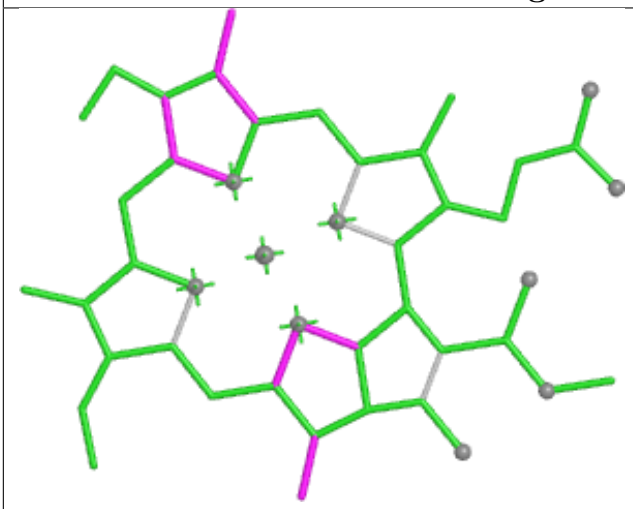


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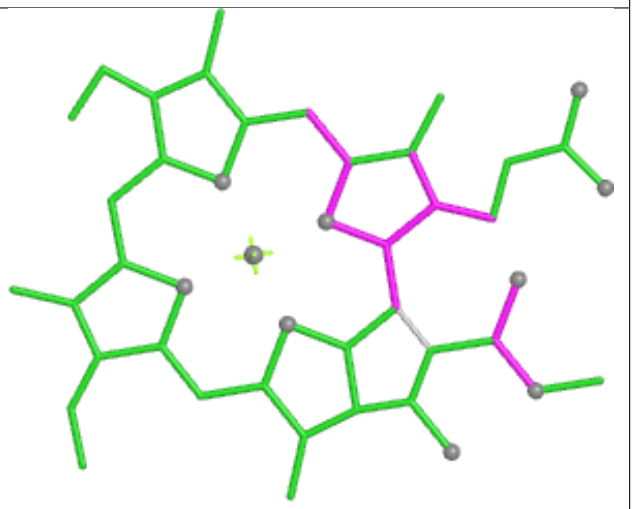


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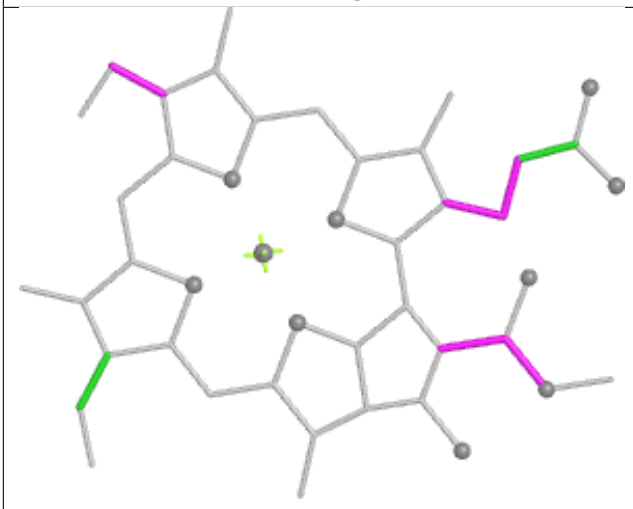
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Bond lengths



Bond angles

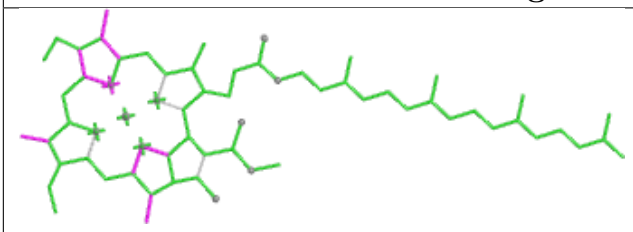


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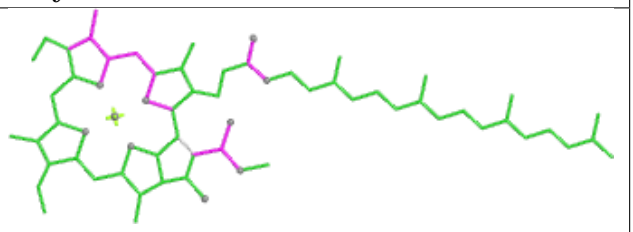


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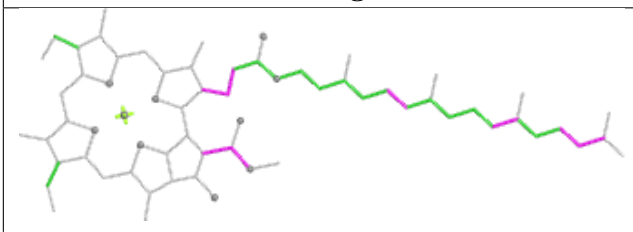
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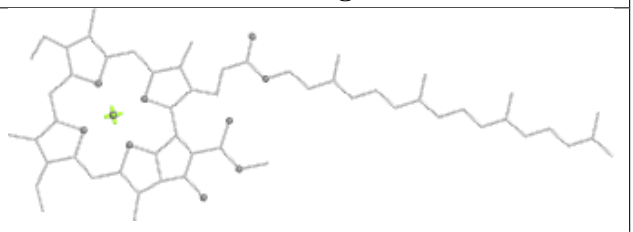
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Bond angles

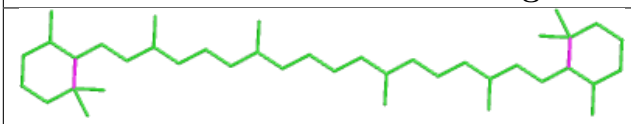


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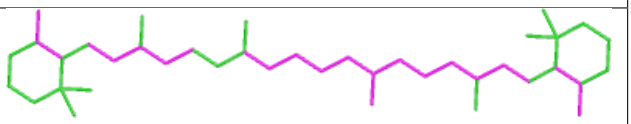


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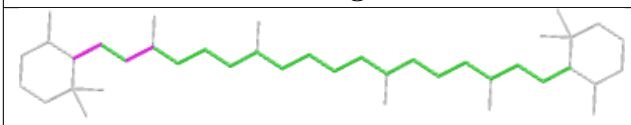
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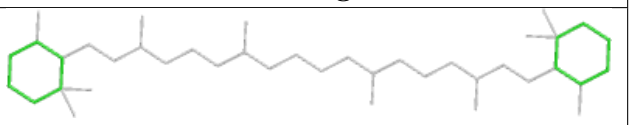
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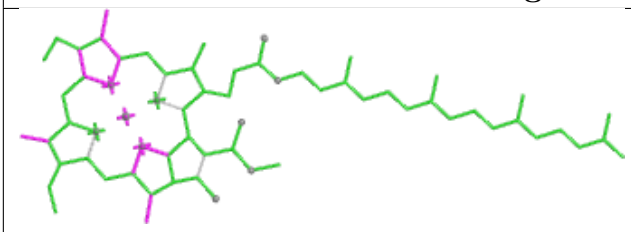


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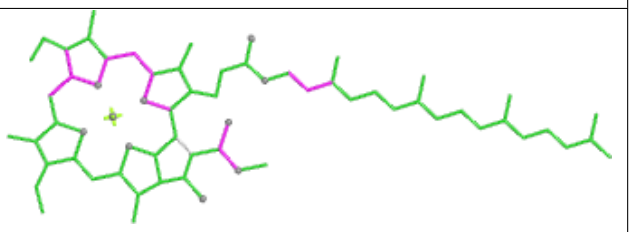


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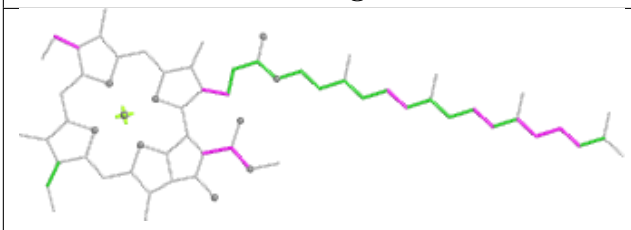
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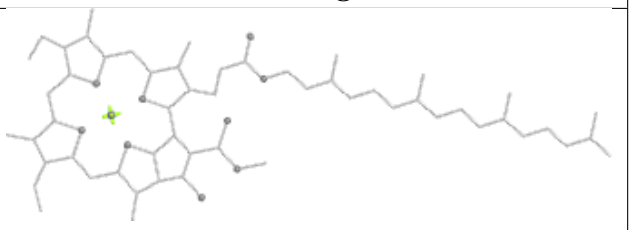
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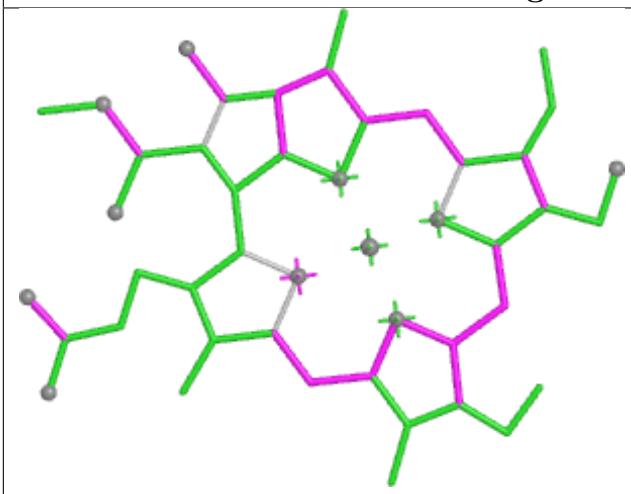


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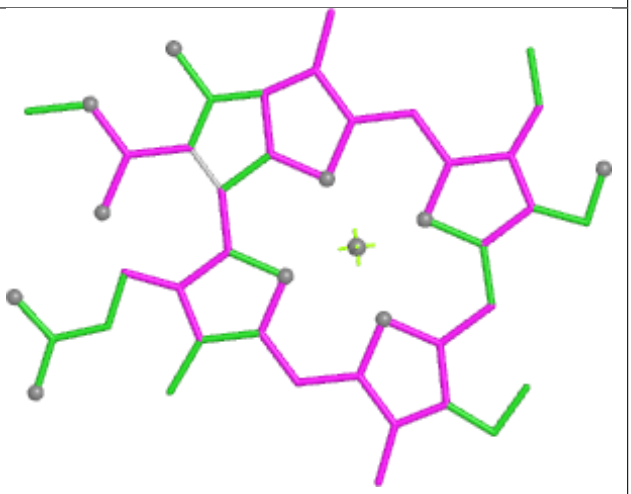


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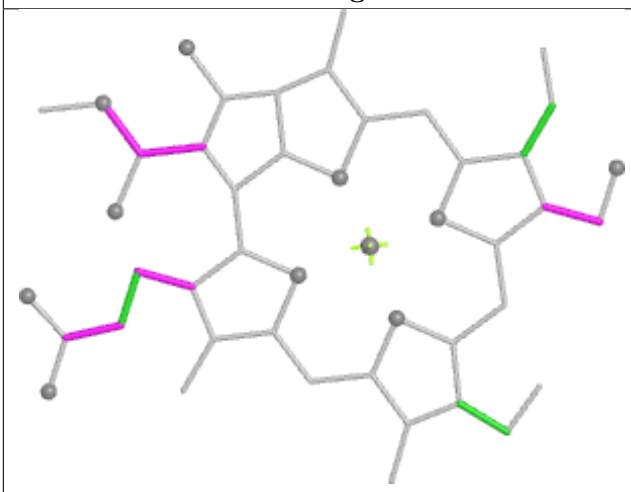
Ligand CHL n 606



Bond lengths



Bond angles

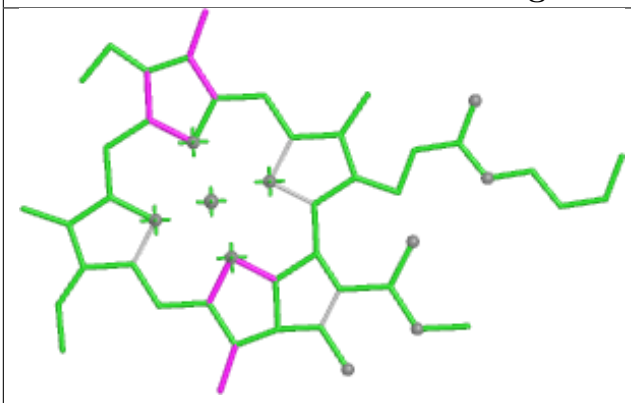


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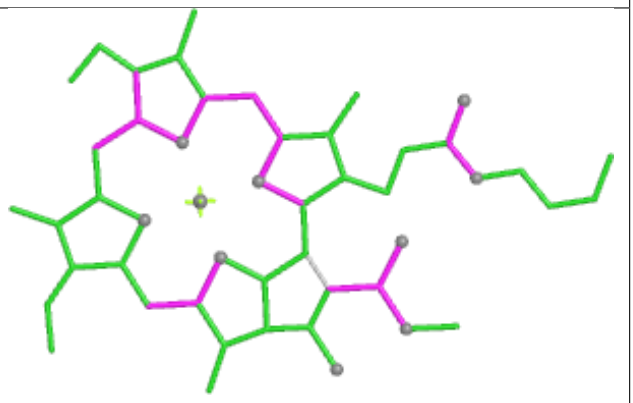


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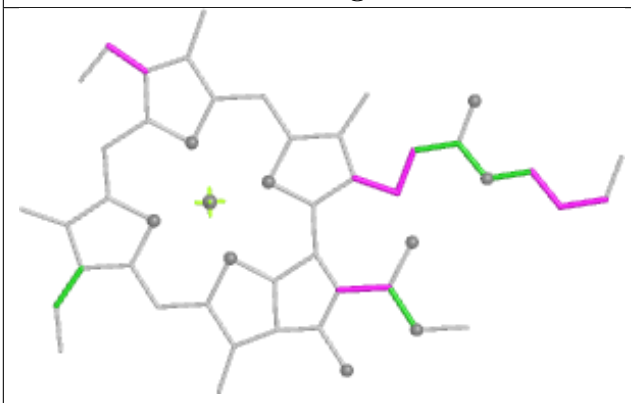
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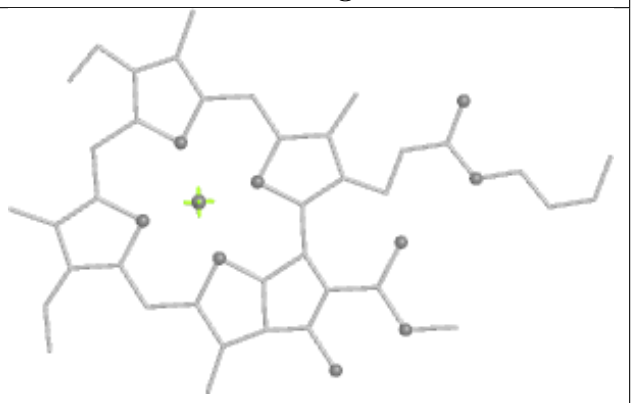
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Bond angles

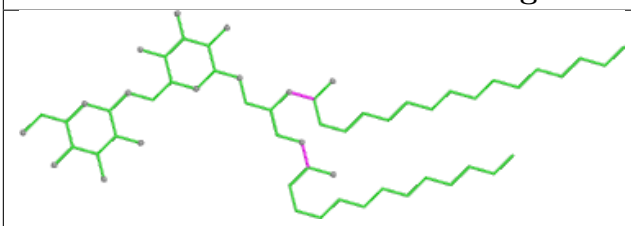


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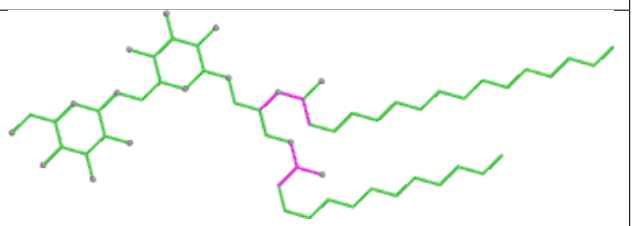


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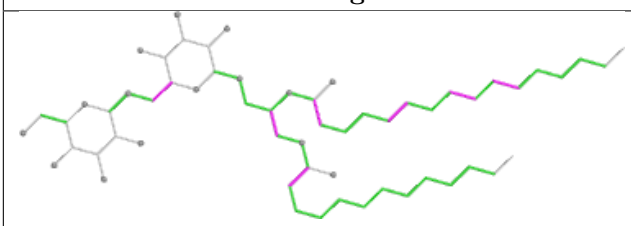
Ligand DGD C 520



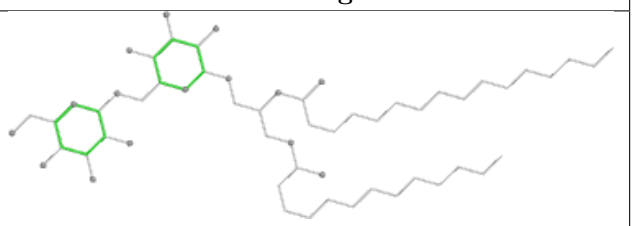
Bond lengths



Bond angles

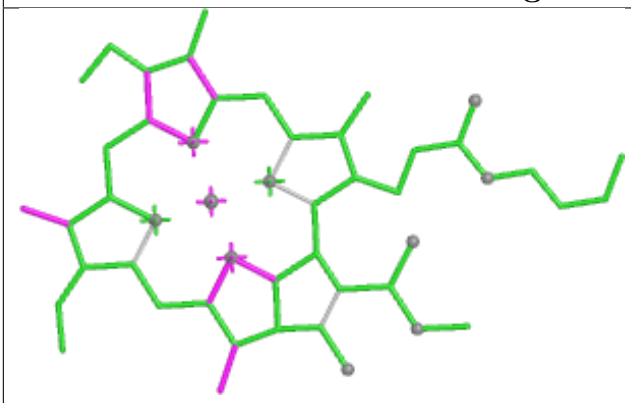


Torsions

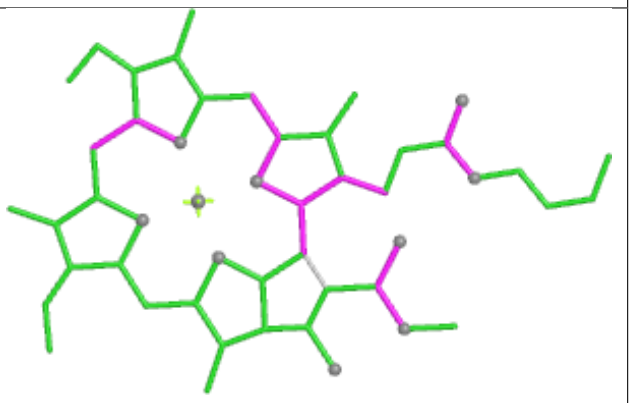


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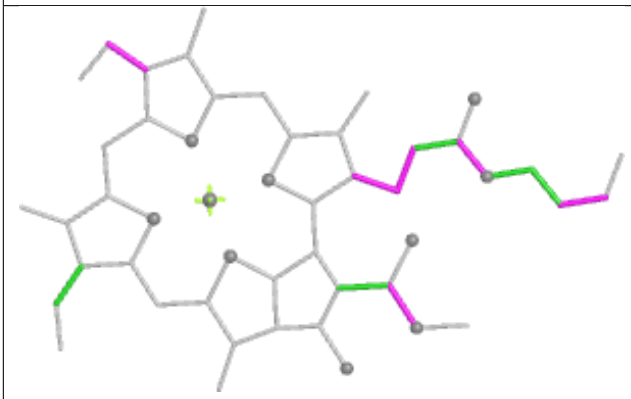
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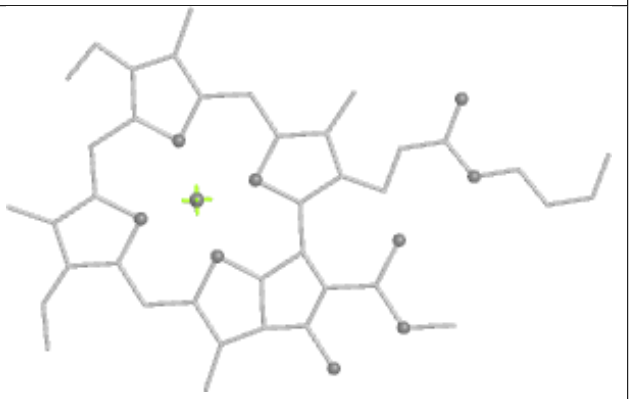
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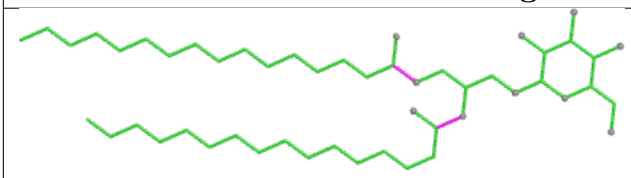


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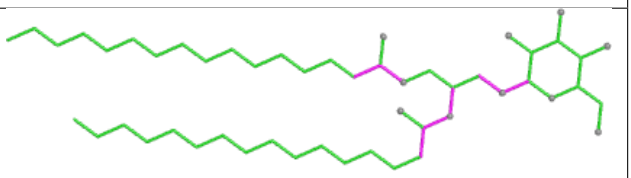


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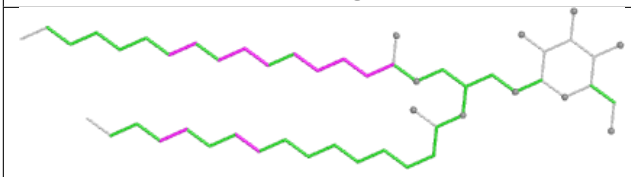
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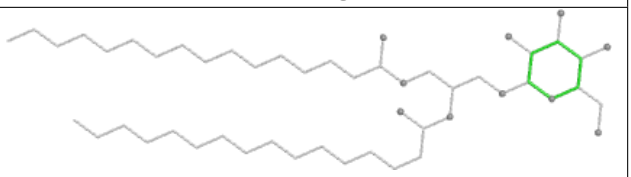
Bond lengths



Bond angles

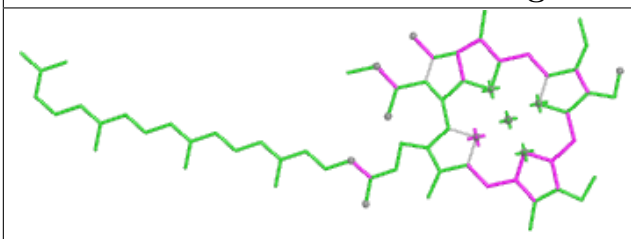


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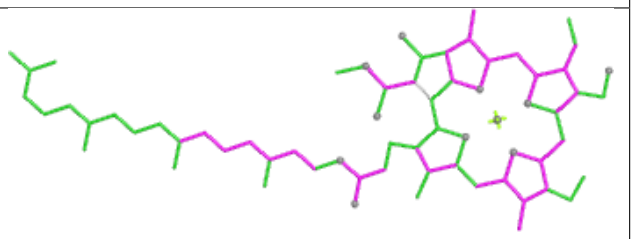


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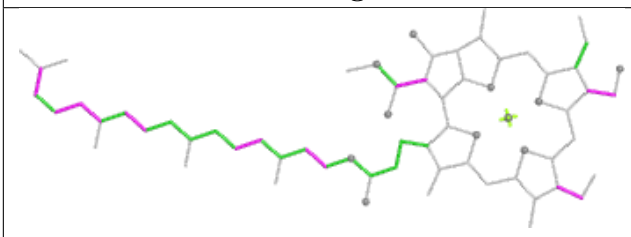
Ligand CHL 0 601



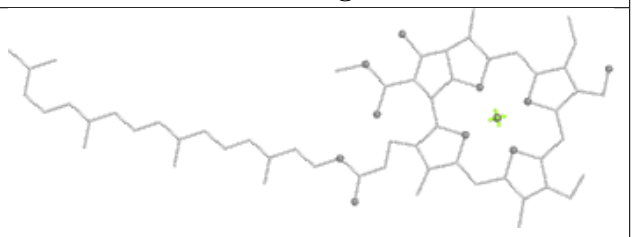
Bond lengths



Bond angles

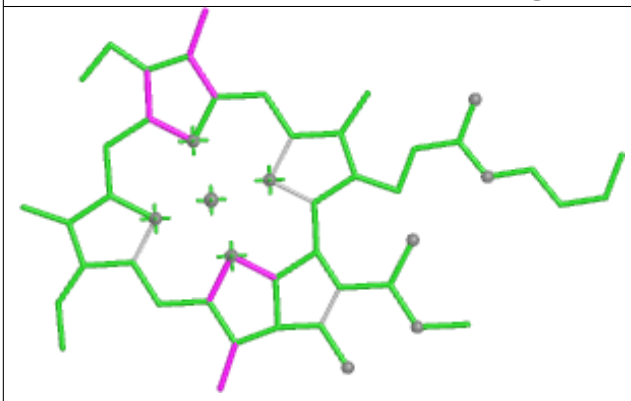


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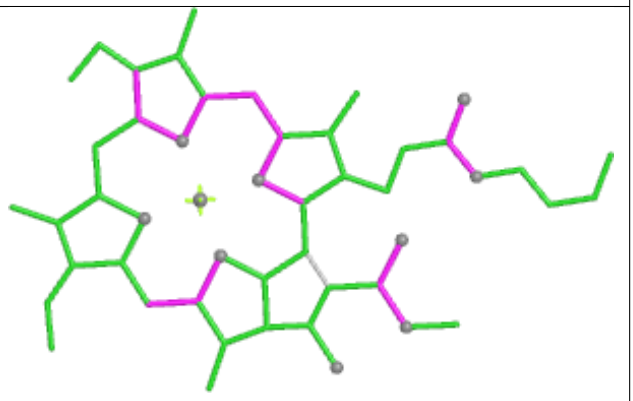


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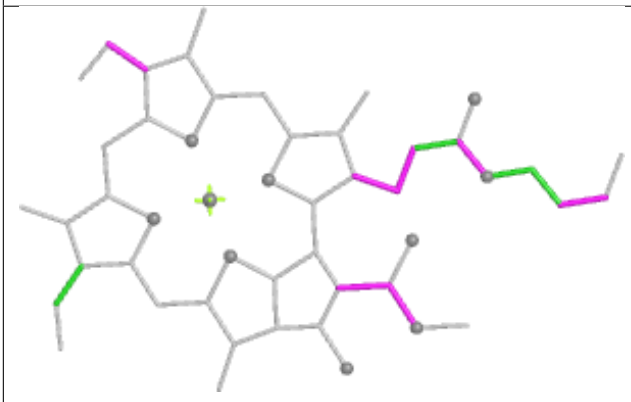
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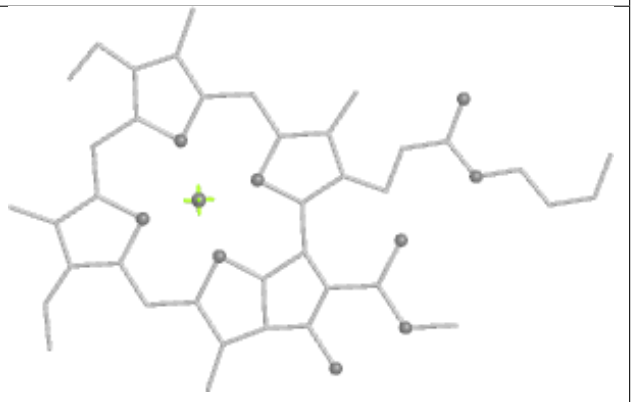
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Bond angles

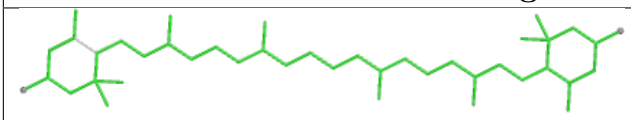


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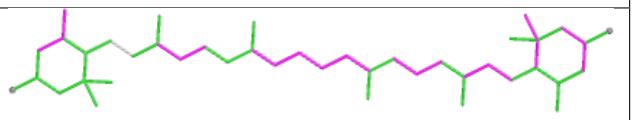


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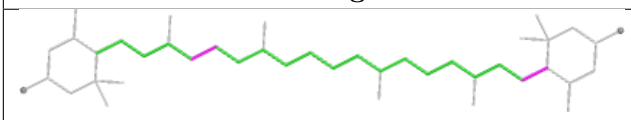
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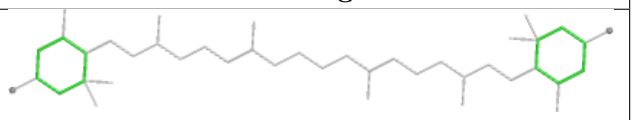
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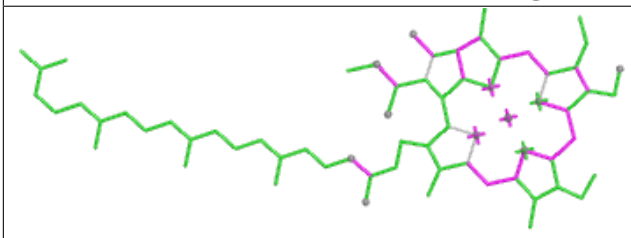


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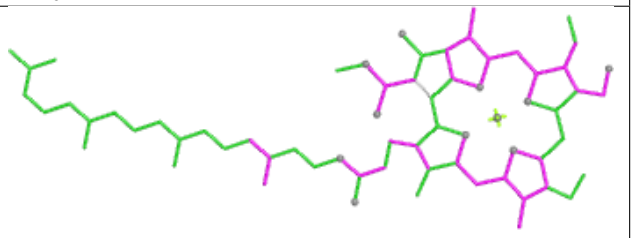


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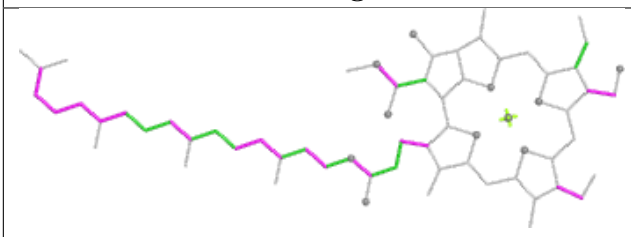
Ligand CHL y 606



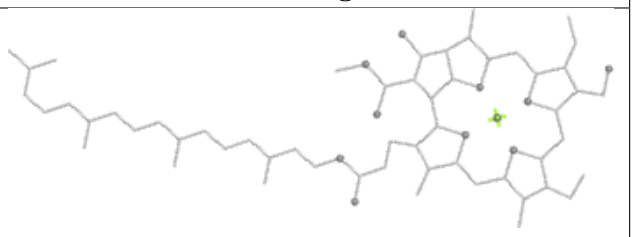
Bond lengths



Bond angles

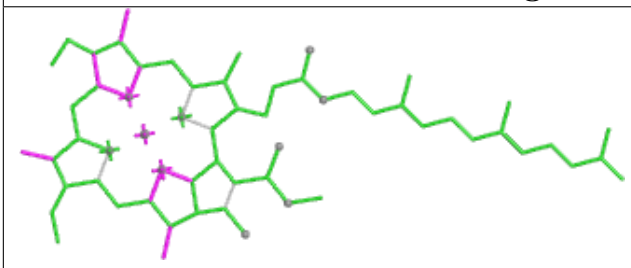


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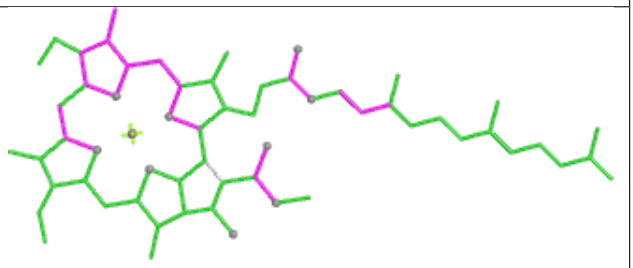


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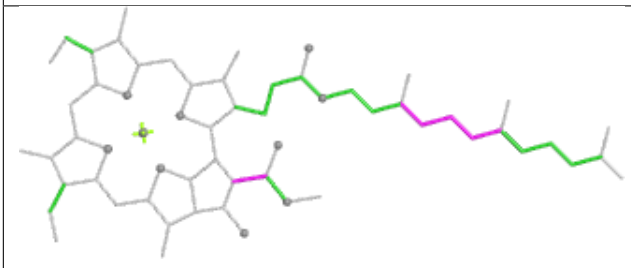
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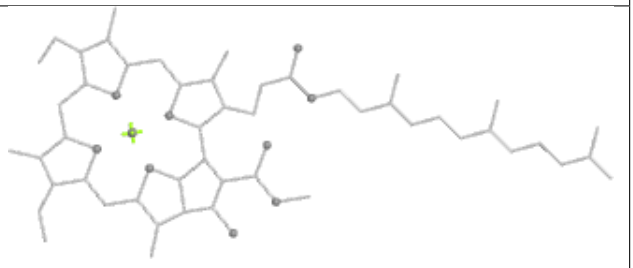
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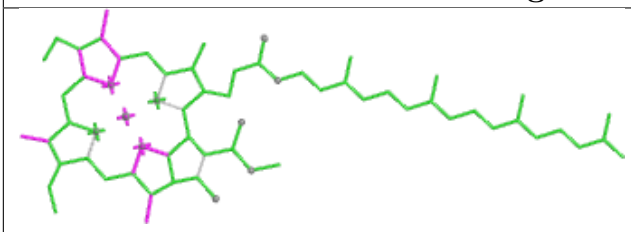


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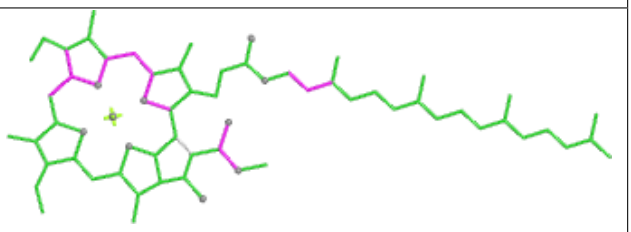


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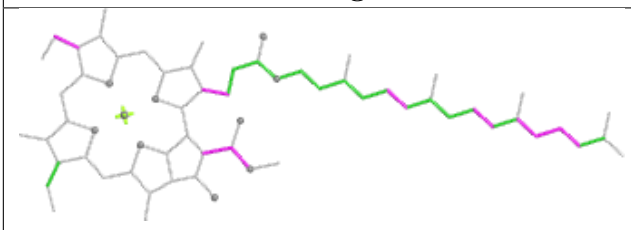
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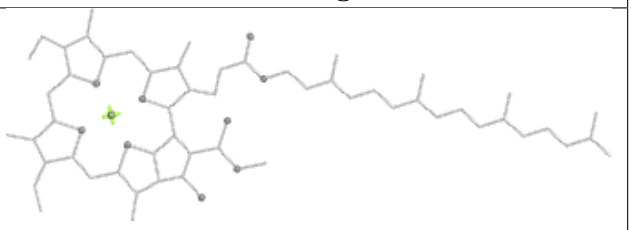
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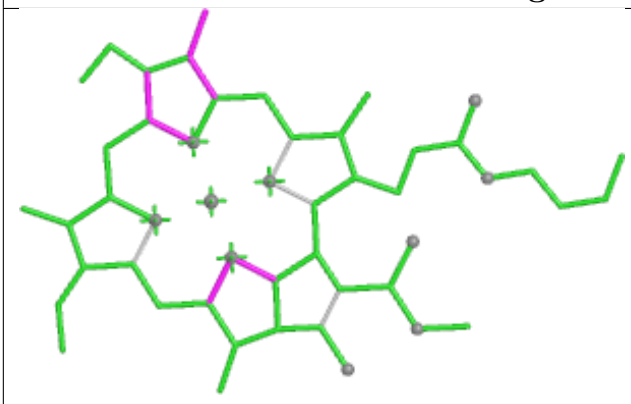


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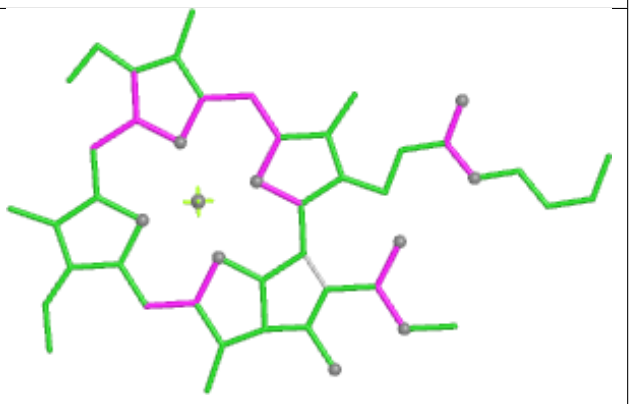


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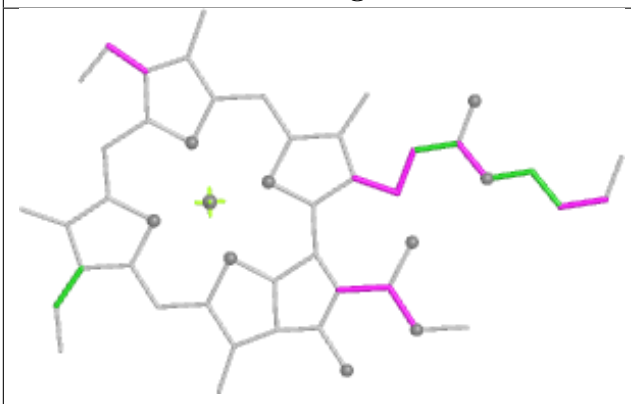
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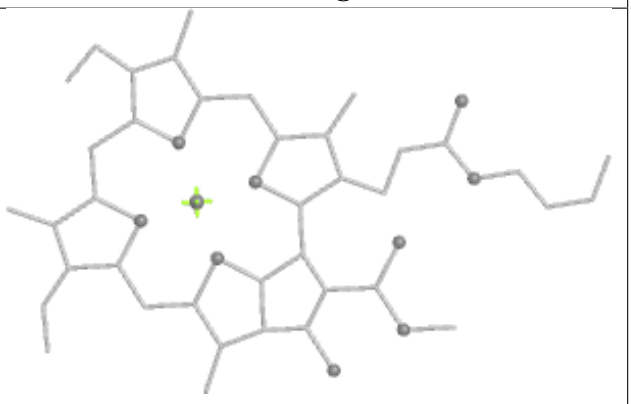
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Bond angles

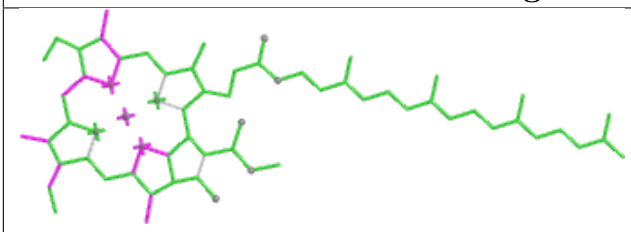


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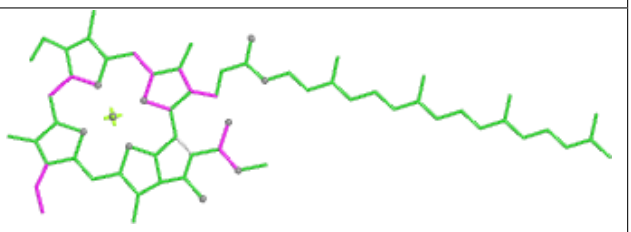


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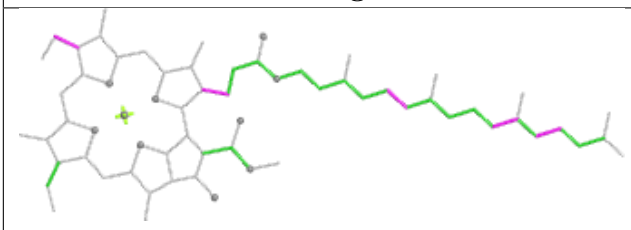
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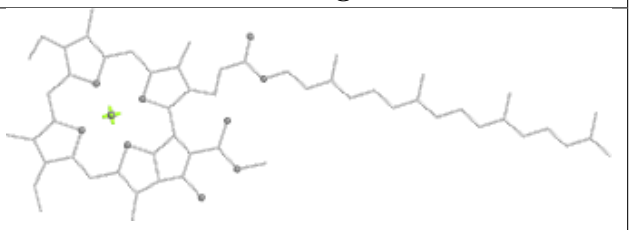
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Bond angles

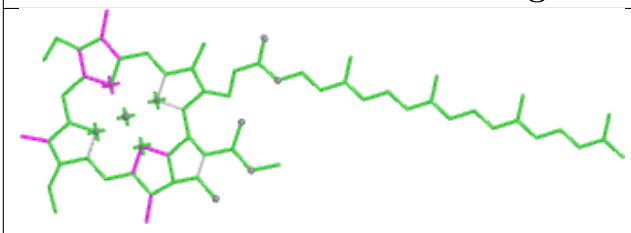


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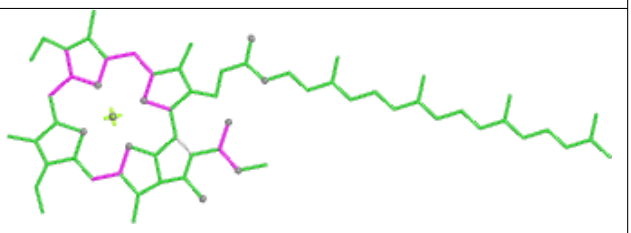


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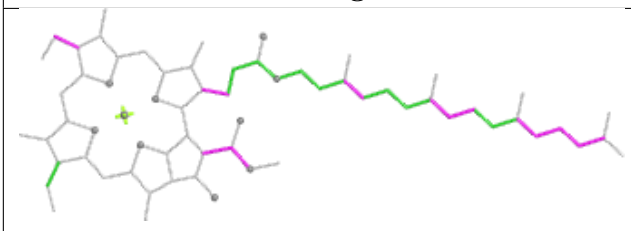
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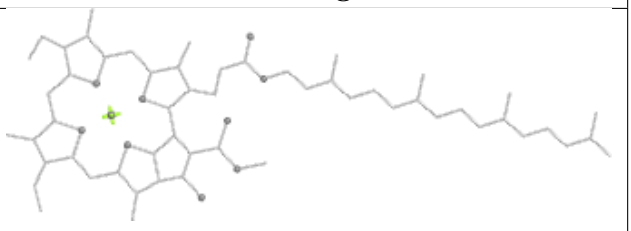
Bond lengths



Bond angles

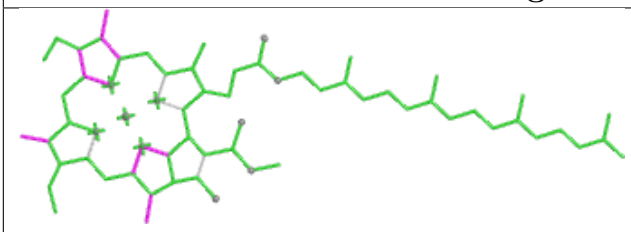


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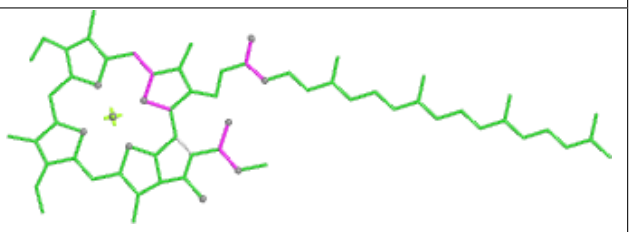


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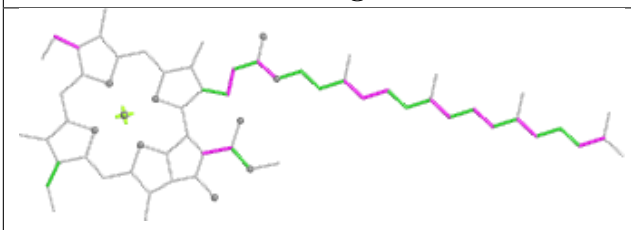
Ligand CLA n 613



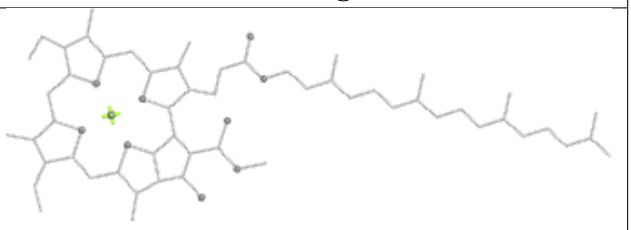
Bond lengths



Bond angles

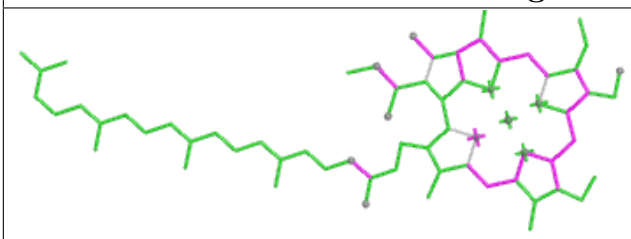


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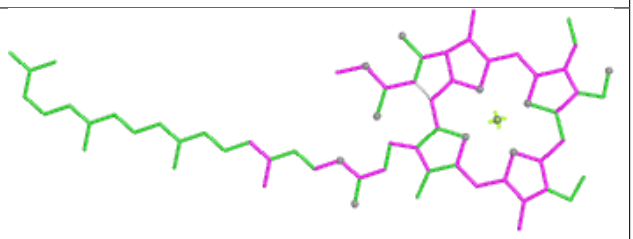


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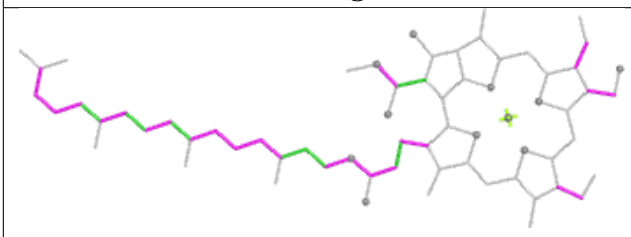
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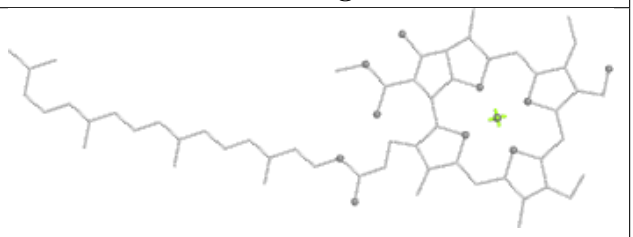
Bond lengths



Bond angles

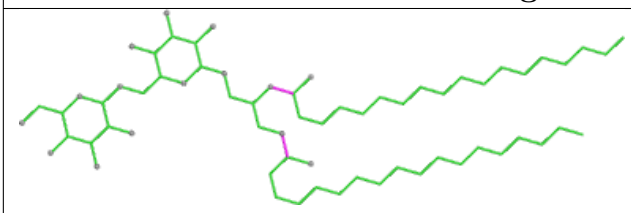


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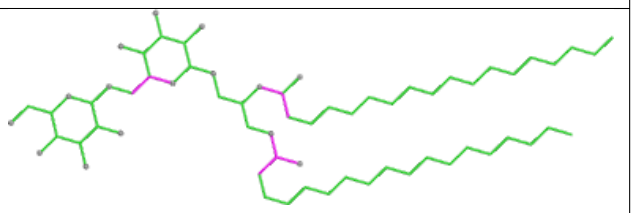


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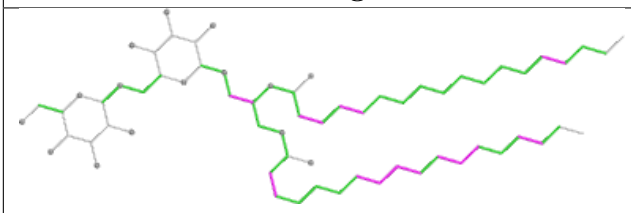
Ligand DGD C 523



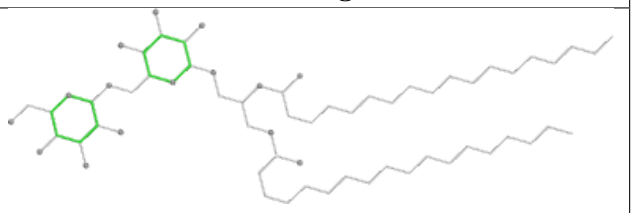
Bond lengths



Bond angles

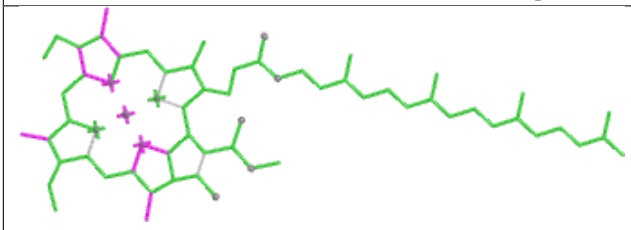


Torsions

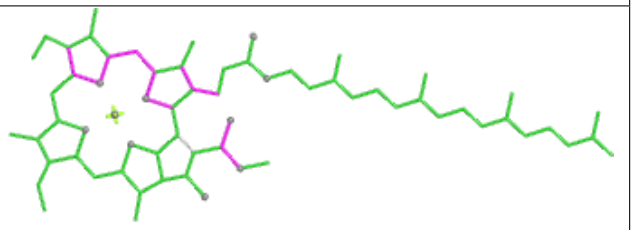


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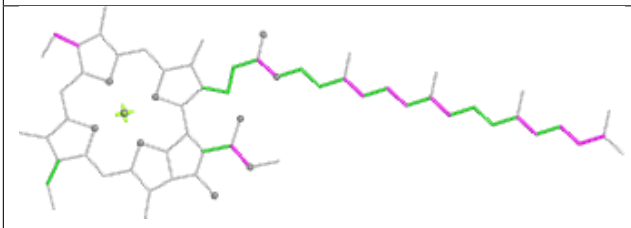
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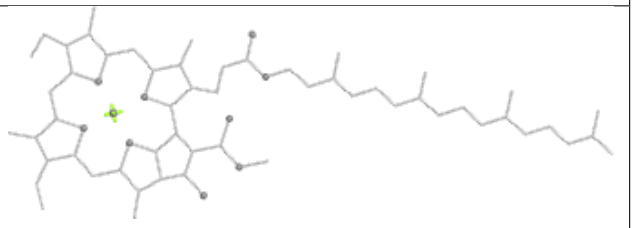
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Bond angles

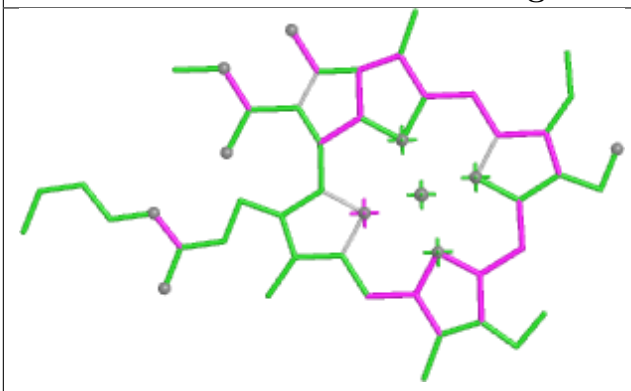


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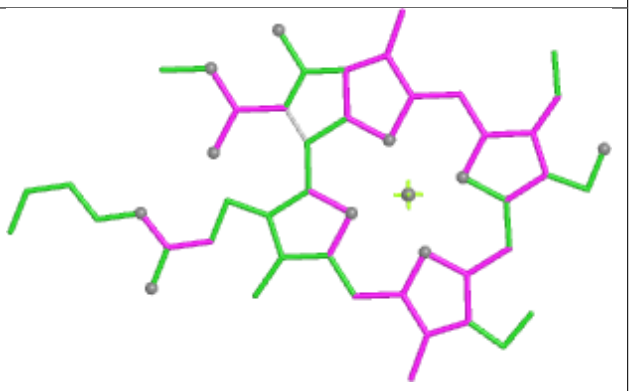


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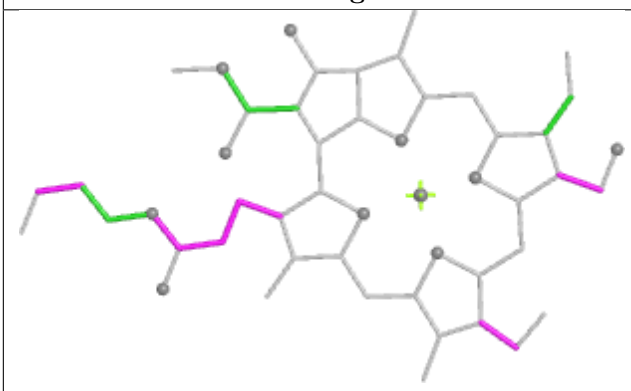
Ligand CHL 2 607



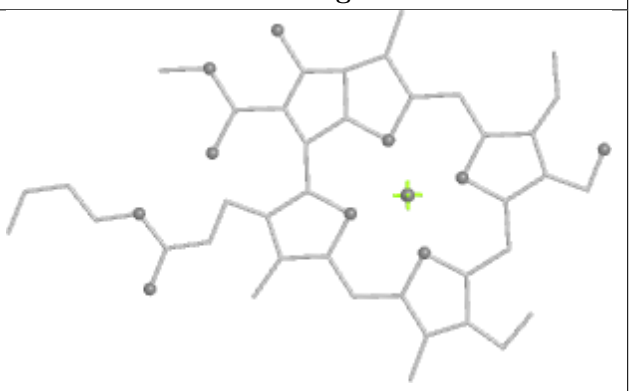
Bond lengths



Bond angles

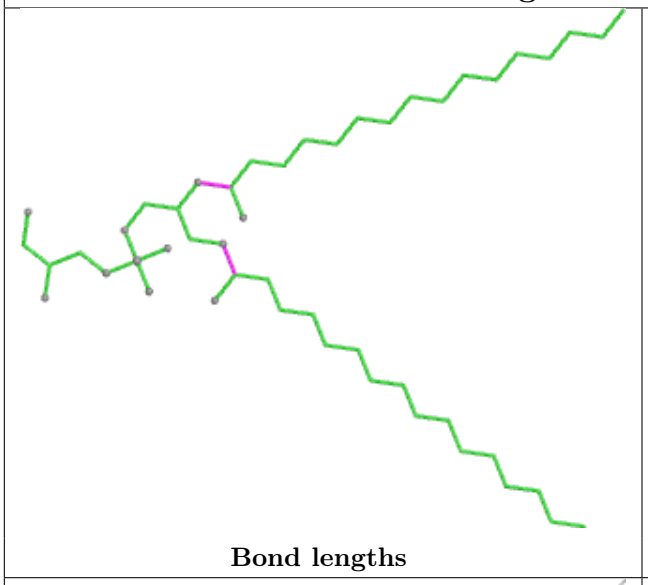


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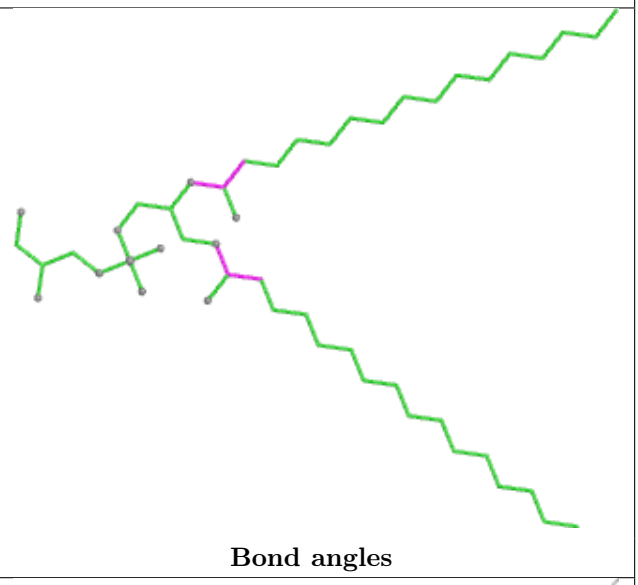


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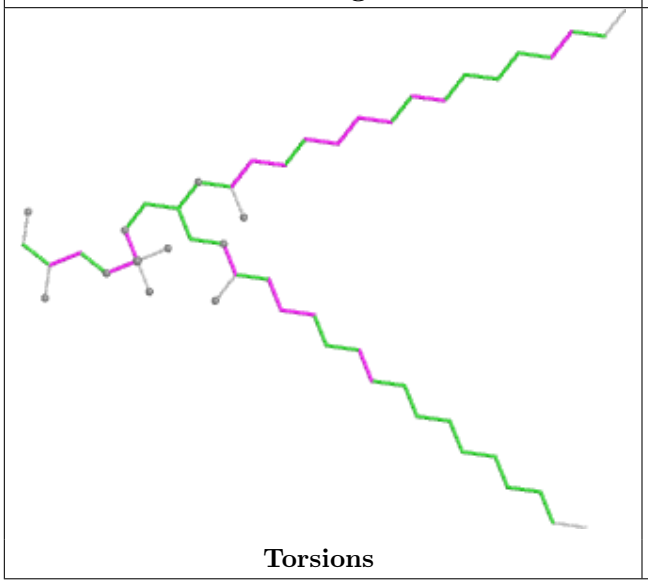
Ligand LHG 9 2630



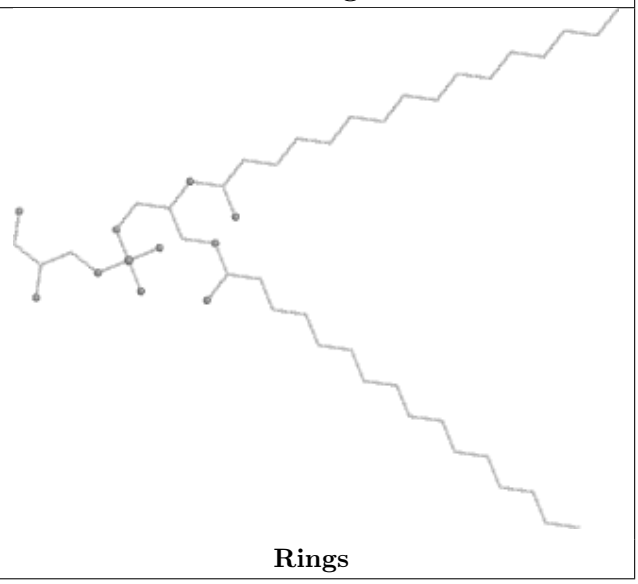
Bond lengths



Bond angles

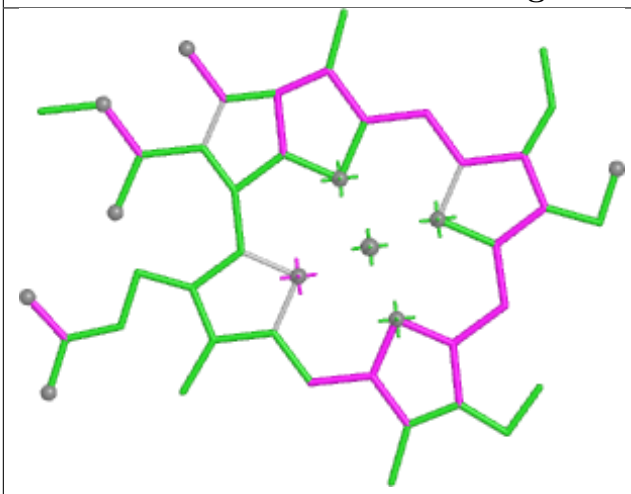


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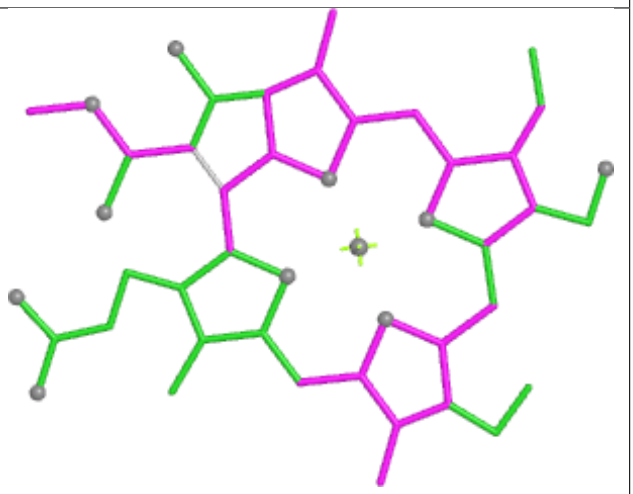


Rings

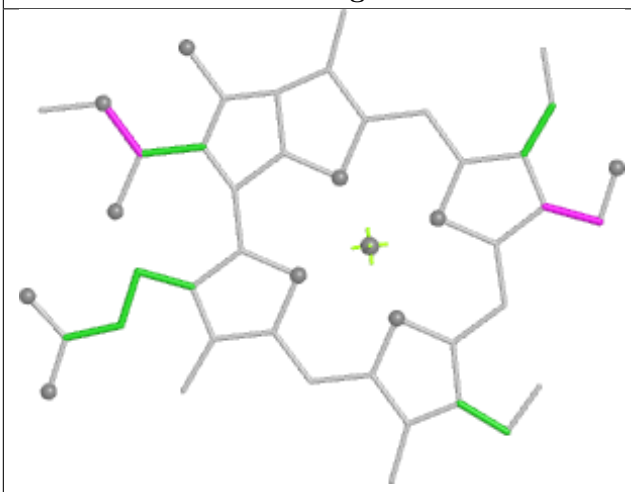
Ligand CHL 5 606



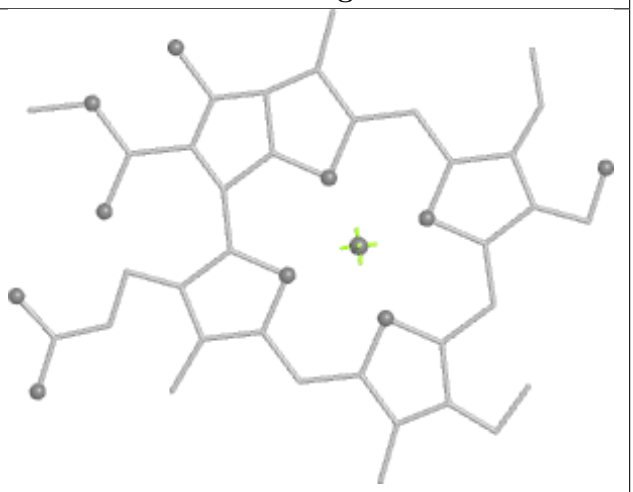
Bond lengths



Bond angles

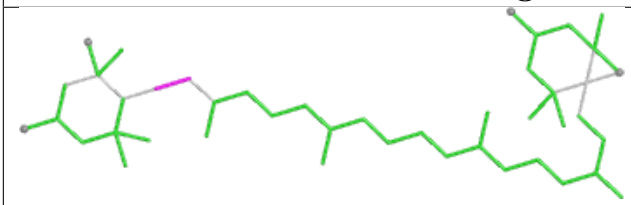


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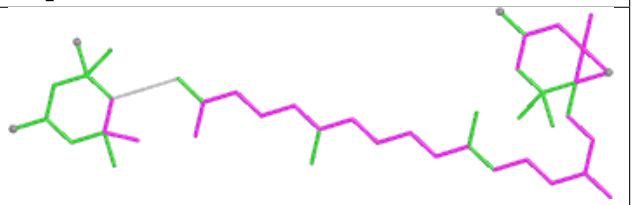


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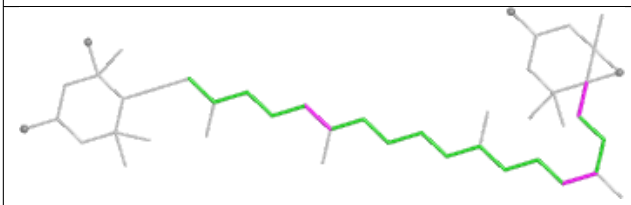
Ligand NEX p 1623



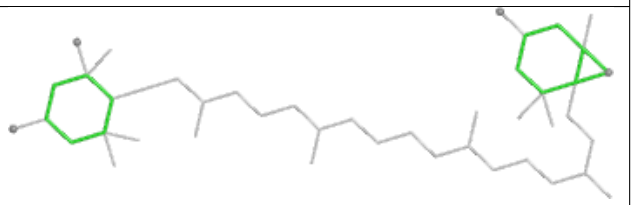
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Bond angles

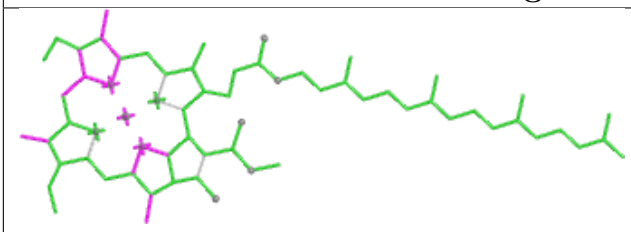


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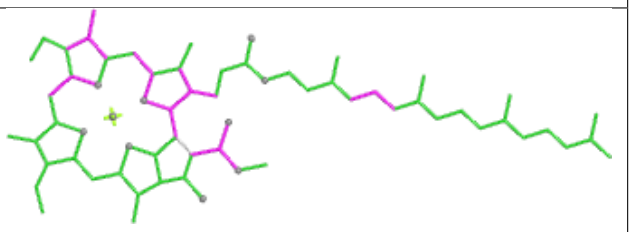


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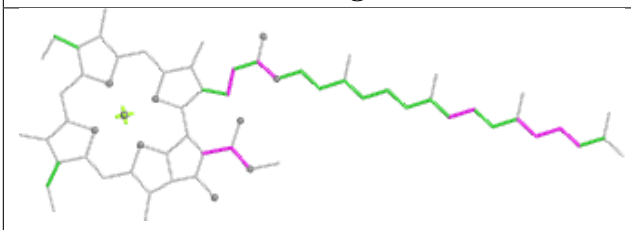
Ligand CLA C 507



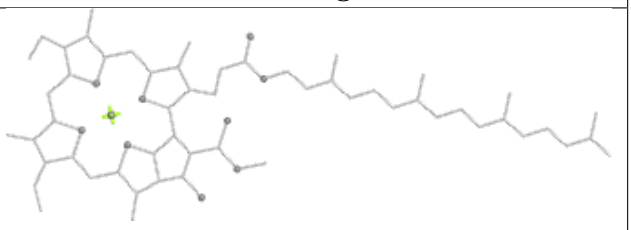
Bond lengths



Bond angles

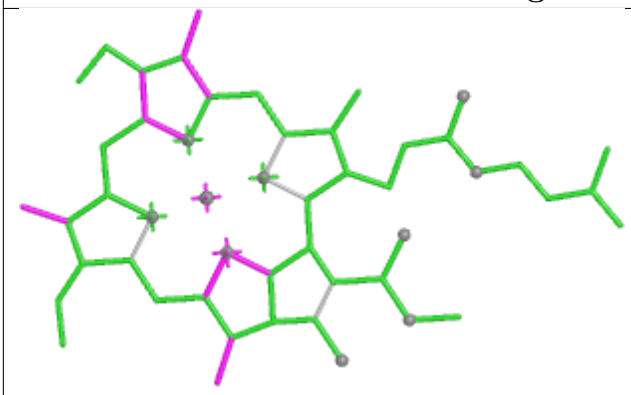


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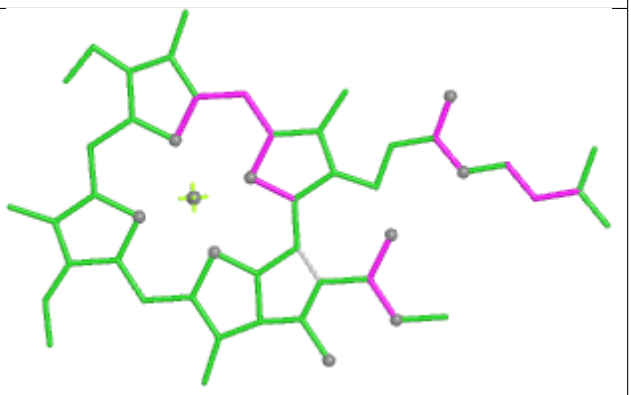


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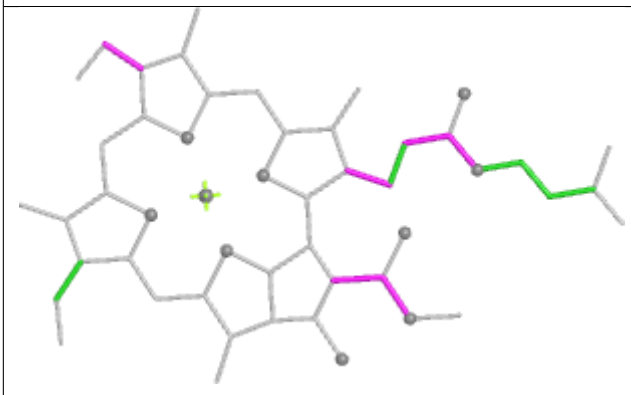
Ligand CLA S 605



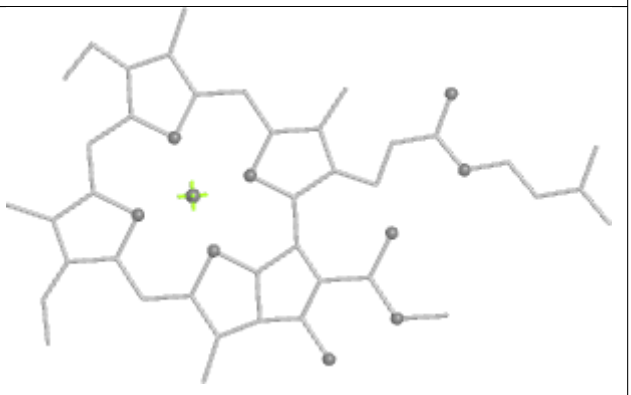
Bond lengths



Bond angles

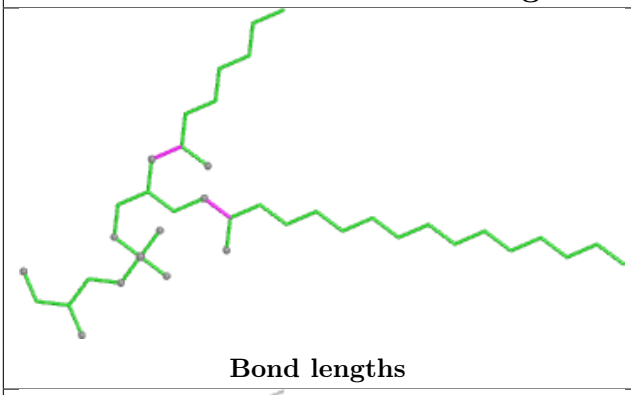


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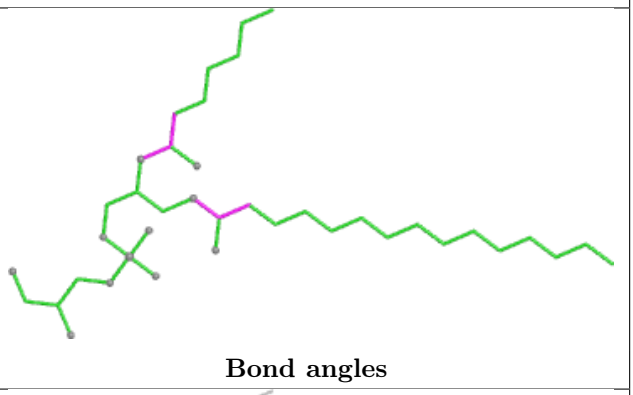


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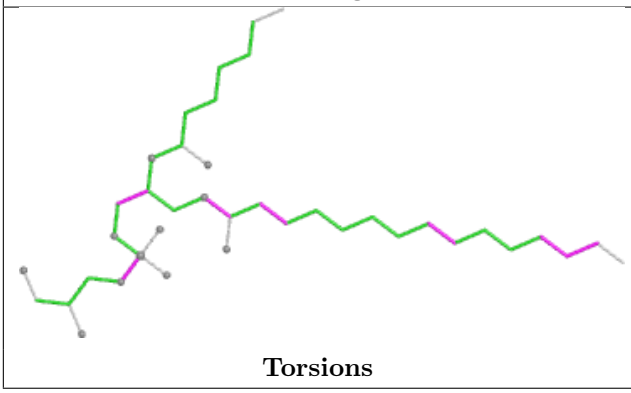
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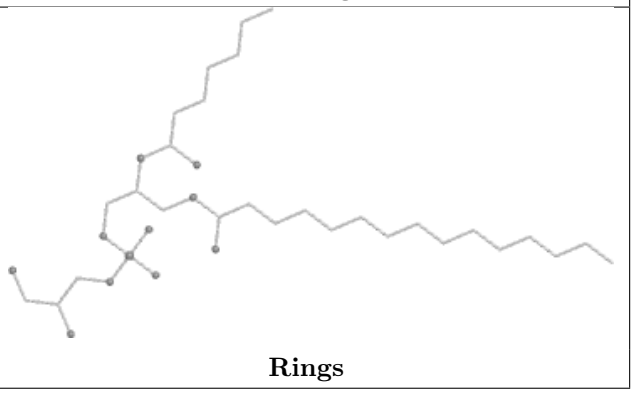
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Bond angles

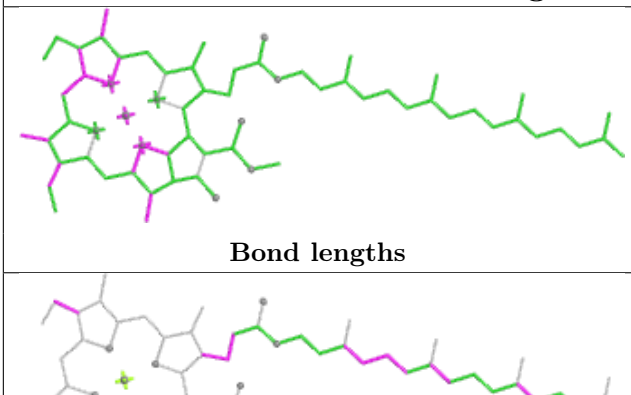


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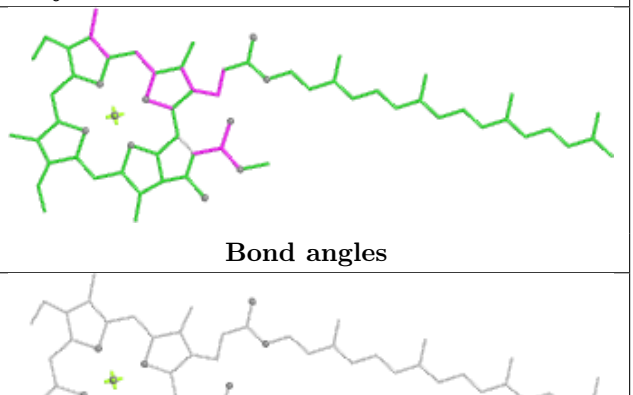


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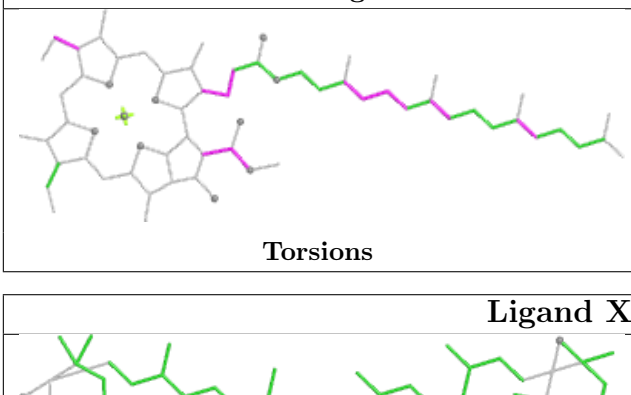
Ligand CLA y 603



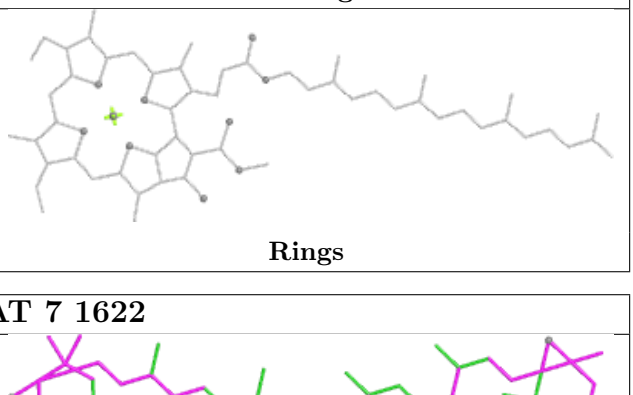
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Bond angles

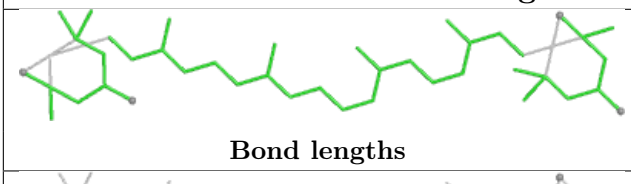


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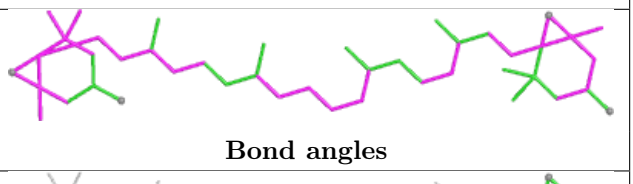


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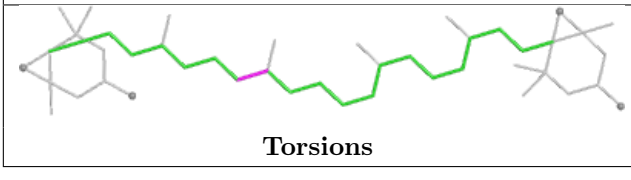
Ligand XAT 7 1622



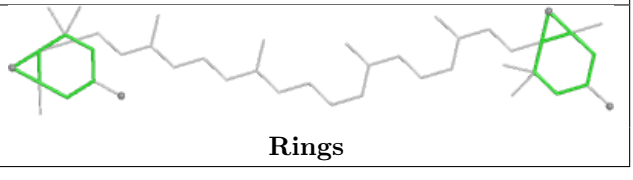
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Bond angles

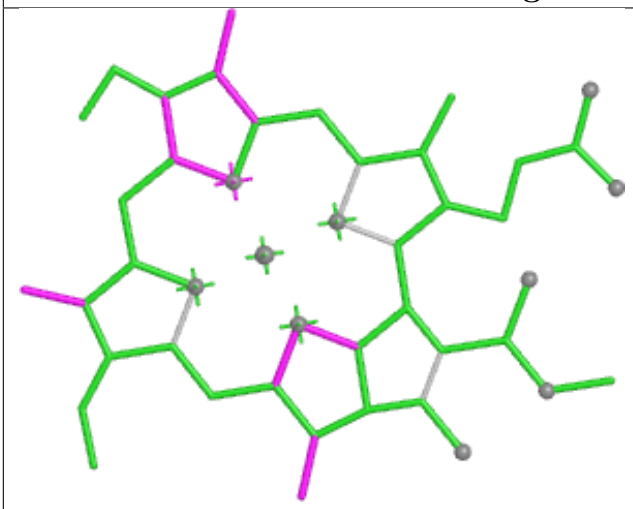


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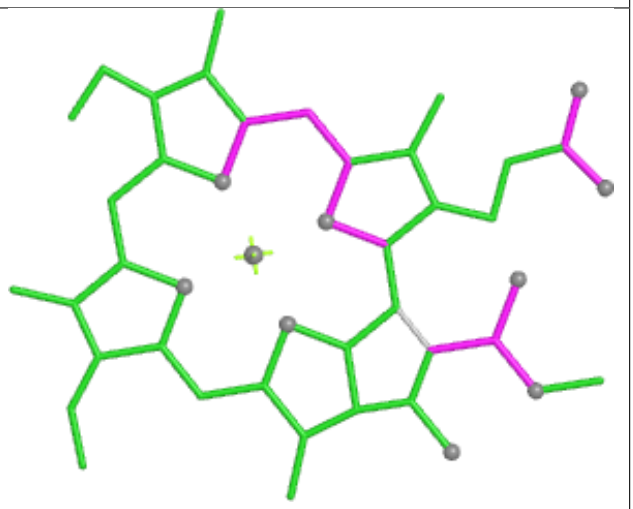


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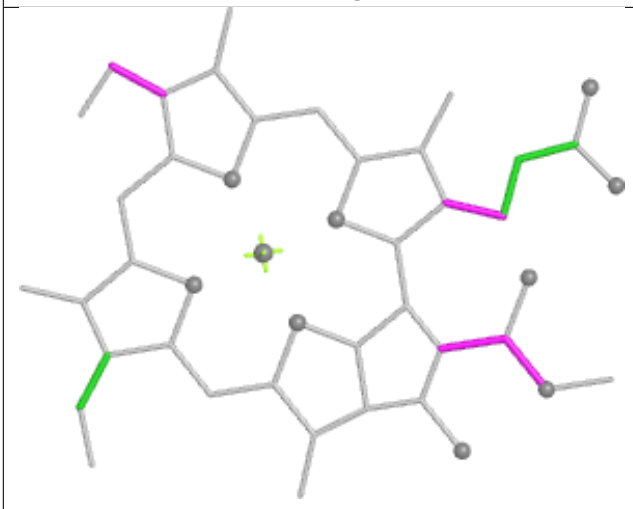
Ligand CLA G 611



Bond lengths



Bond angles

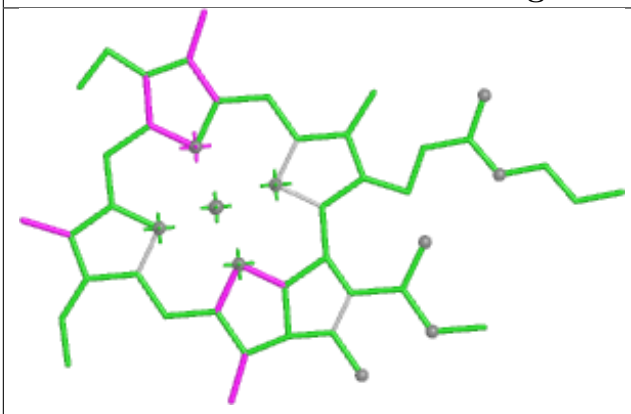


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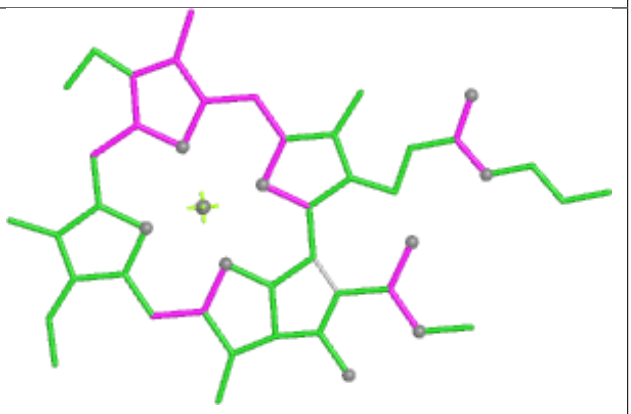


Rings

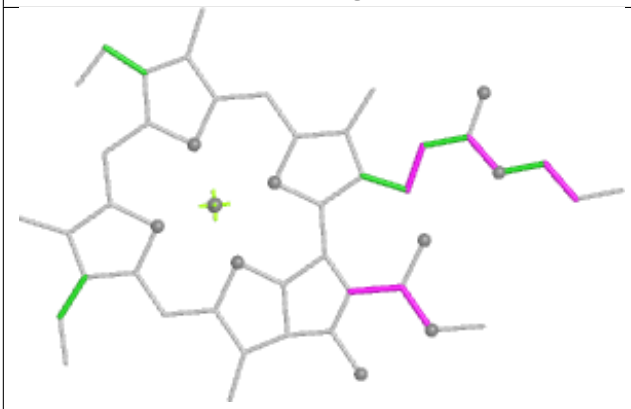
Ligand CLA S 614



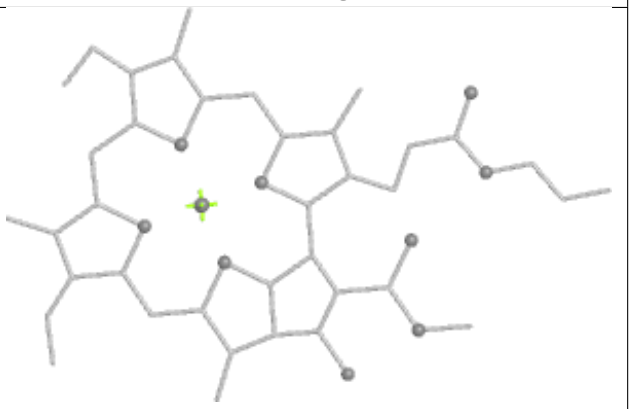
Bond lengths



Bond angles

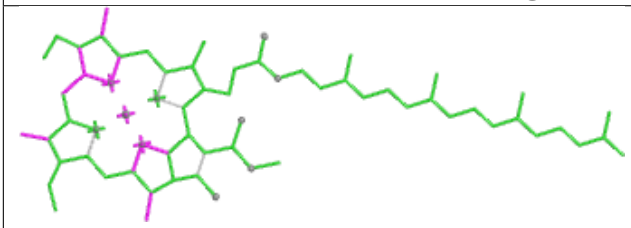


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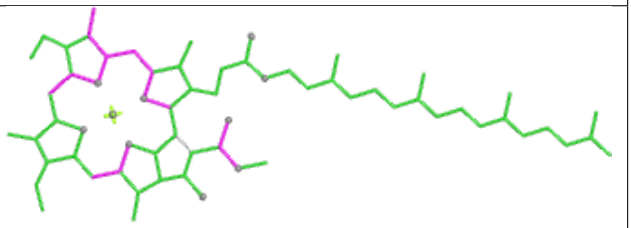


Rings

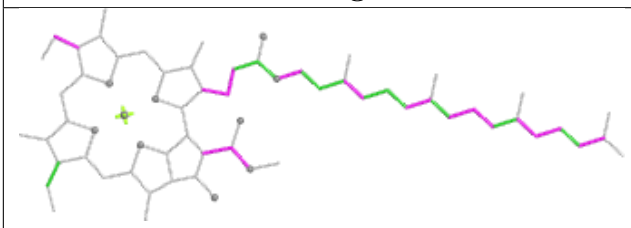
Ligand CLA Y 604



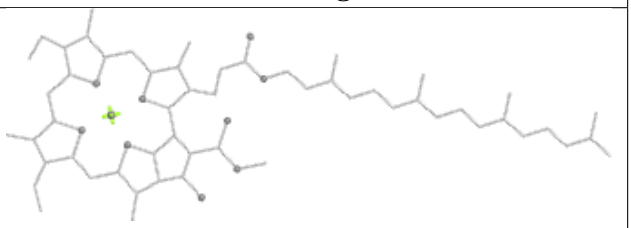
Bond lengths



Bond angles

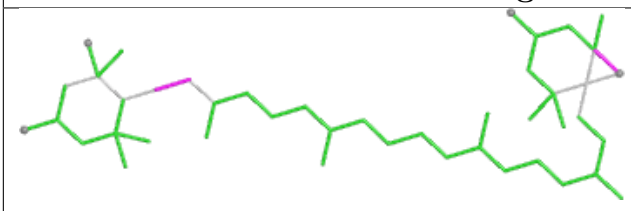


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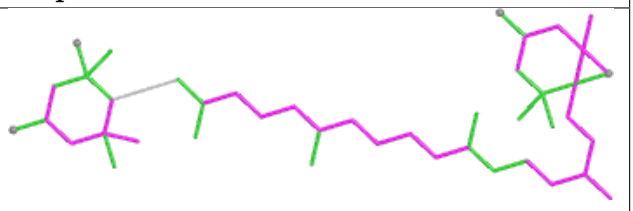


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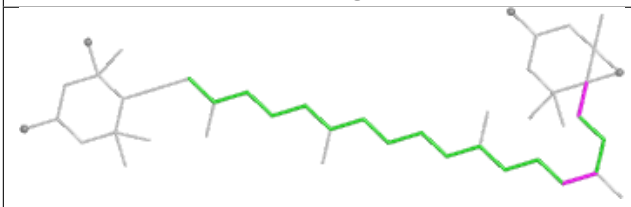
Ligand NEX q 1623



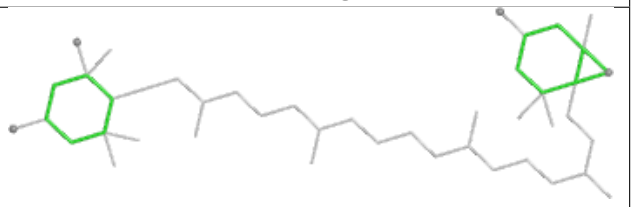
Bond lengths



Bond angles

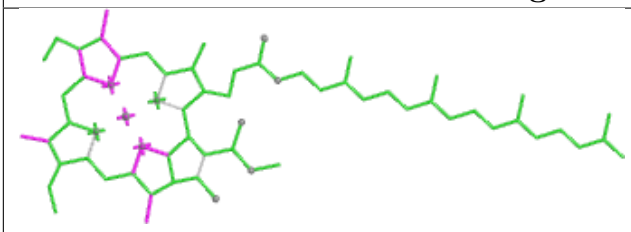


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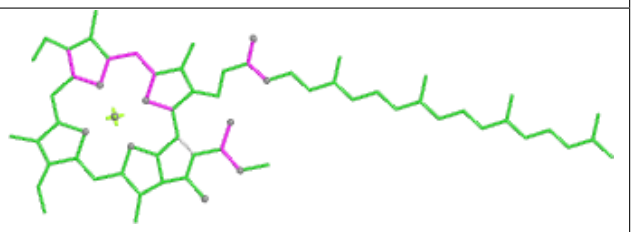


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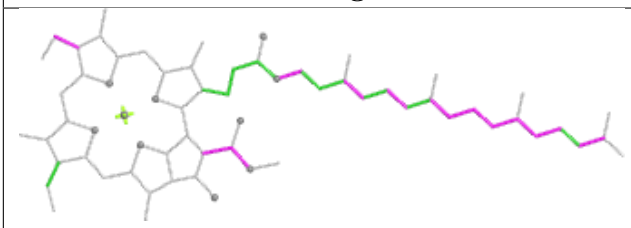
Ligand CLA c 506



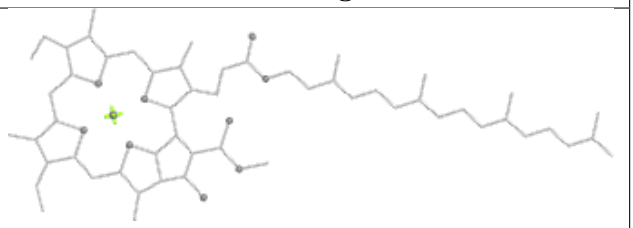
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Bond angles

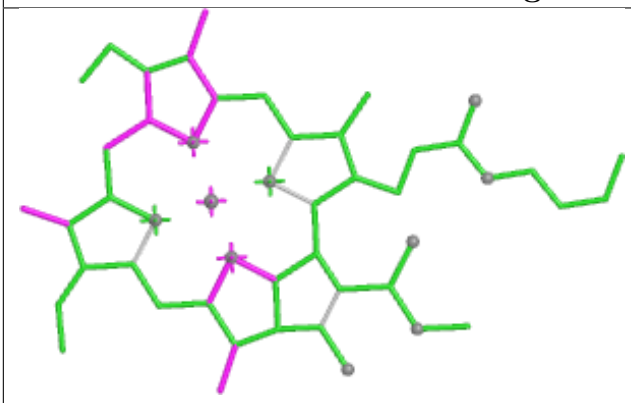


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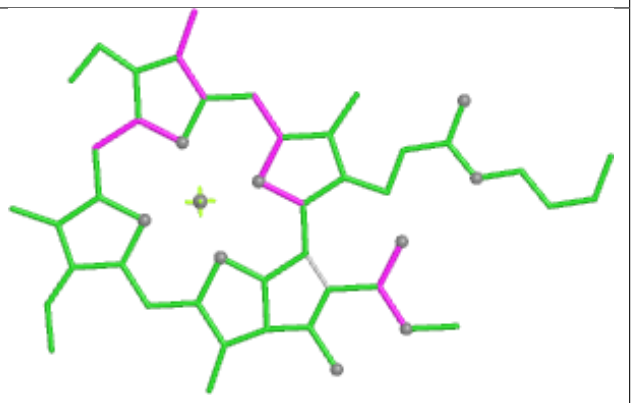


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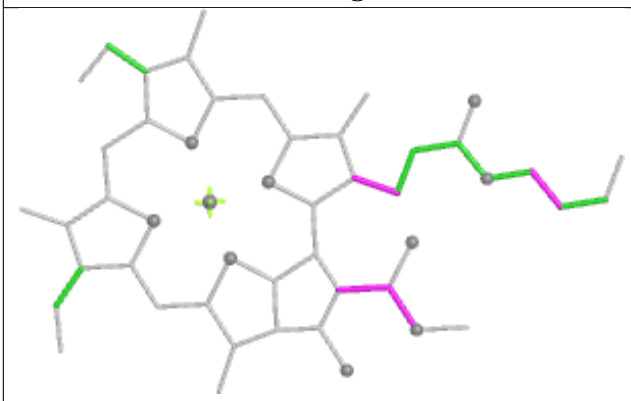
Ligand CLA A 407



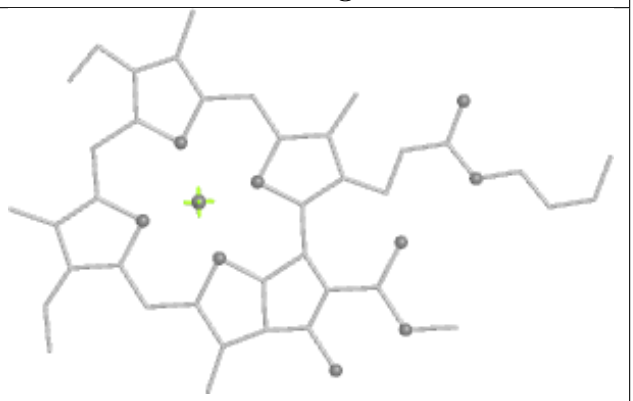
Bond lengths



Bond angles

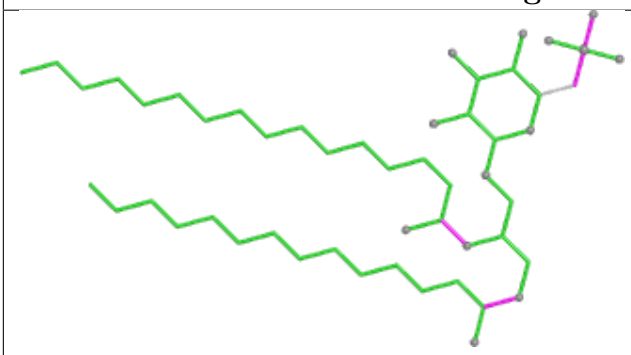


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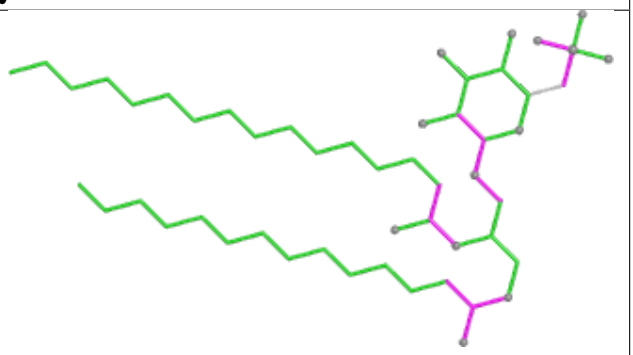


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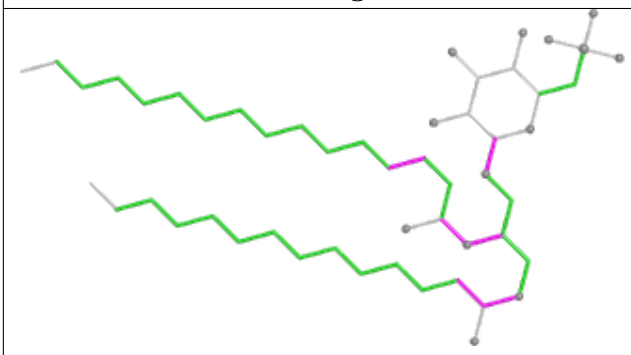
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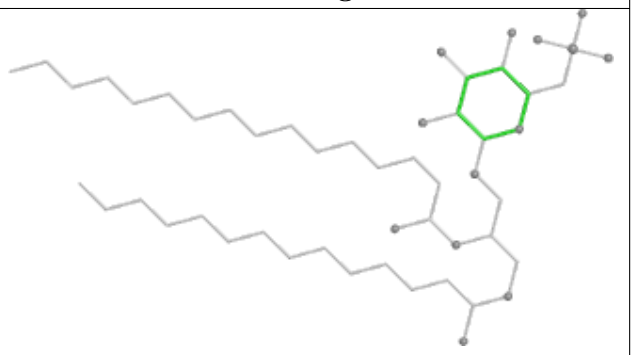
Bond lengths



Bond angles

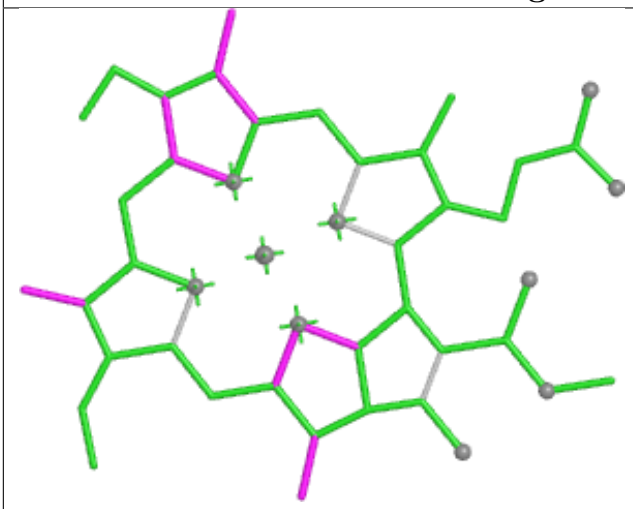


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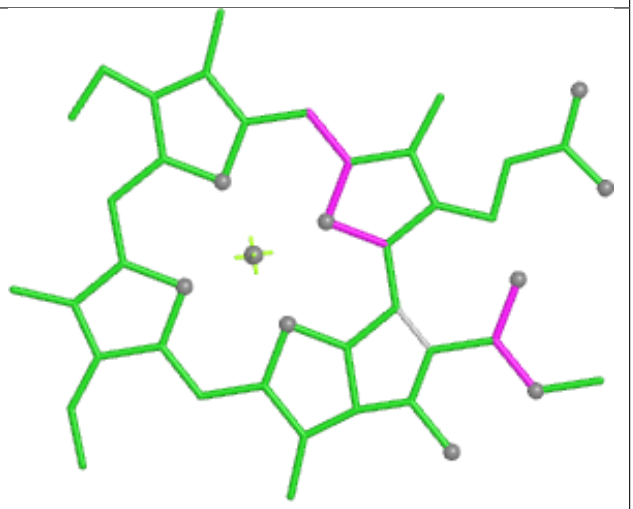


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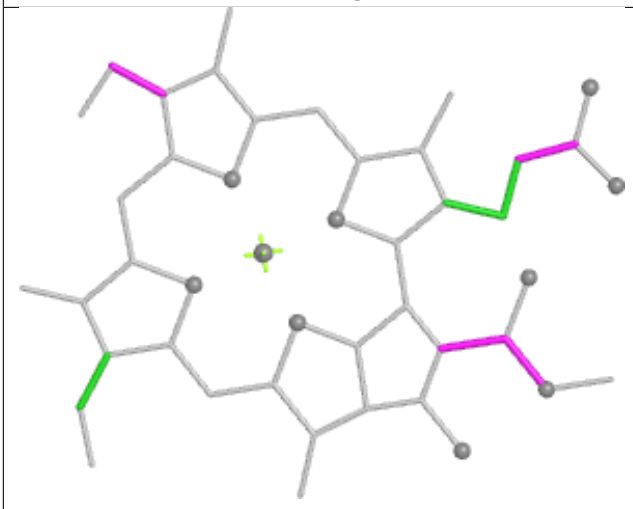
Ligand CLA 4 611



Bond lengths



Bond angles

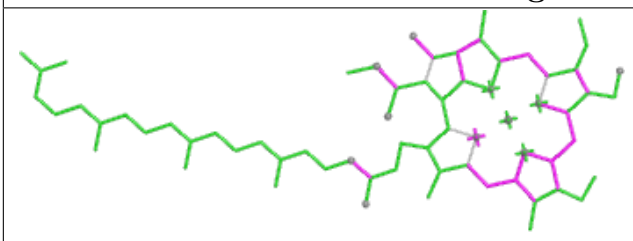


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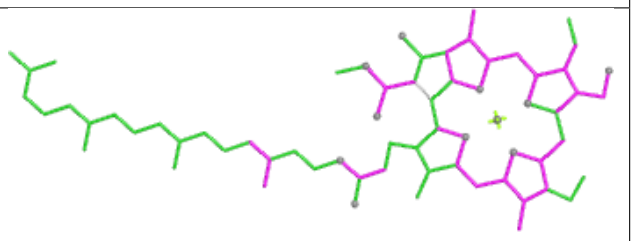


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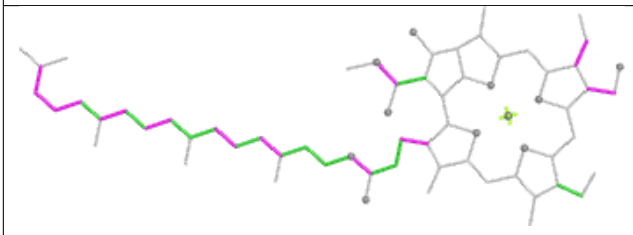
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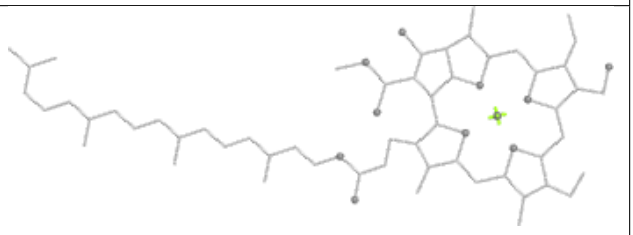
Bond lengths



Bond angles

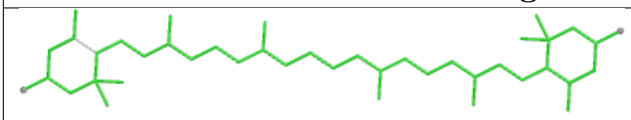


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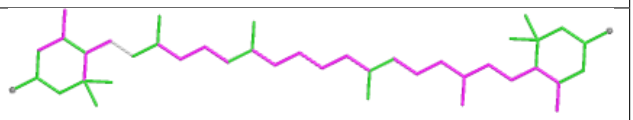


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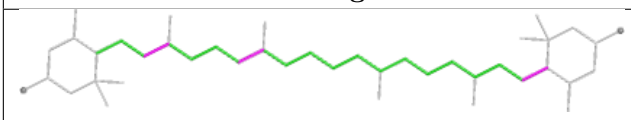
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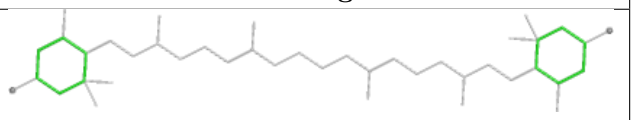
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Bond angles

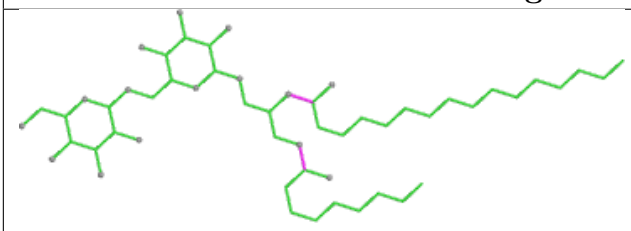


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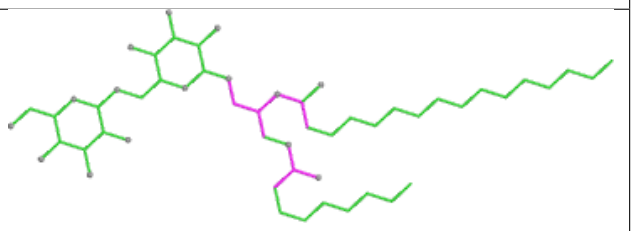


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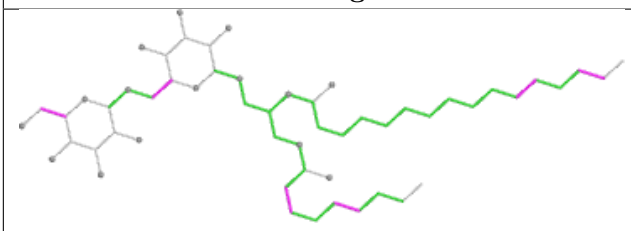
Ligand DGD c 518



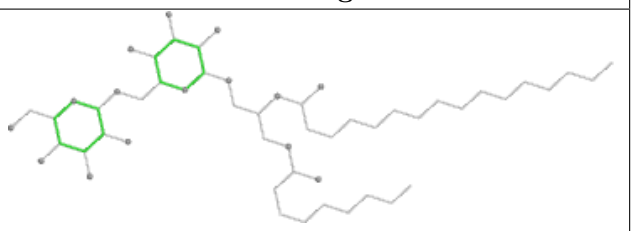
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Bond angles

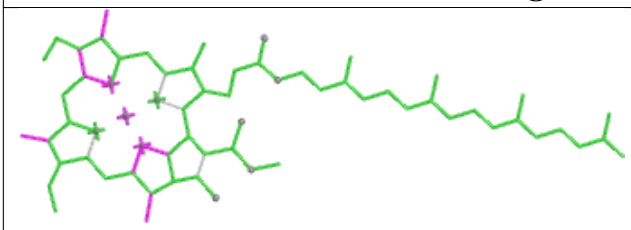


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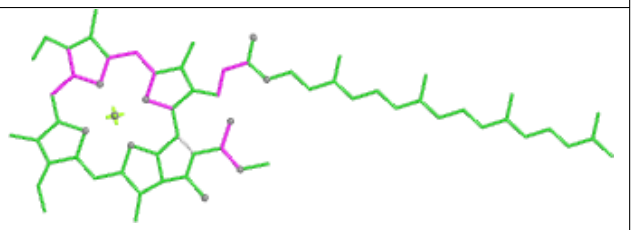


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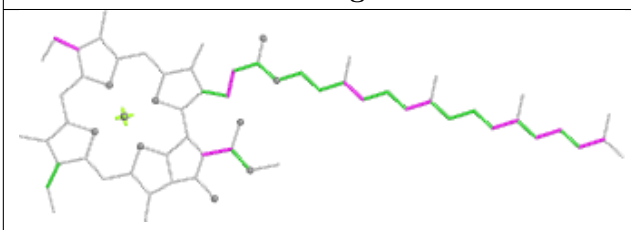
Ligand CLA b 604



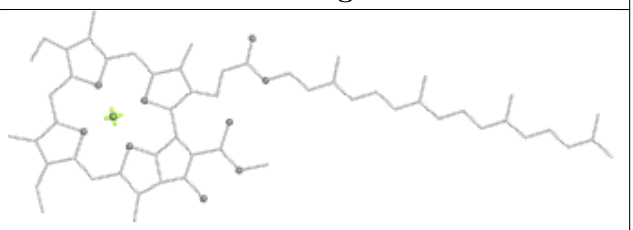
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Bond angles

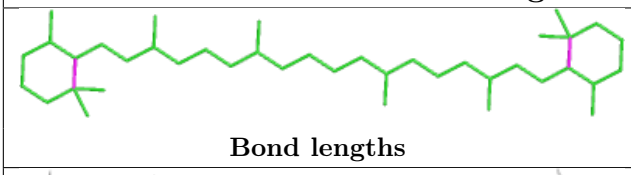


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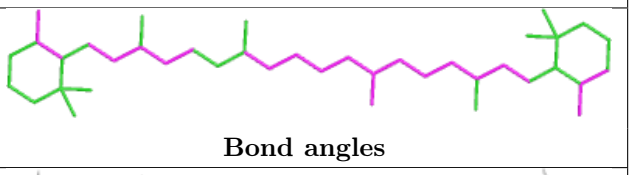


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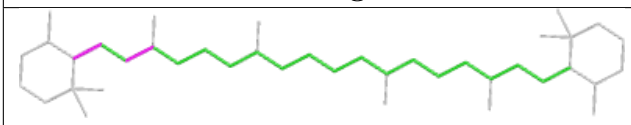
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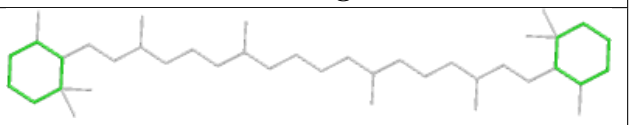
Bond lengths



Bond angles

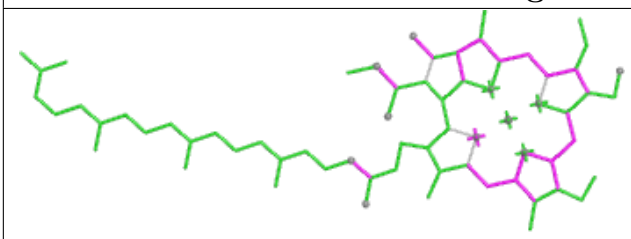


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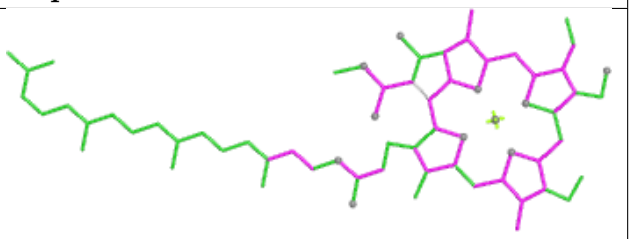


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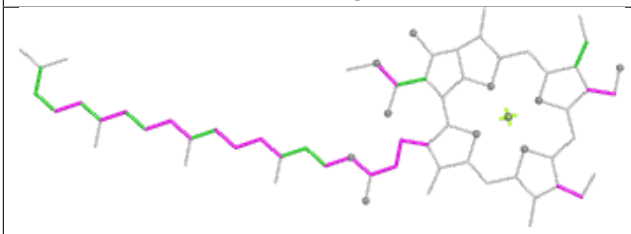
Ligand CHL p 607



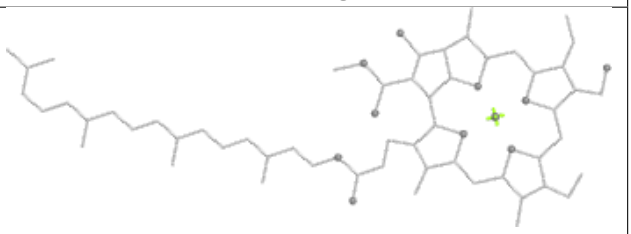
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Bond angles

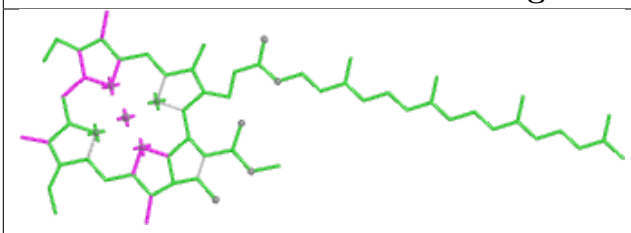


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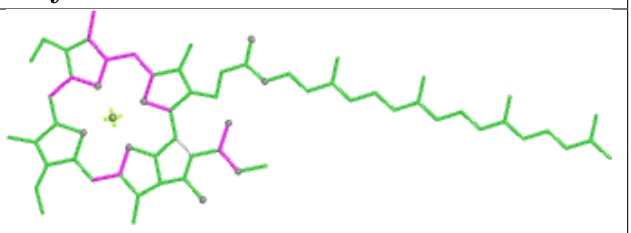


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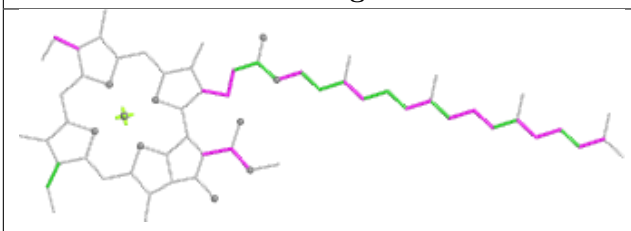
Ligand CLA y 604



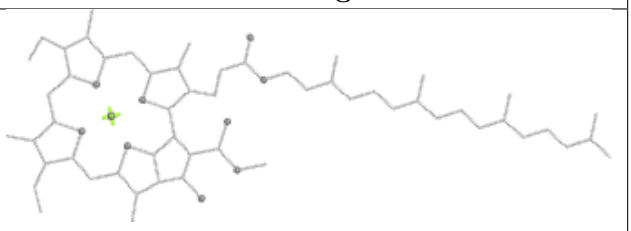
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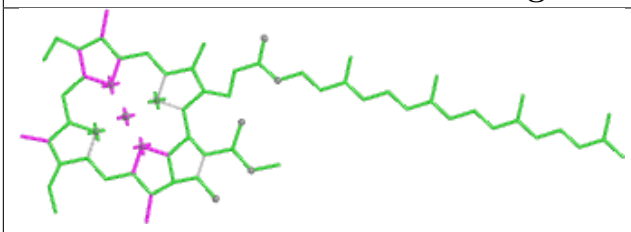


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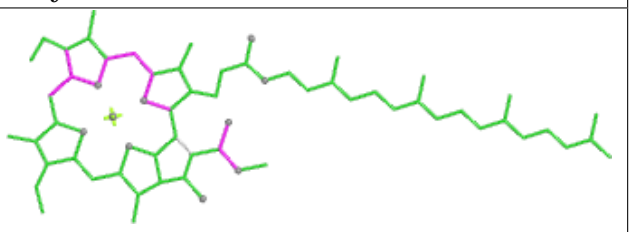


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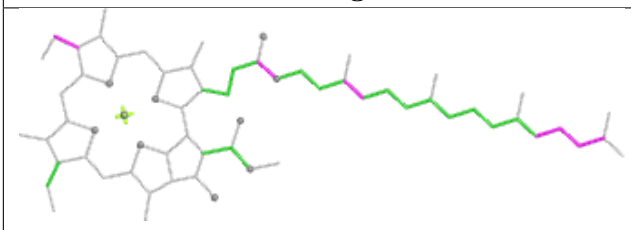
Ligand CLA y 611



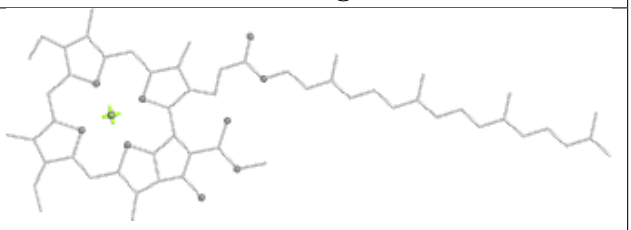
Bond lengths



Bond angles

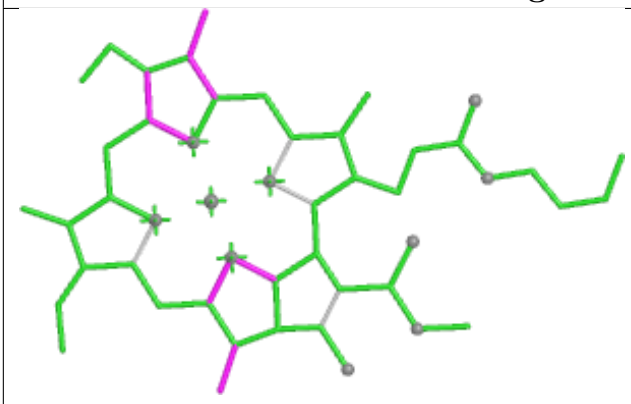


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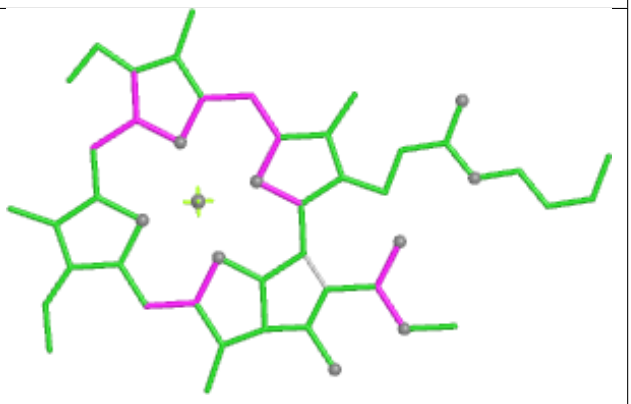


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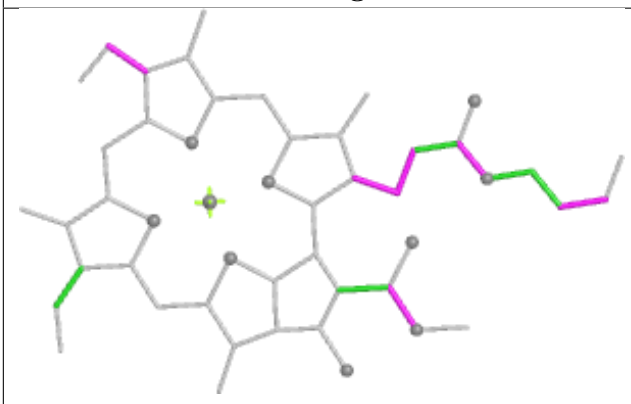
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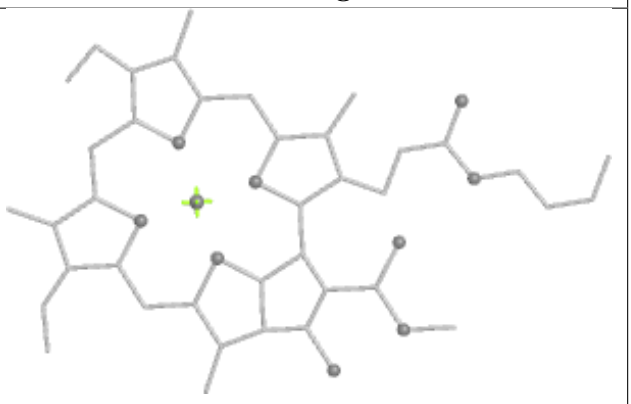
Bond lengths



Bond angles

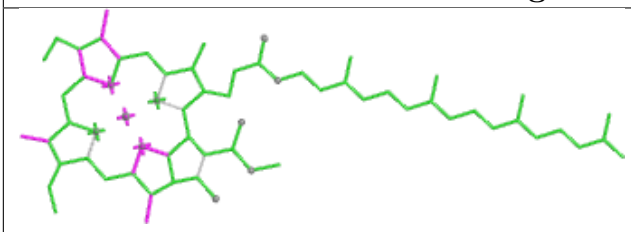


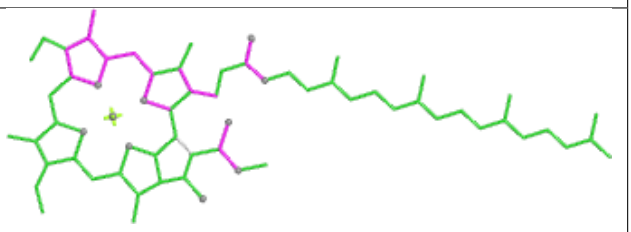
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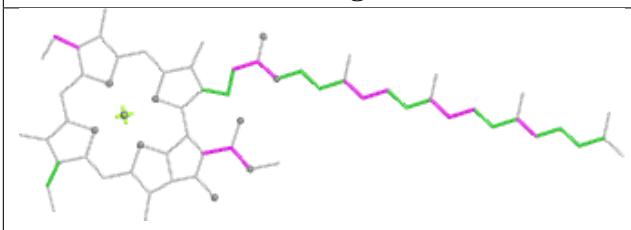


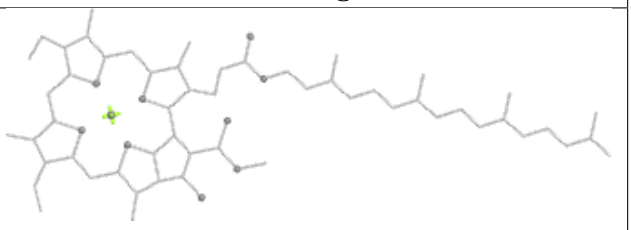
Rings

Ligand CLA 1 612

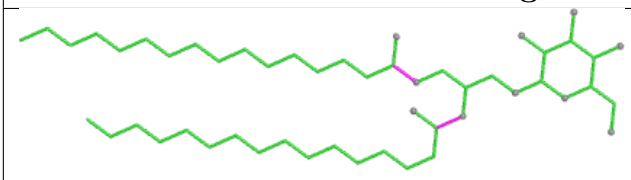

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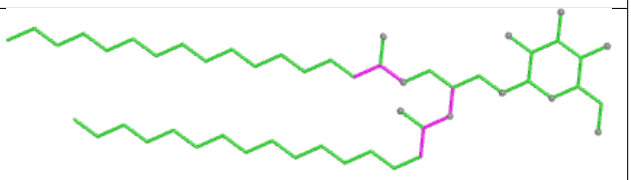

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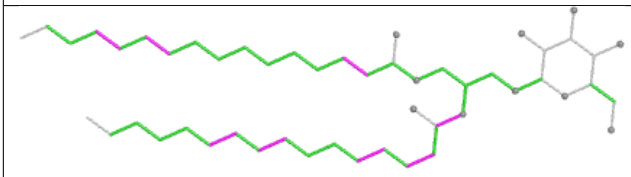

Torsions

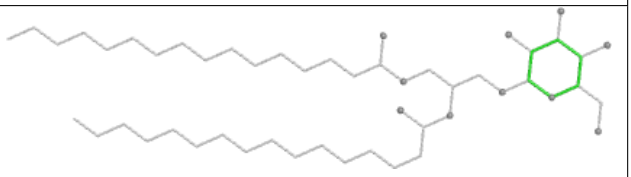

Rings

Ligand LMG B 622

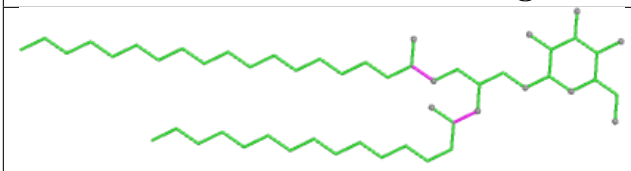

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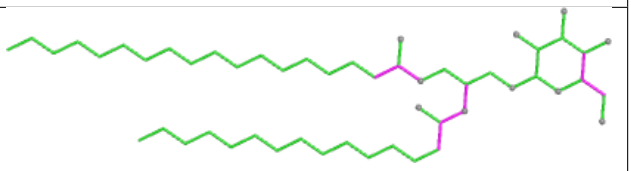

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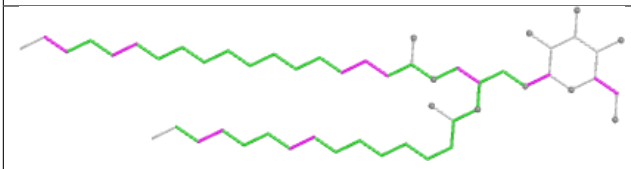

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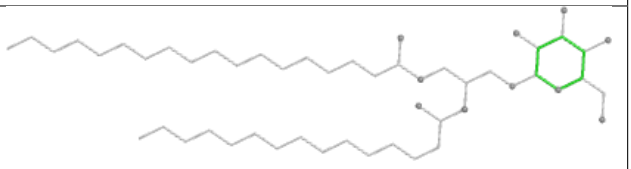

Rings

Ligand LMG s 2631

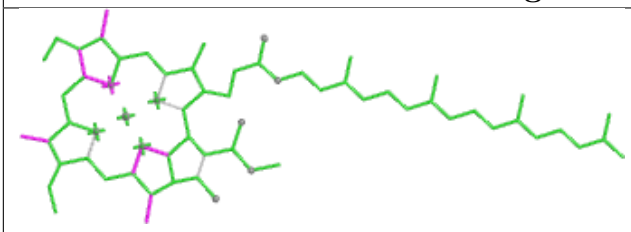

Bond lengths


Bond angles

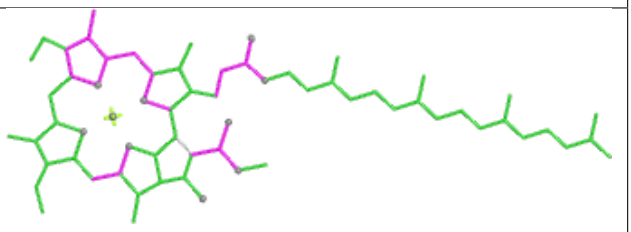

Torsions


Rings

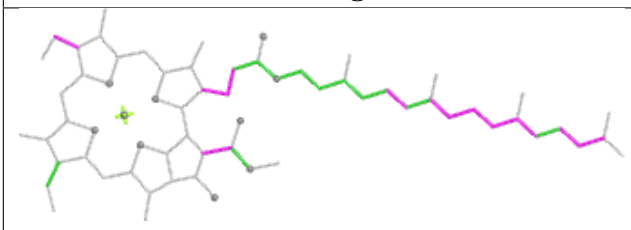
Ligand CLA B 607



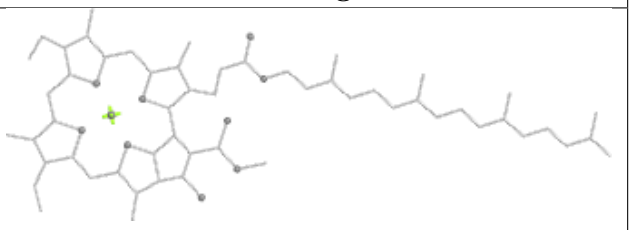
Bond lengths



Bond angles



Torsions



Rings

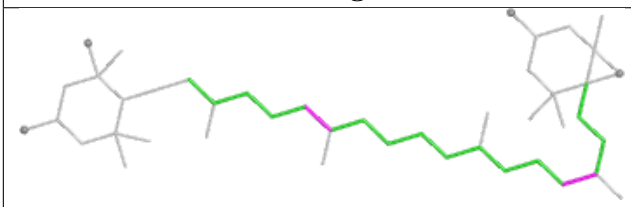
Ligand NEX s 1623



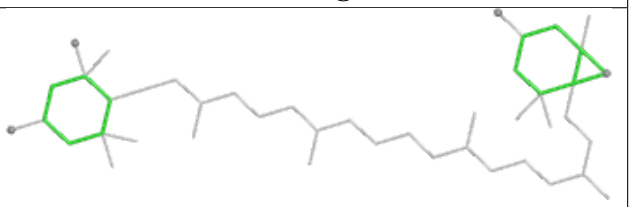
Bond lengths



Bond angles

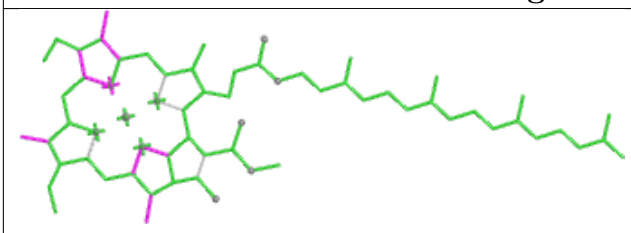


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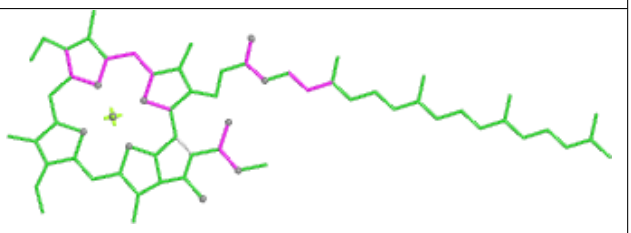


Rings

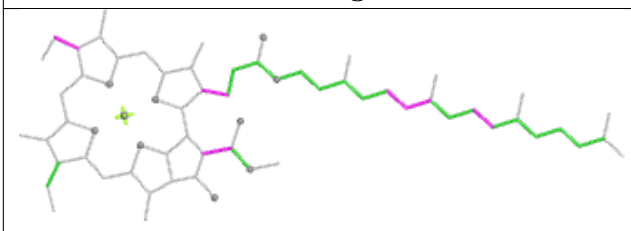
Ligand CLA n 610



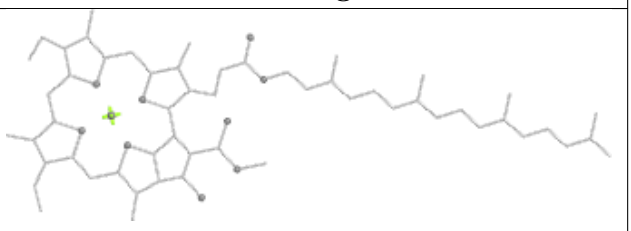
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Bond angles

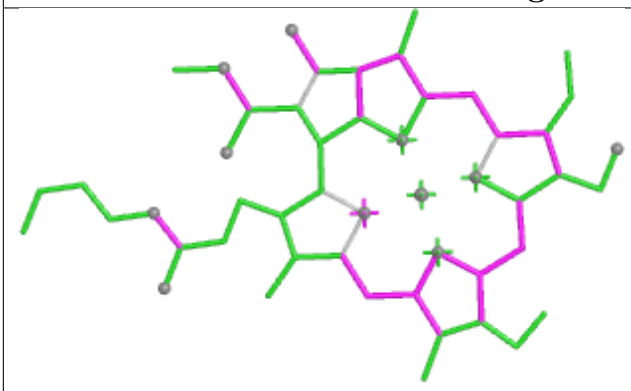


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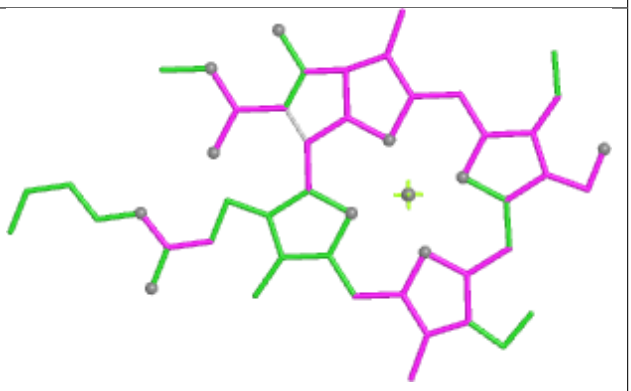


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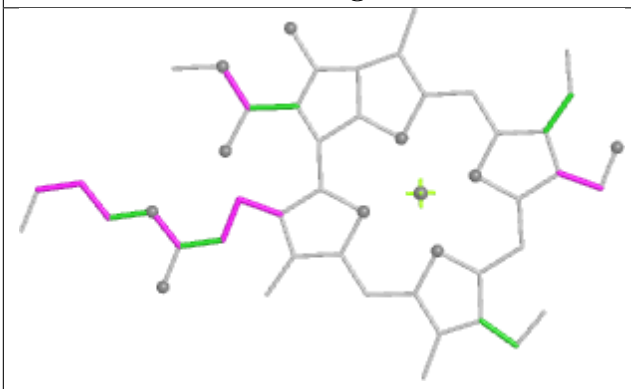
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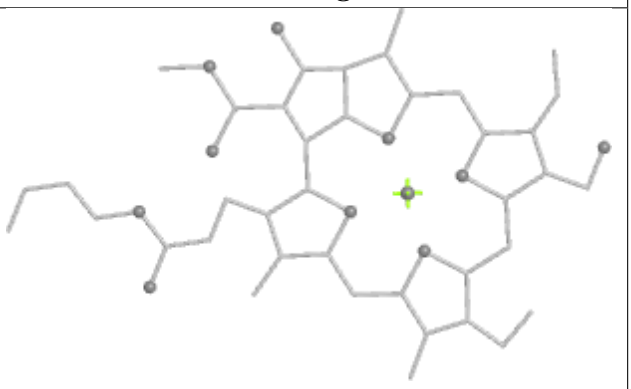
Bond lengths



Bond angles

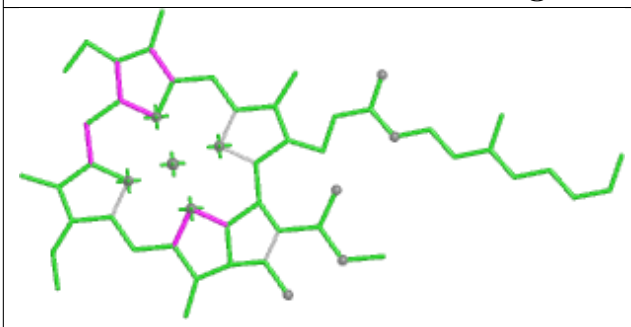


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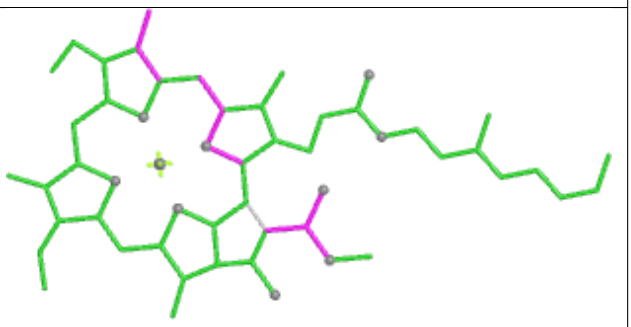


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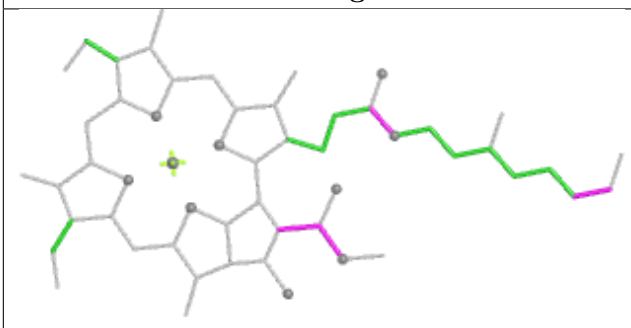
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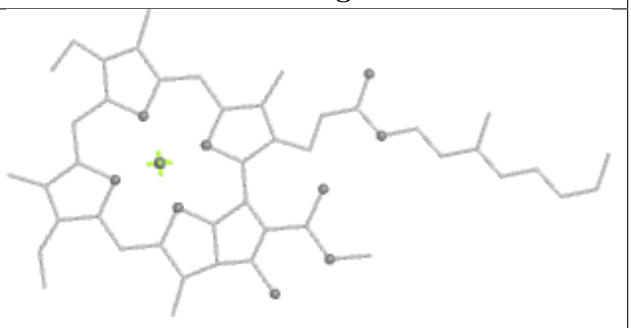
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Bond angles

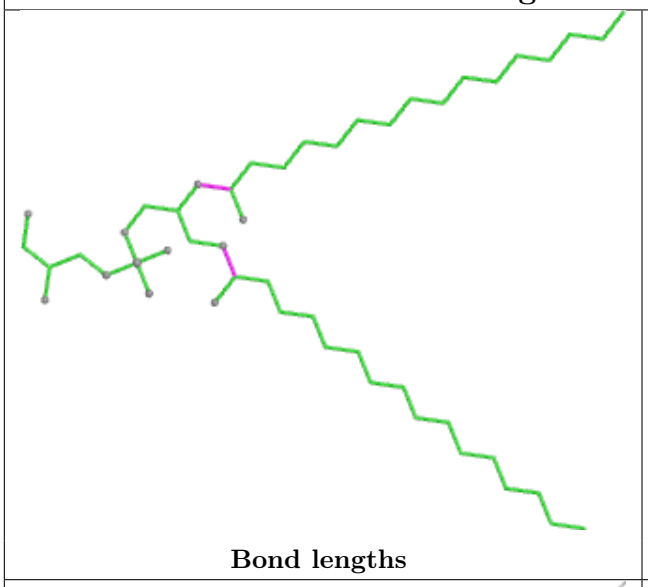


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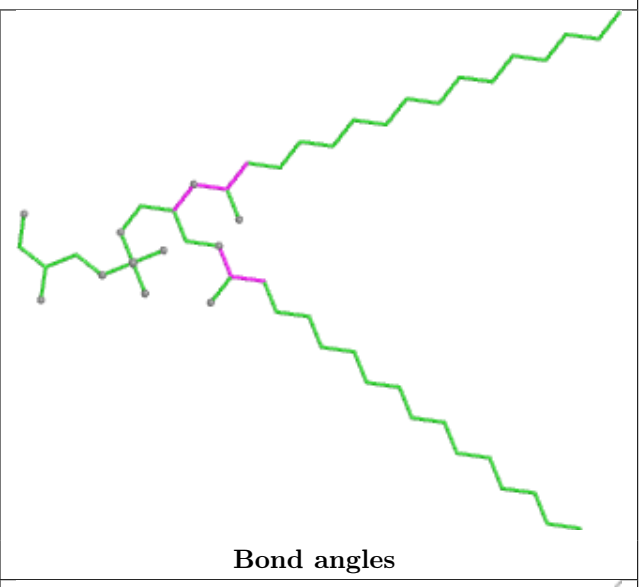


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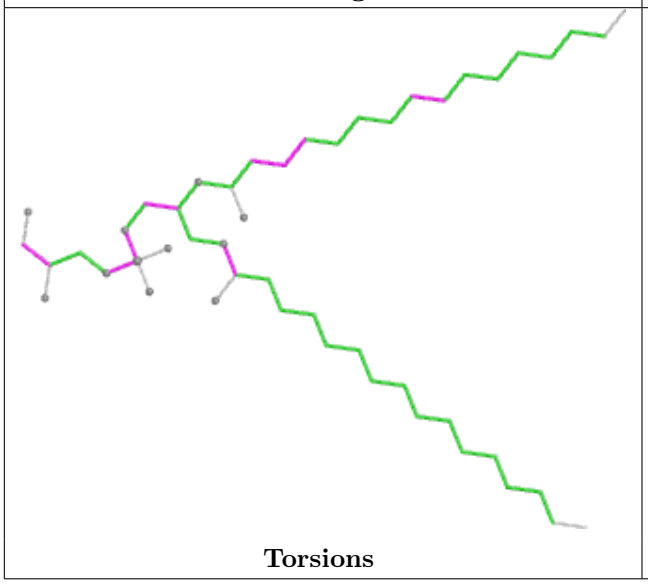
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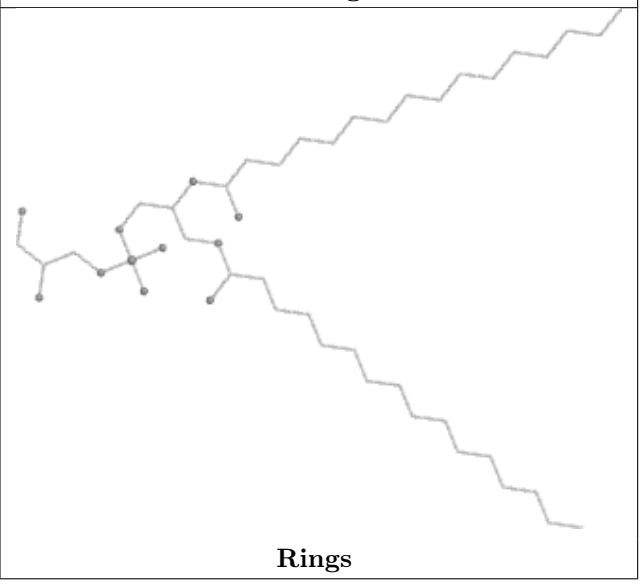
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Bond angles

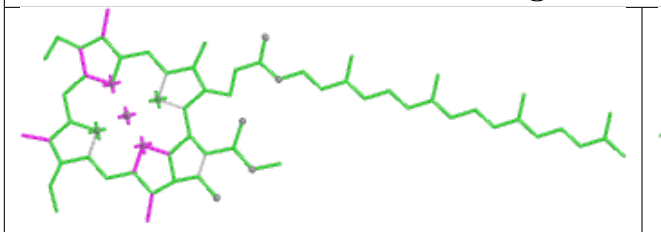


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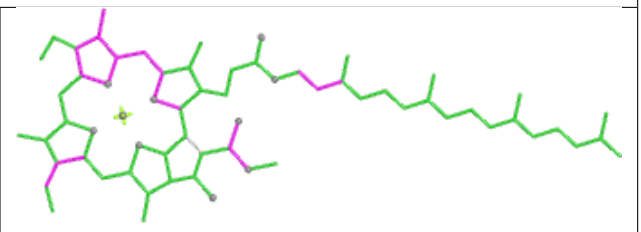


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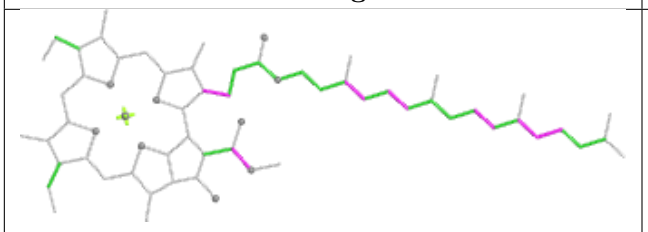
Ligand CLA b 612



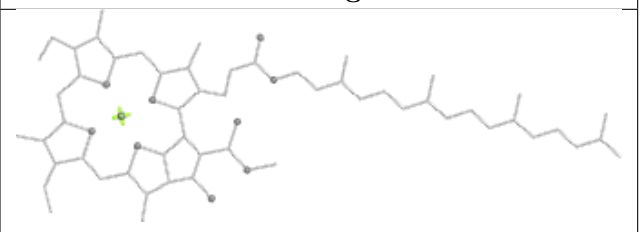
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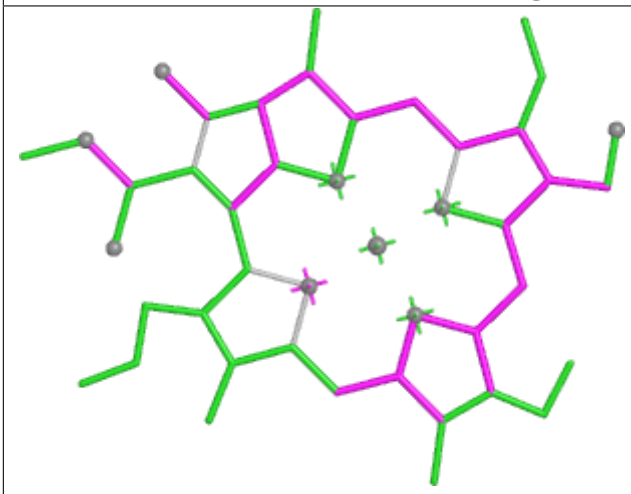
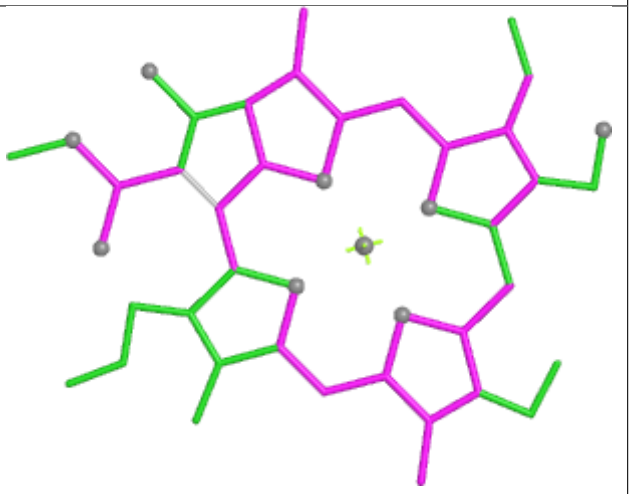
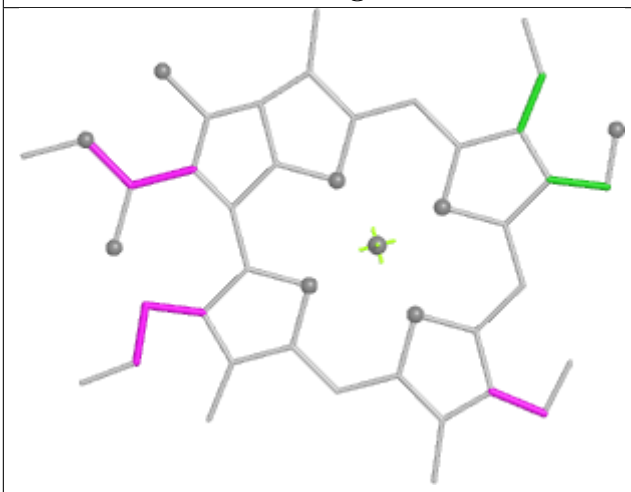
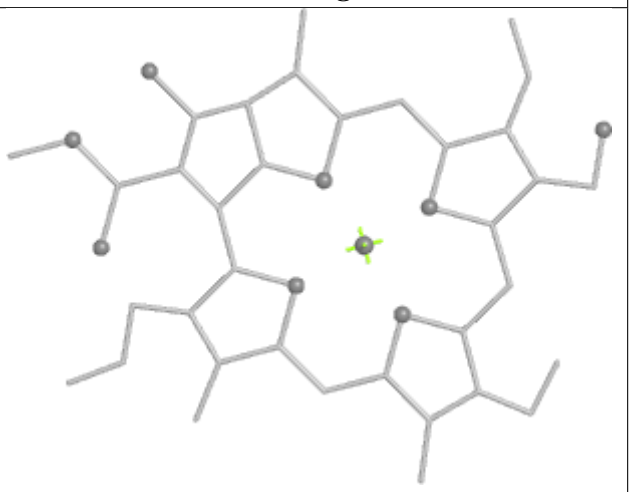
Bond angles

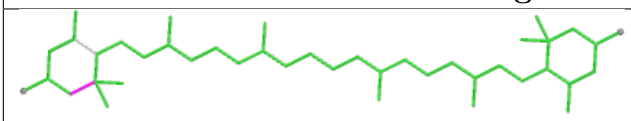
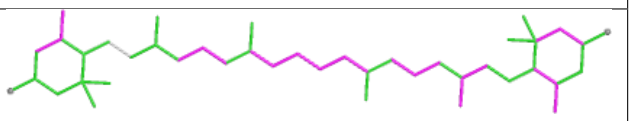
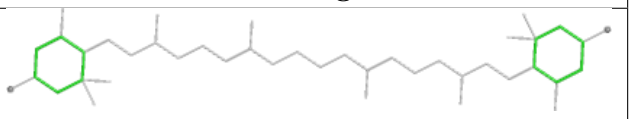


Torsions

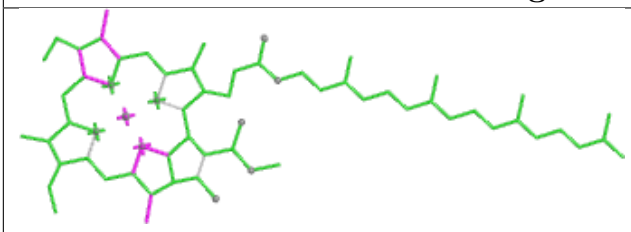


Rings

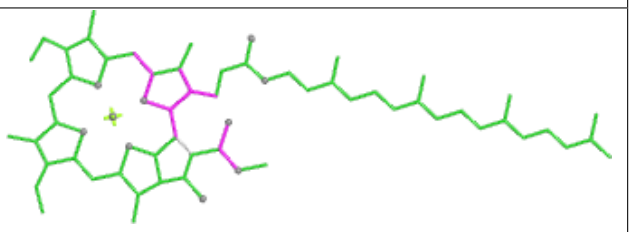
Ligand CHL 2 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT N 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

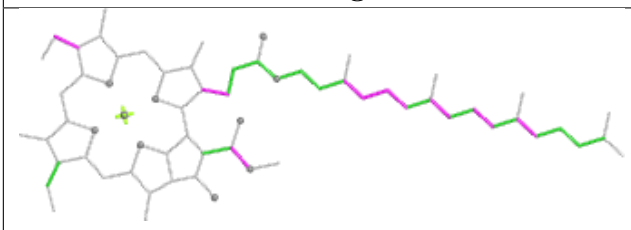
Ligand CLA 3 603



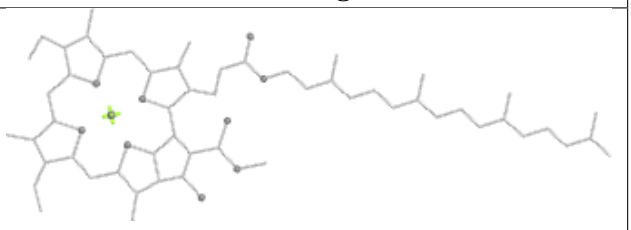
Bond lengths



Bond angles

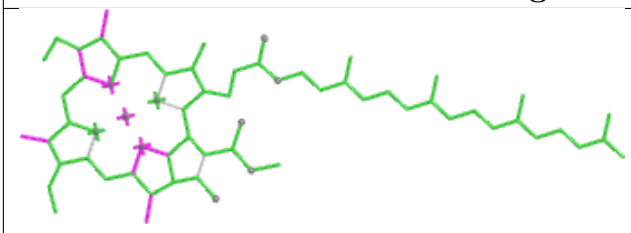


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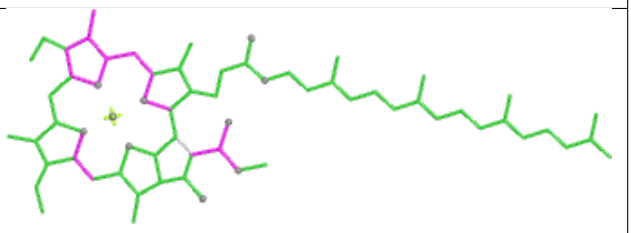


Rings

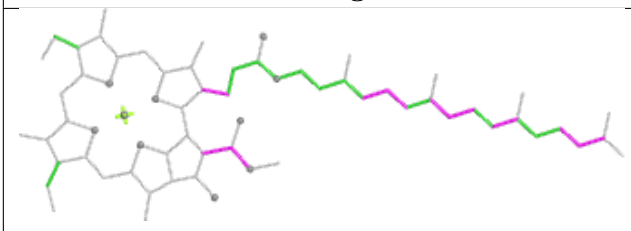
Ligand CLA c 508



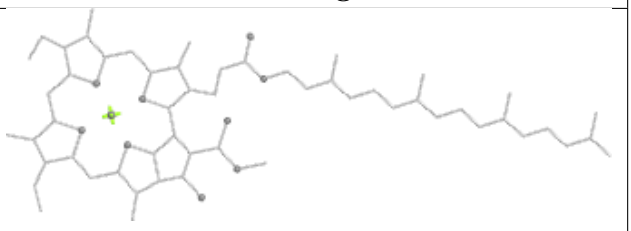
Bond lengths



Bond angles

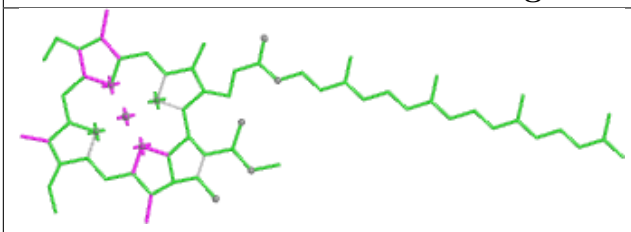


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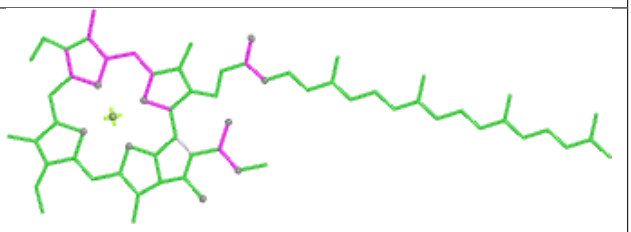


Rings

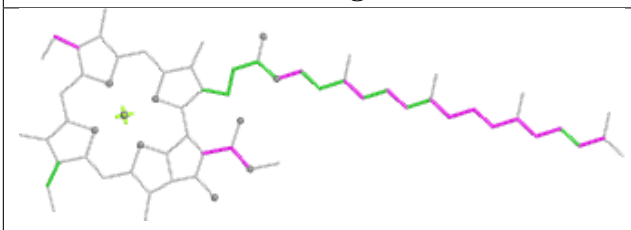
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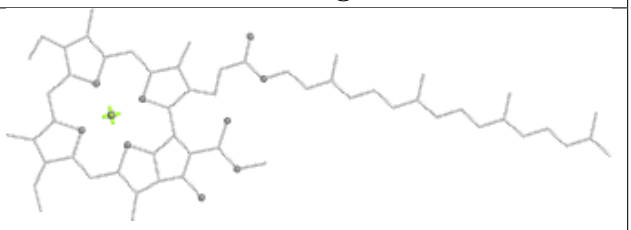
Bond lengths



Bond angles

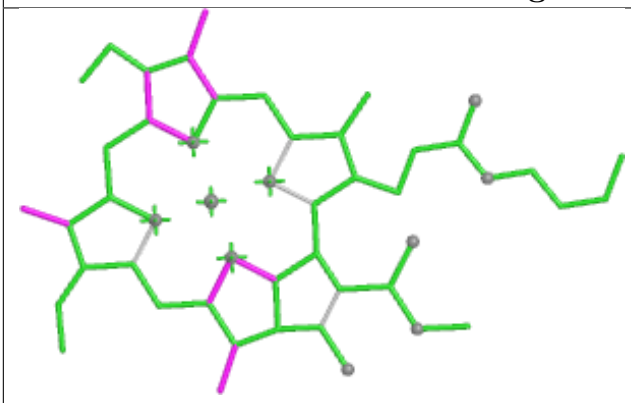


Torsions

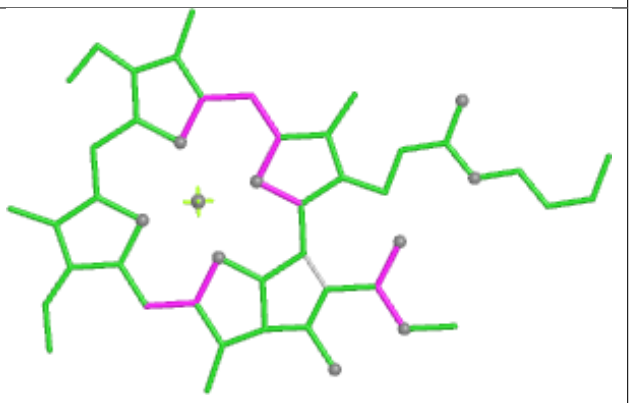


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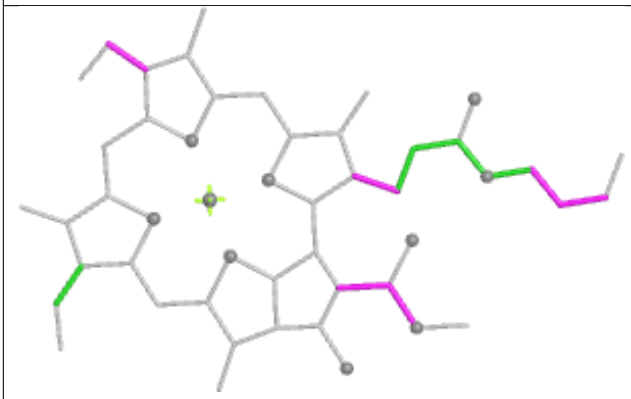
Ligand CLA 9 604



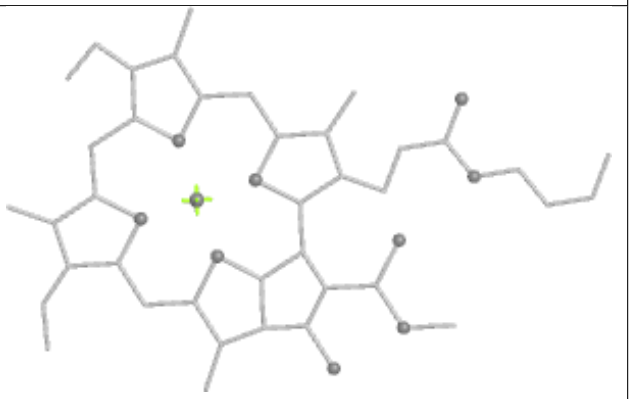
Bond lengths



Bond angles



Torsions

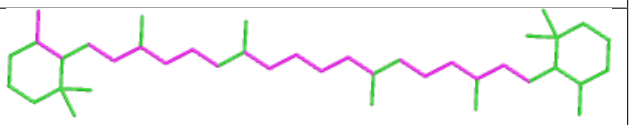


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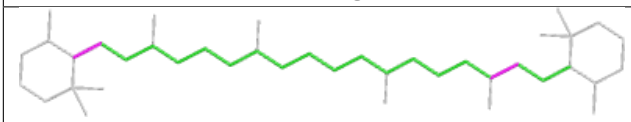
Ligand BCR c 514



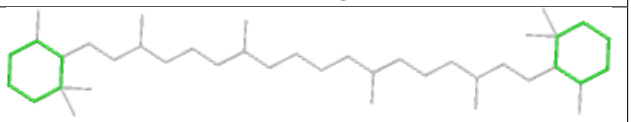
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Bond angles

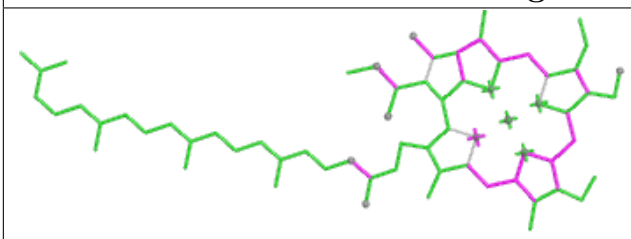


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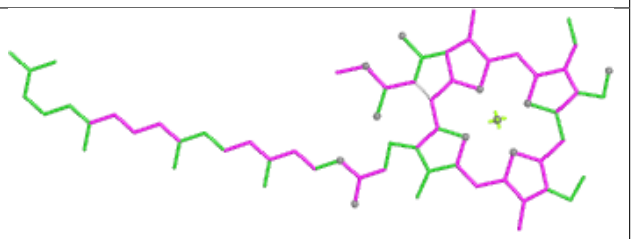


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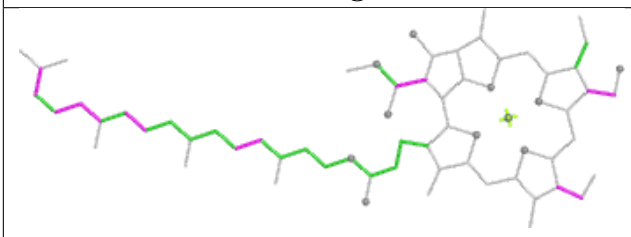
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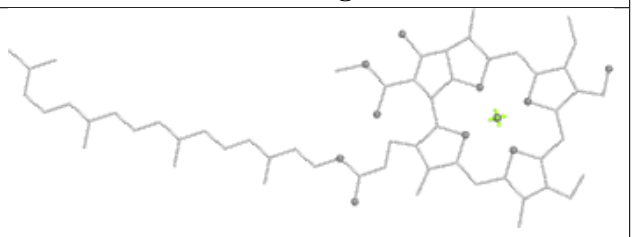
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Bond angles

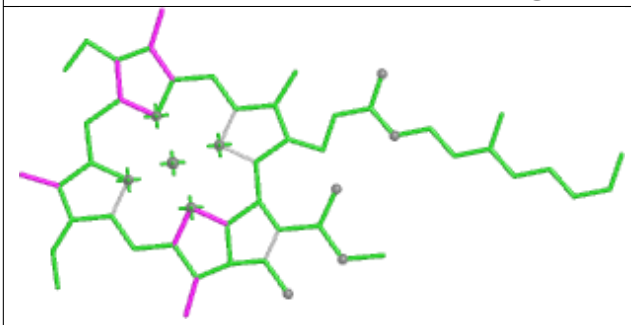


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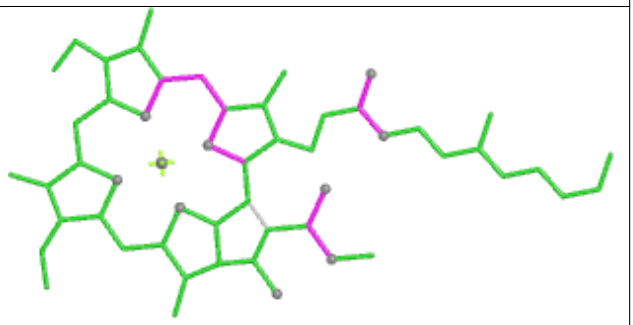


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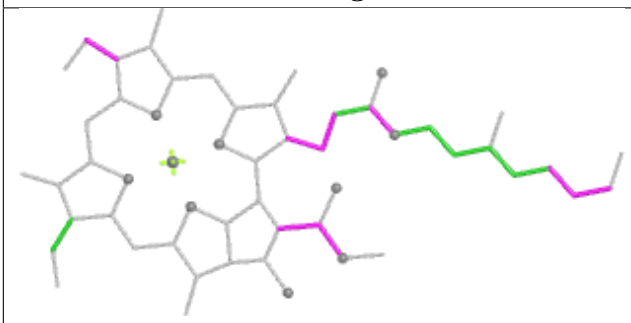
Ligand CLA 7 614



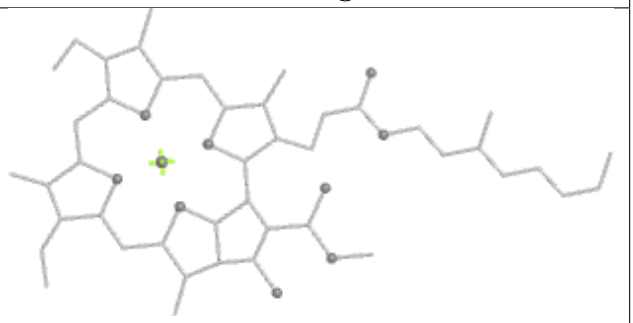
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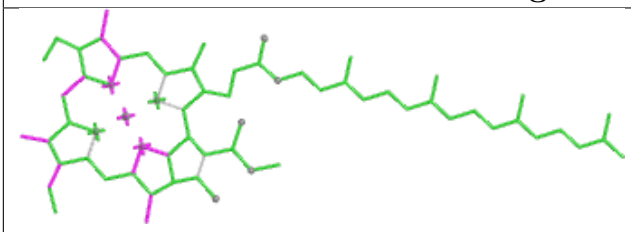


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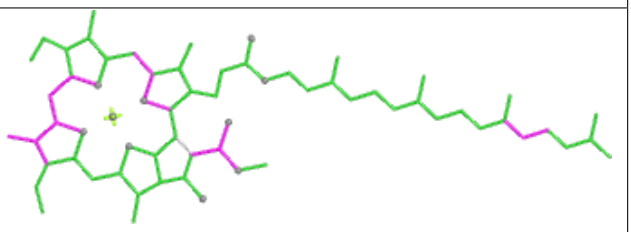


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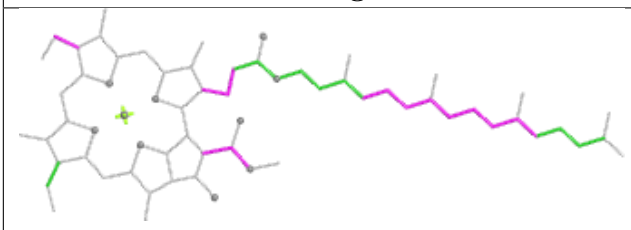
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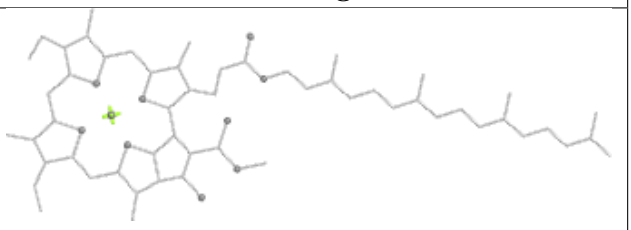
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Bond angles

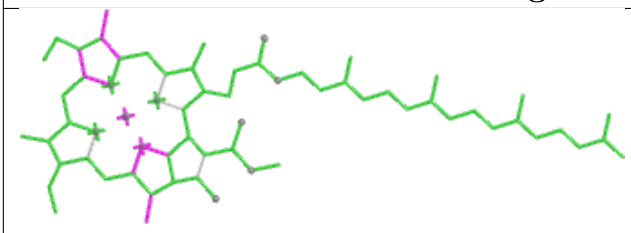


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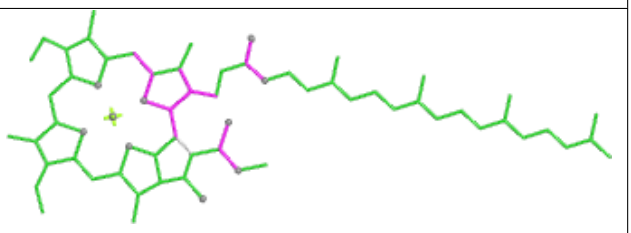


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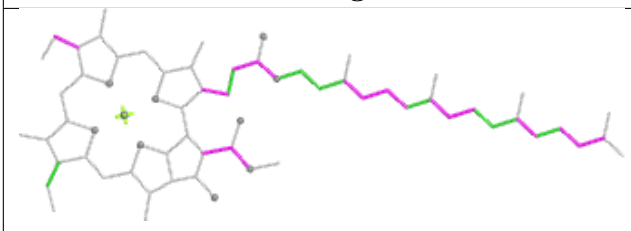
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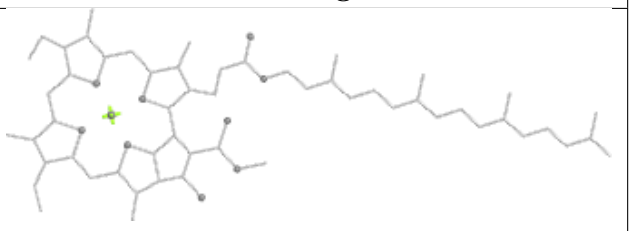
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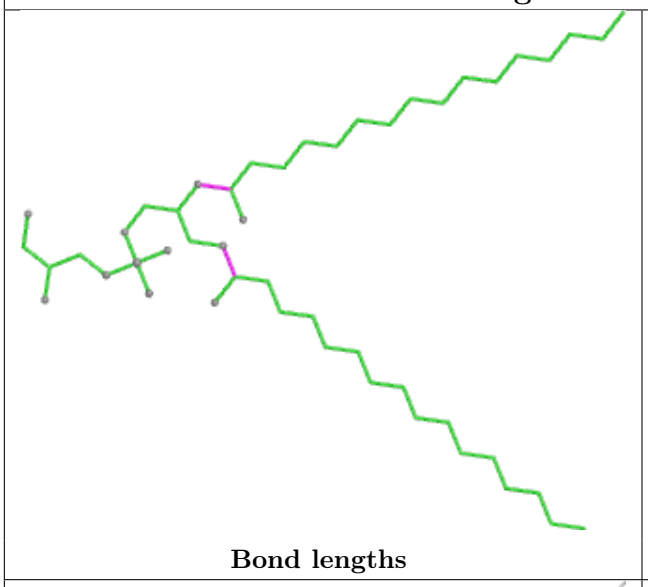


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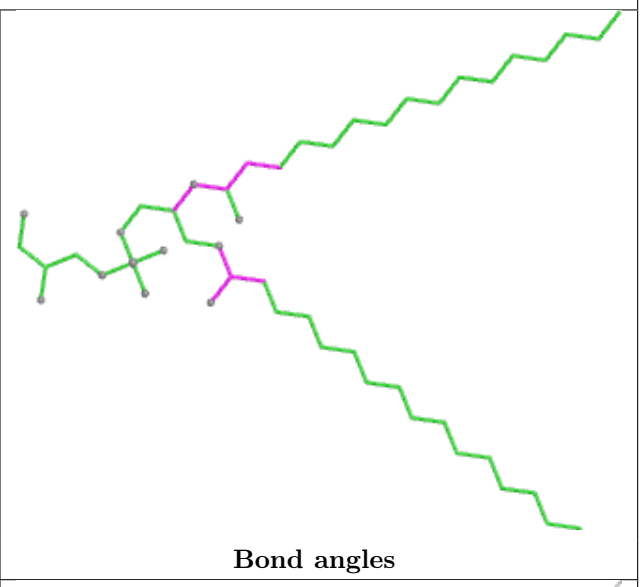


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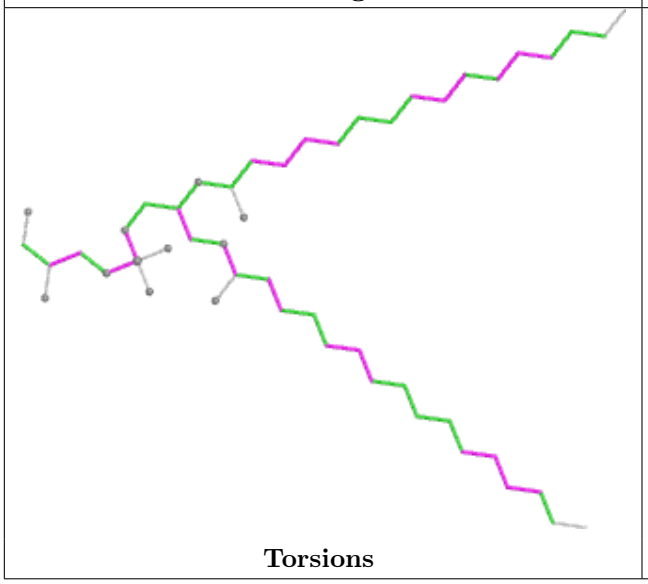
Ligand LHG Y 2630



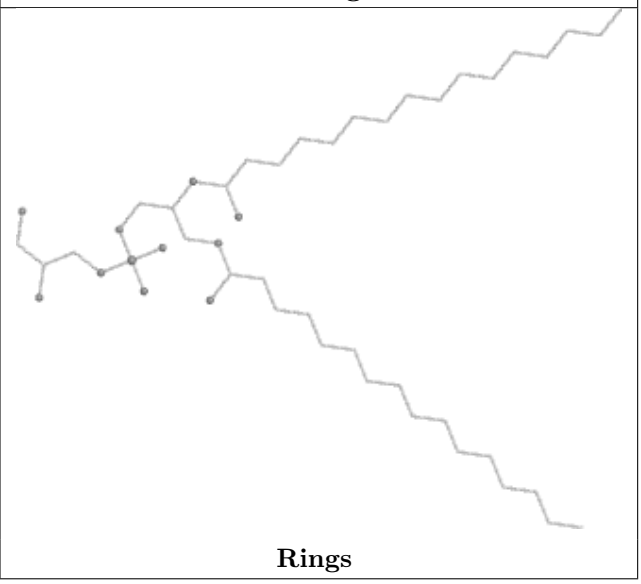
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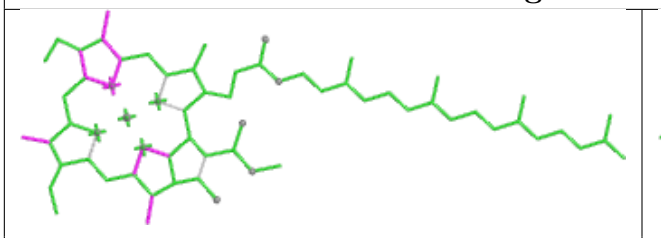


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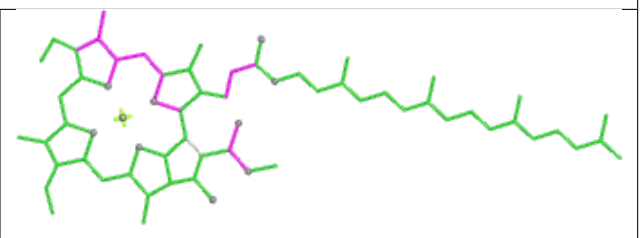


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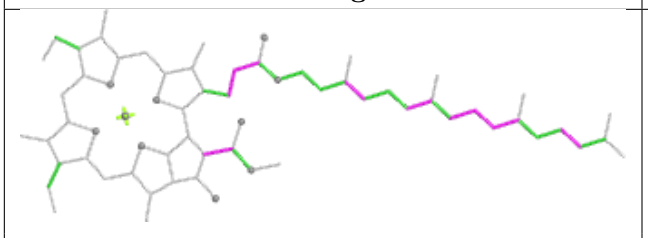
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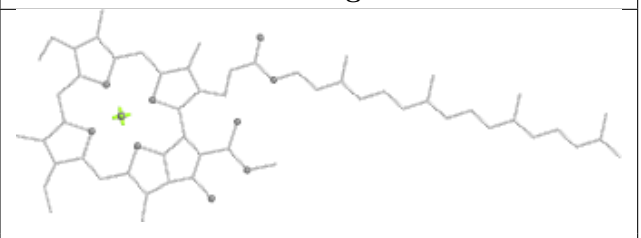
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Bond angles

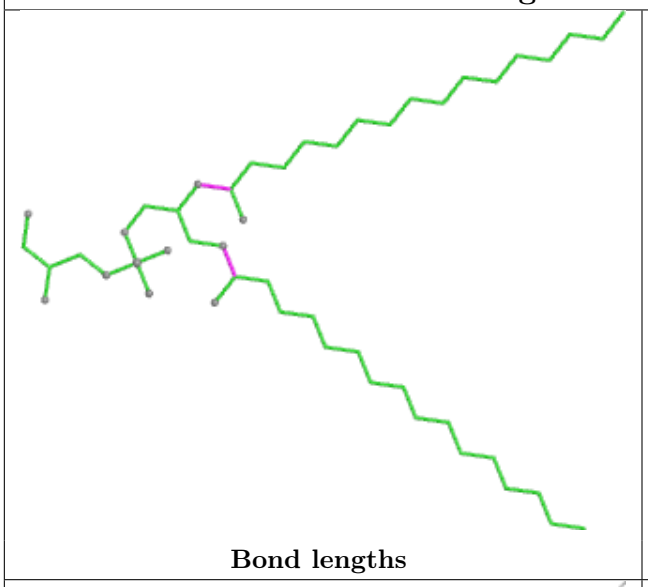


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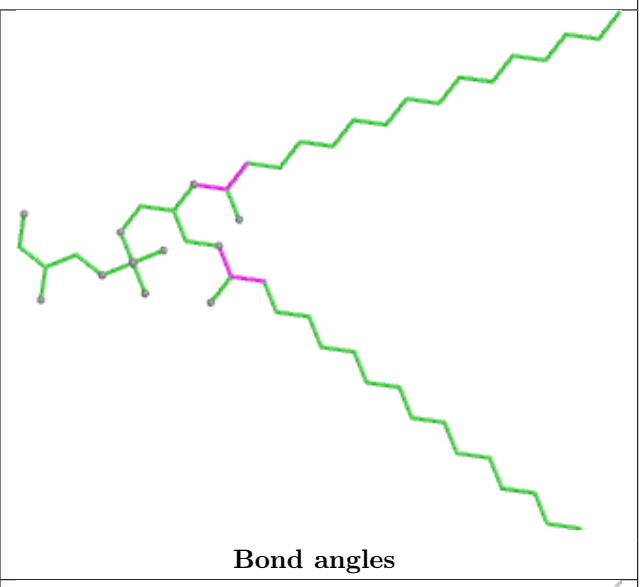


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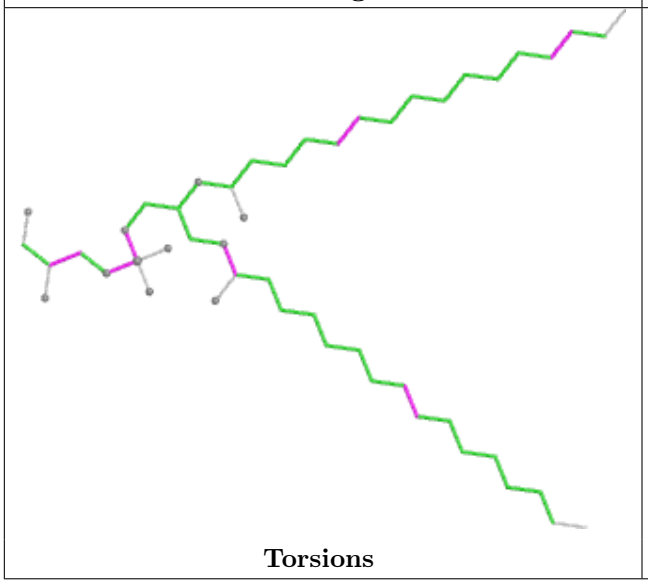
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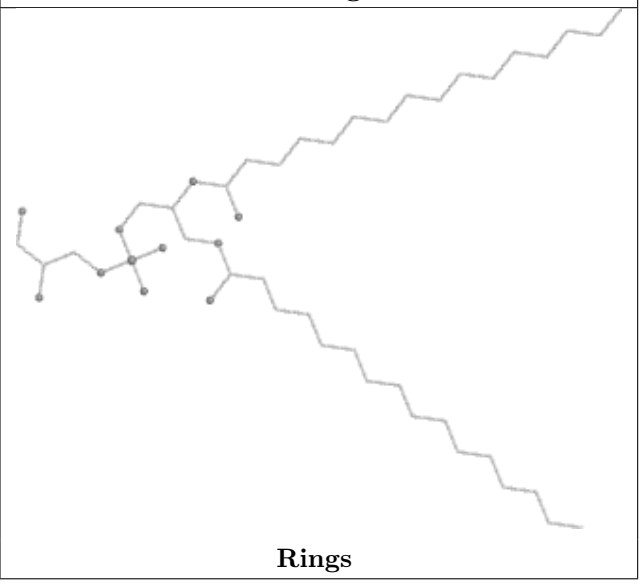
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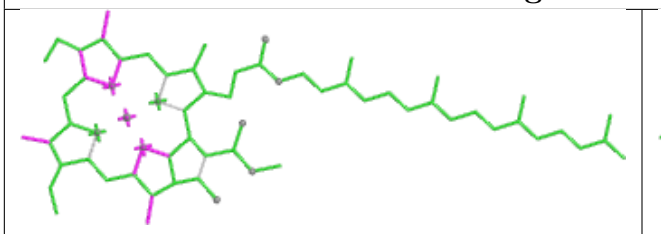


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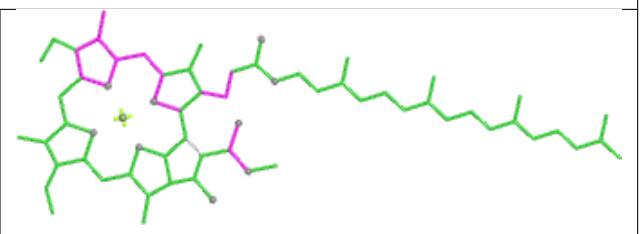


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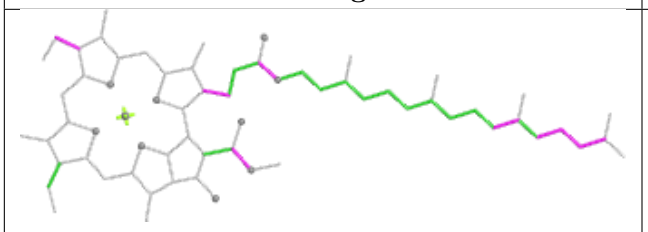
Ligand CLA A 405



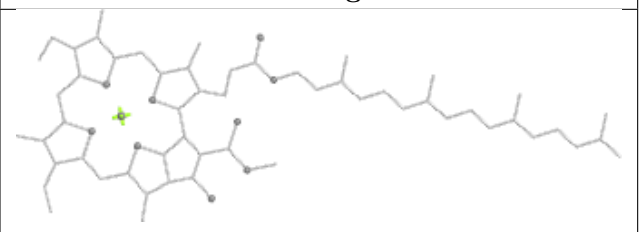
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Bond angles

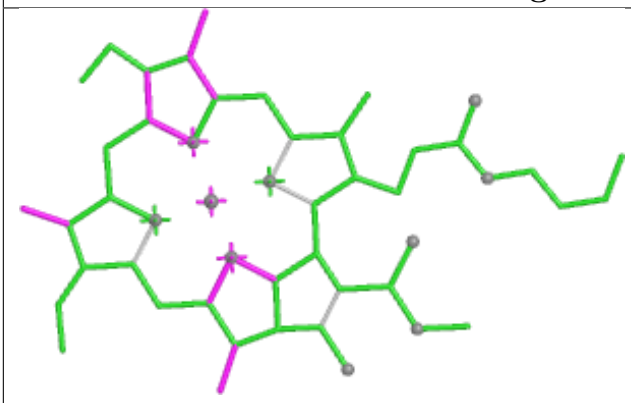


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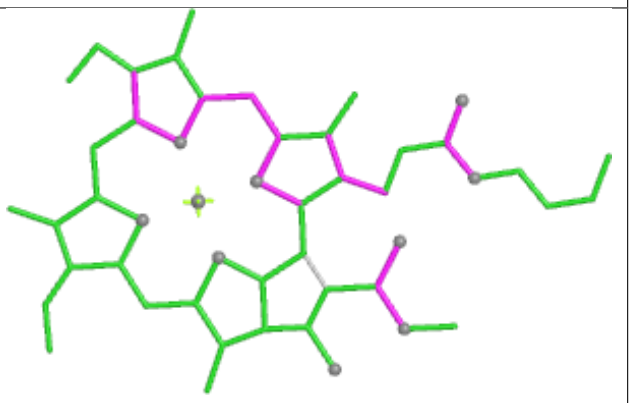


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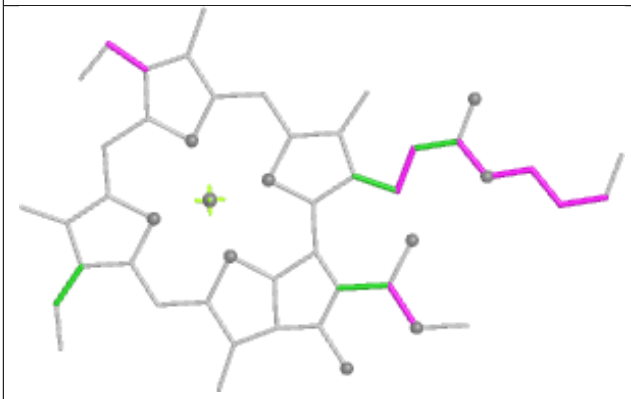
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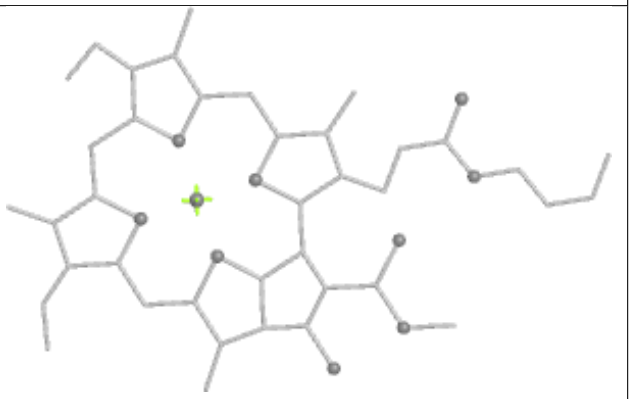
Bond lengths



Bond angles



Torsions

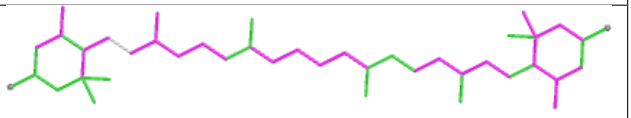


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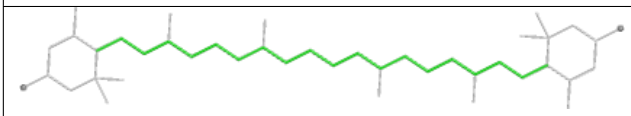
Ligand LUT s 1621



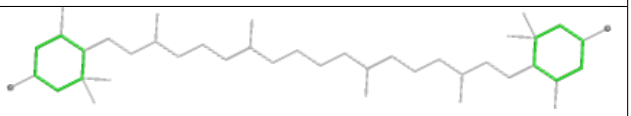
Bond lengths



Bond angles

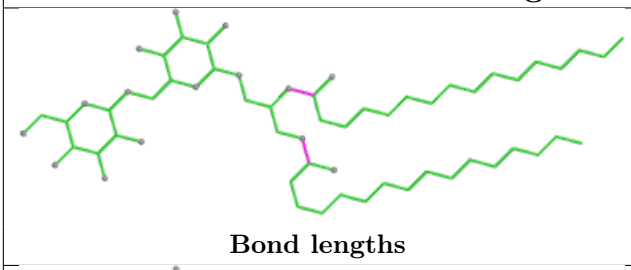


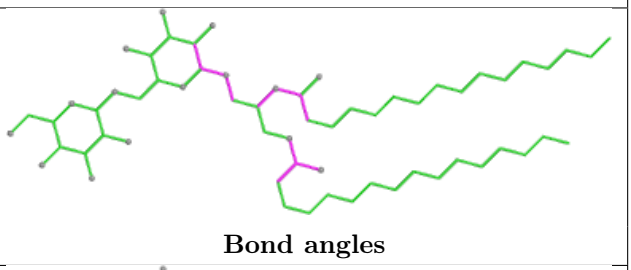
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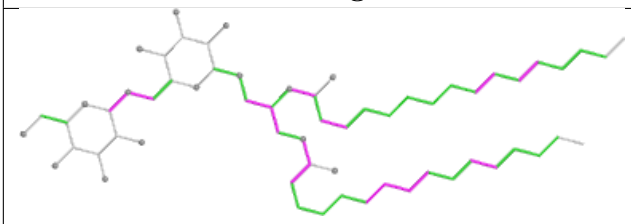


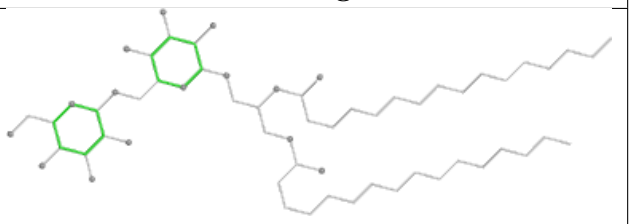
Rings

Ligand DGD c 519

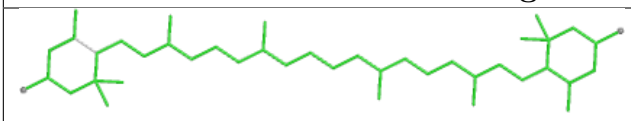

Bond lengths

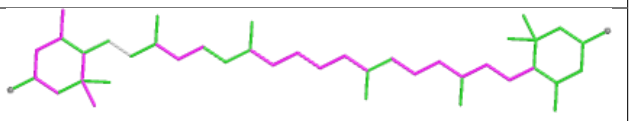

Bond angles


Torsions

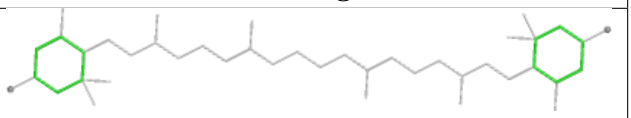

Rings

Ligand LUT 5 1620


Bond lengths

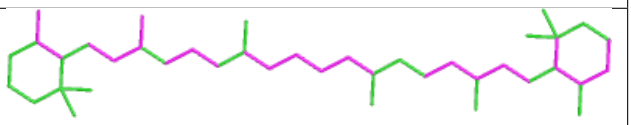

Bond angles

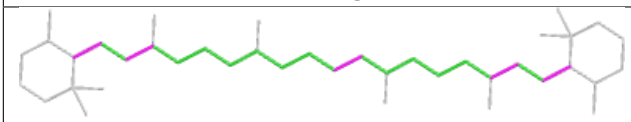

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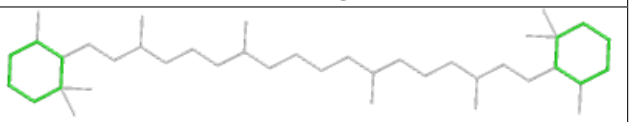

Rings

Ligand BCR C 516

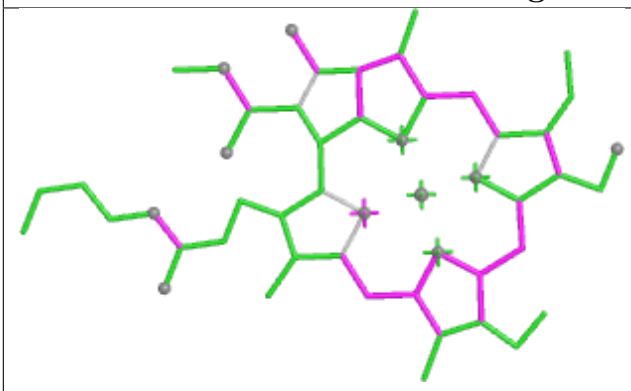

Bond lengths


Bond angles

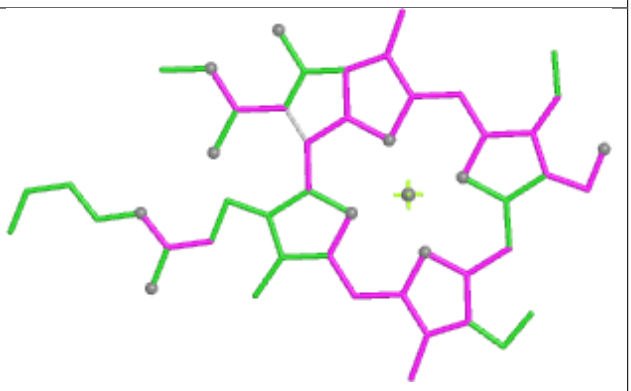

Torsions


Rings

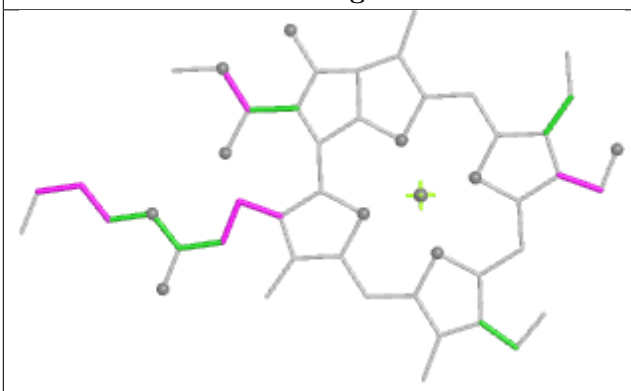
Ligand CHL 1 608



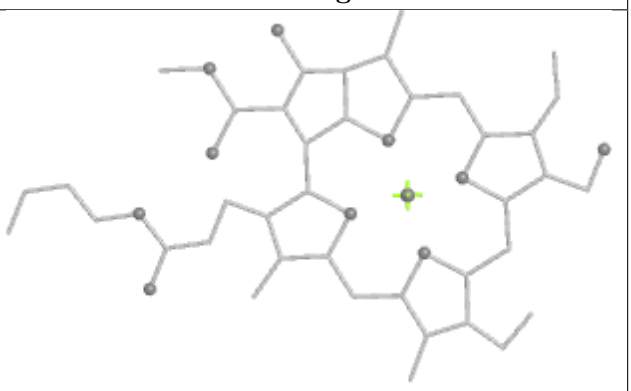
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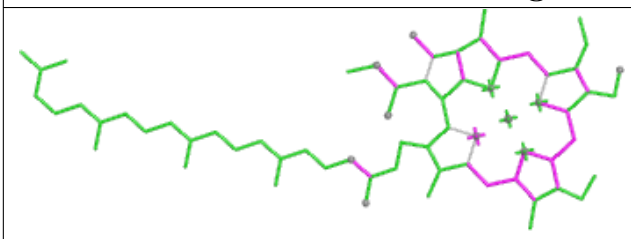


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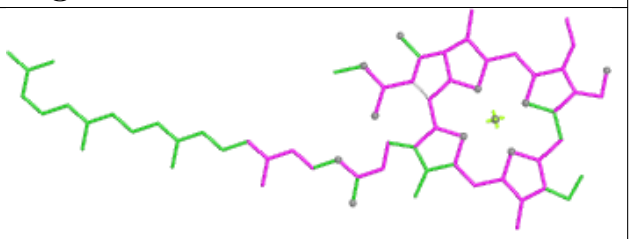


Rings

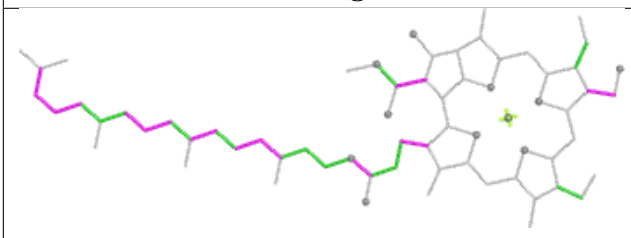
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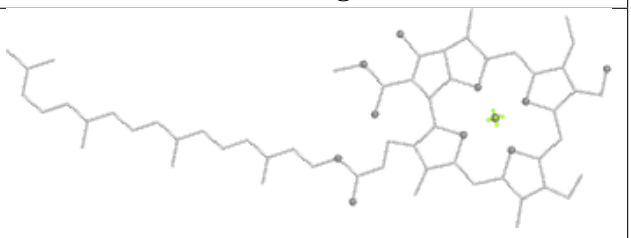
Bond lengths



Bond angles

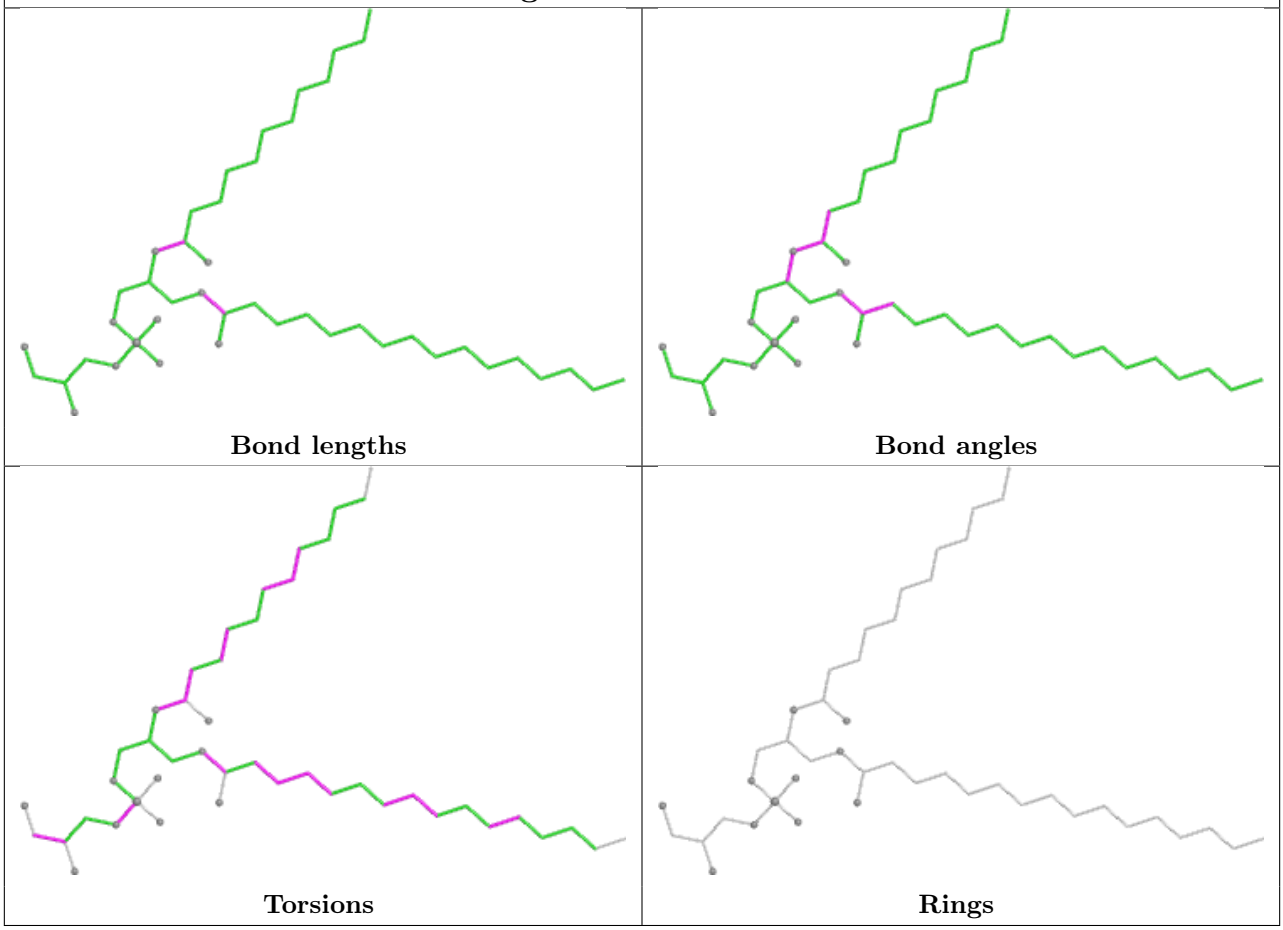


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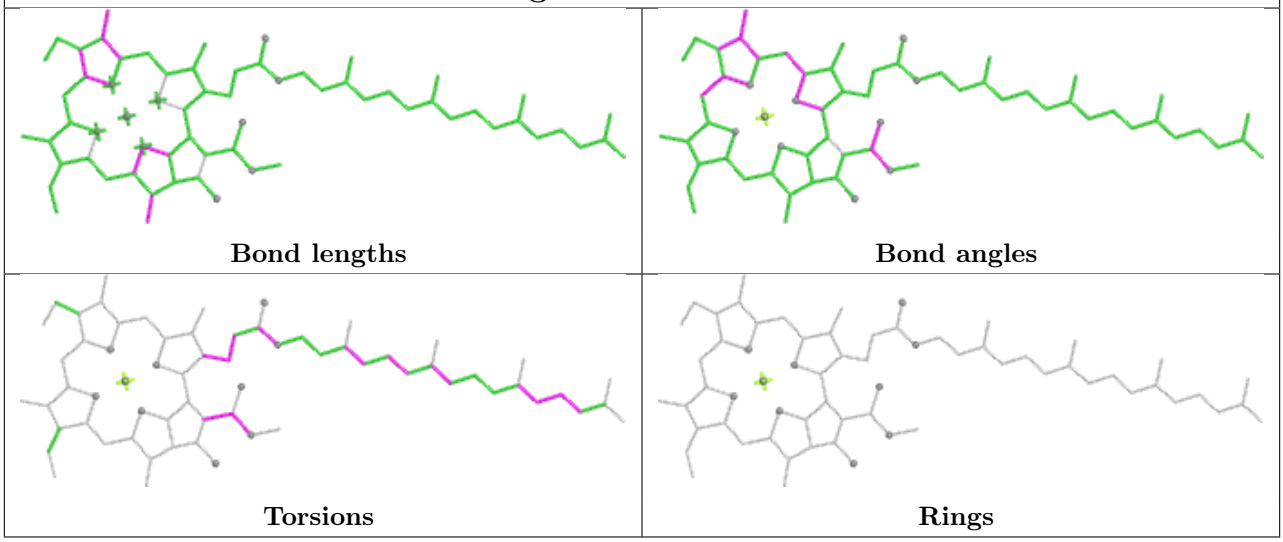


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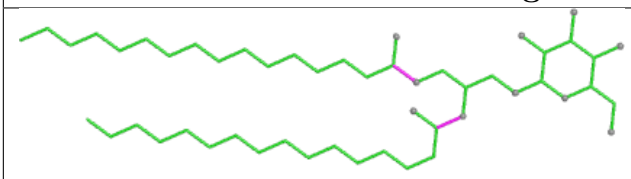
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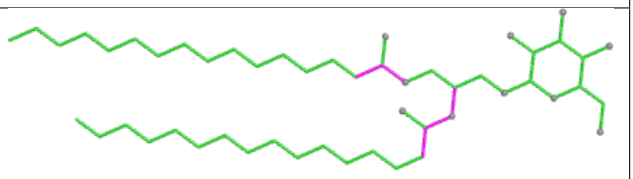
Ligand CLA 4 613



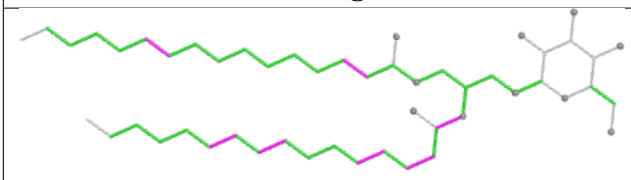
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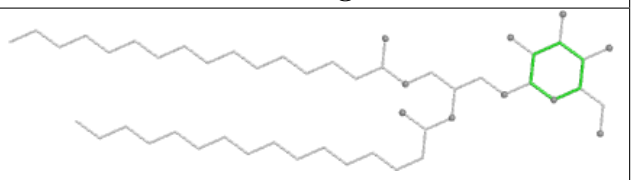
Bond lengths



Bond angles

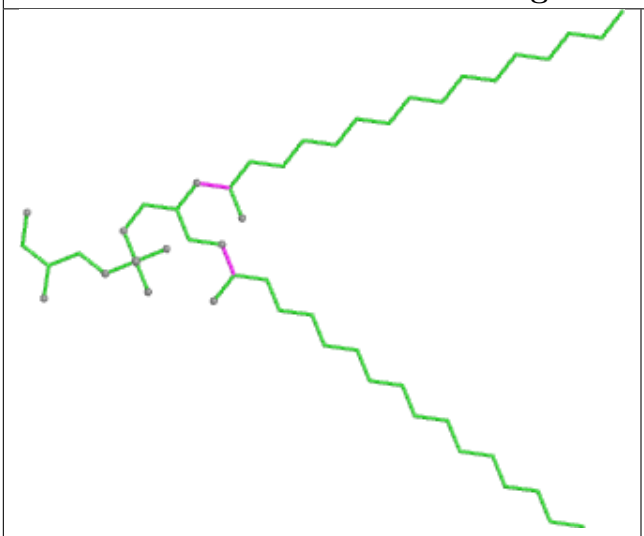


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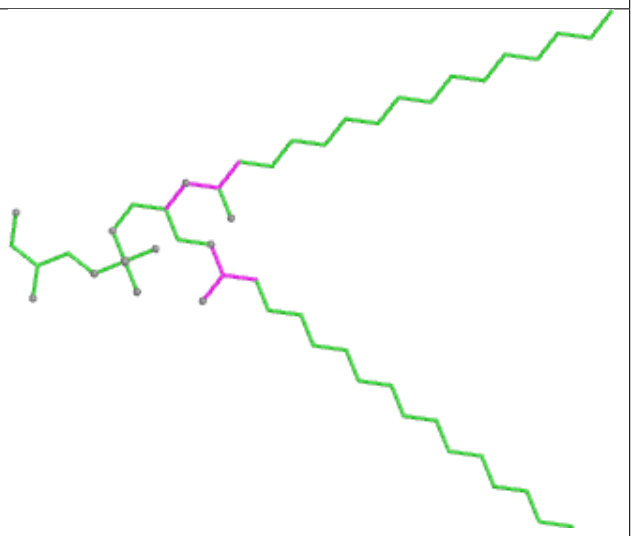


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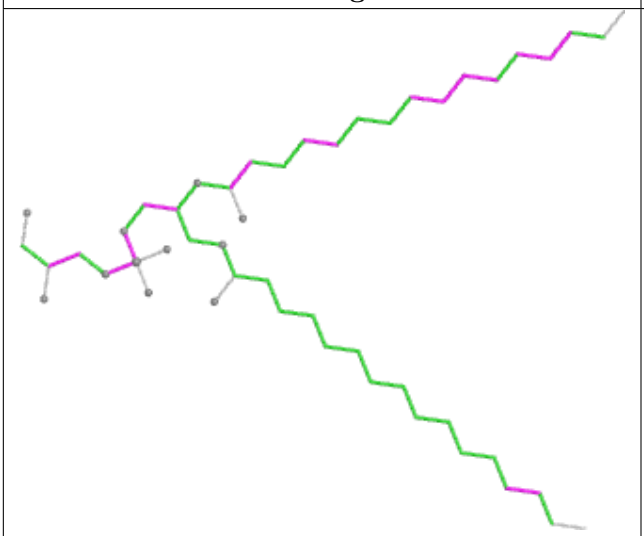
Ligand LHG l 101



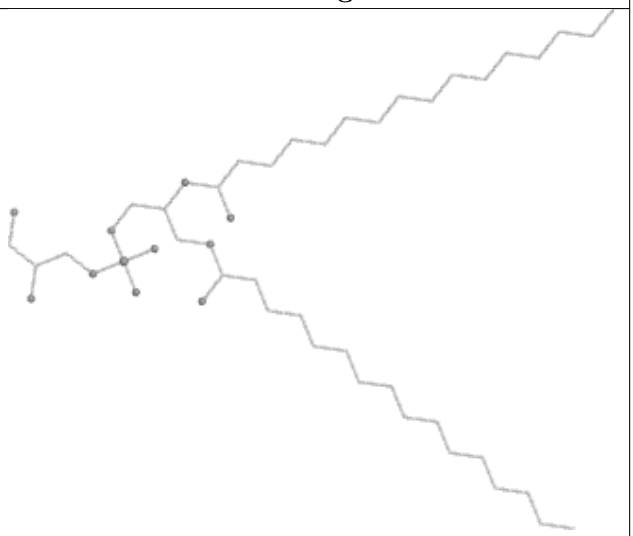
Bond lengths



Bond angles

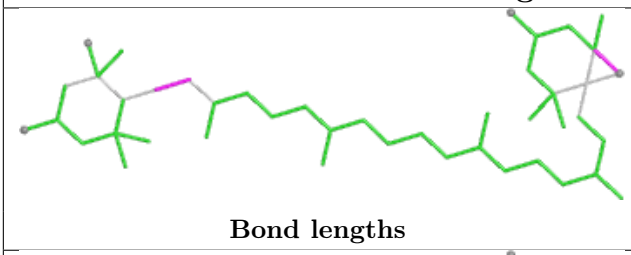


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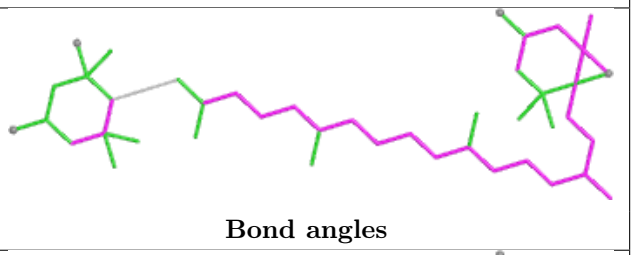


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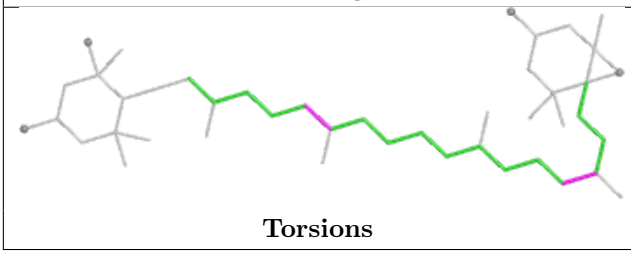
Ligand NEX S 1623



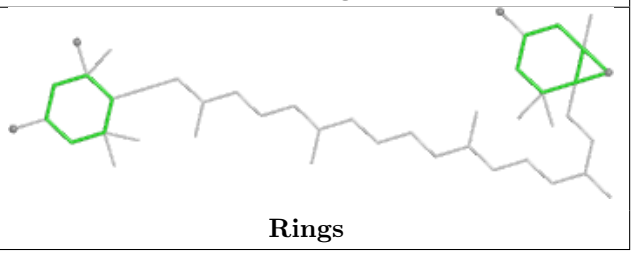
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Bond angles

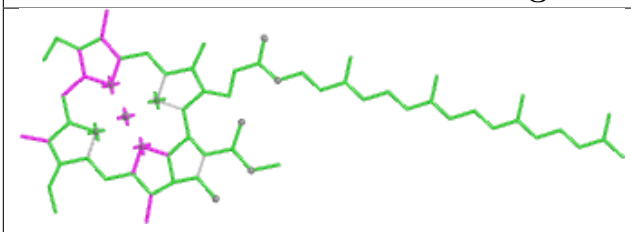


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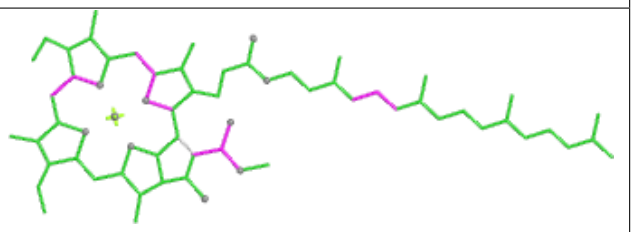


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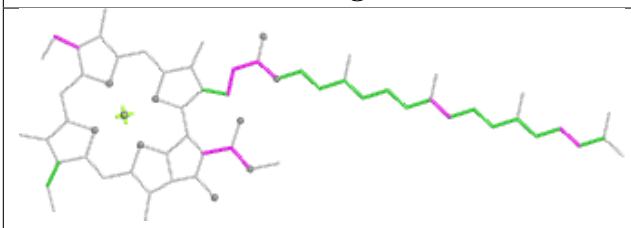
Ligand CLA c 501



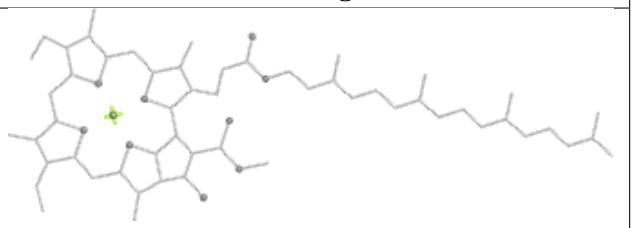
Bond lengths



Bond angles

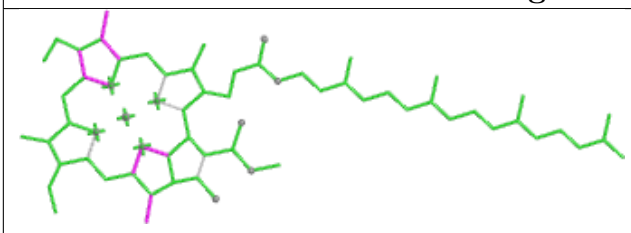


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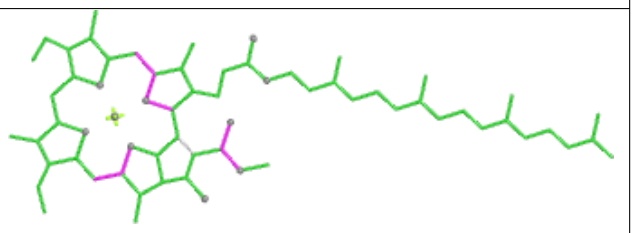


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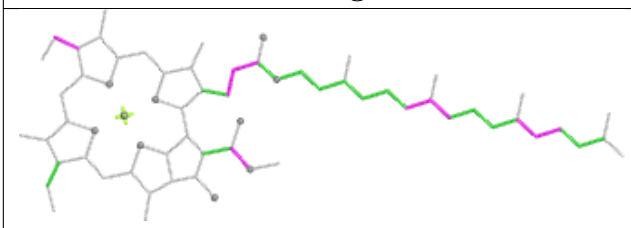
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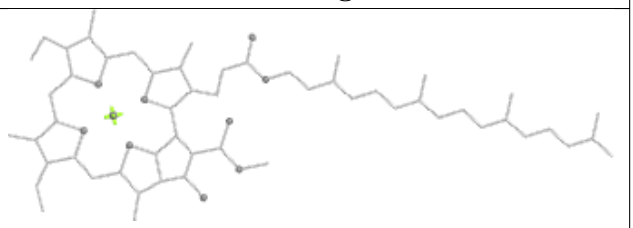
Bond lengths



Bond angles

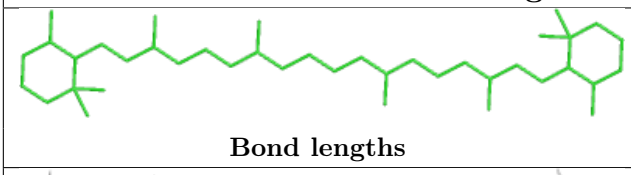


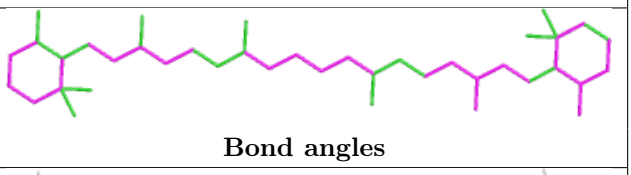
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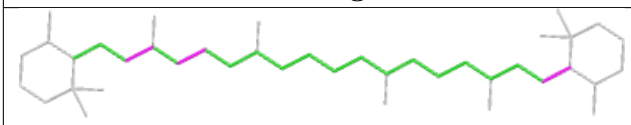


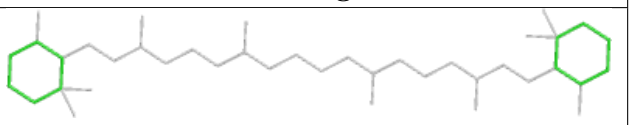
Rings

Ligand BCR h 101


Bond lengths

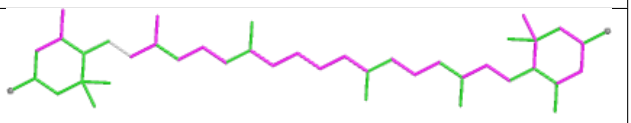

Bond angles

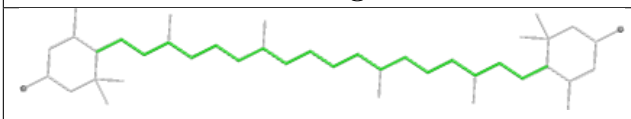

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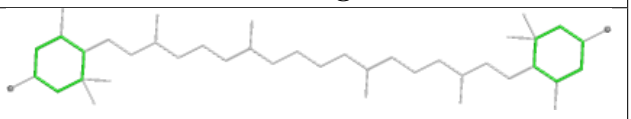

Rings

Ligand LUT 3 1621

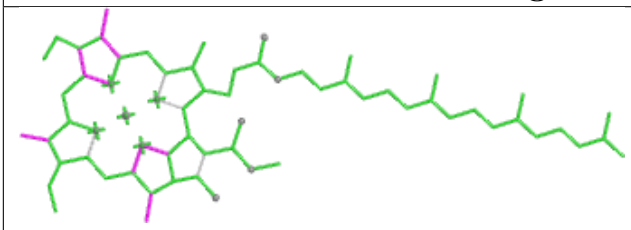

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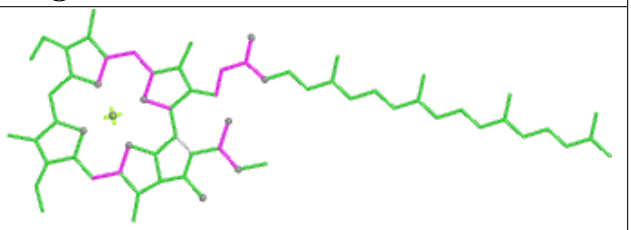

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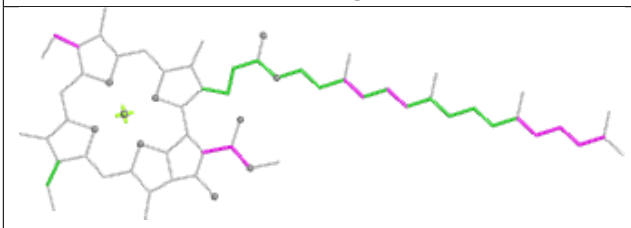

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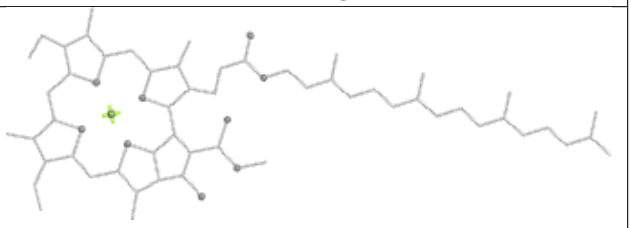

Rings

Ligand CLA g 610

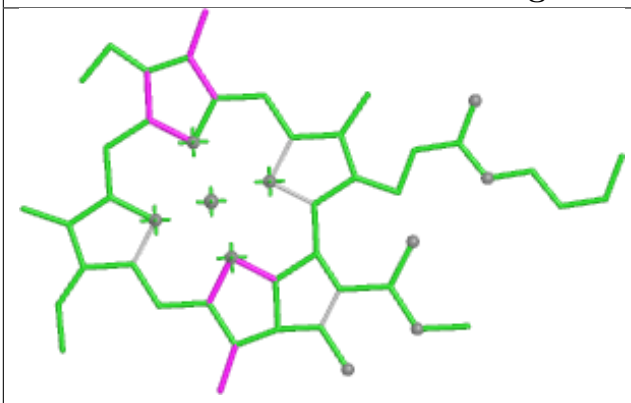

Bond lengths


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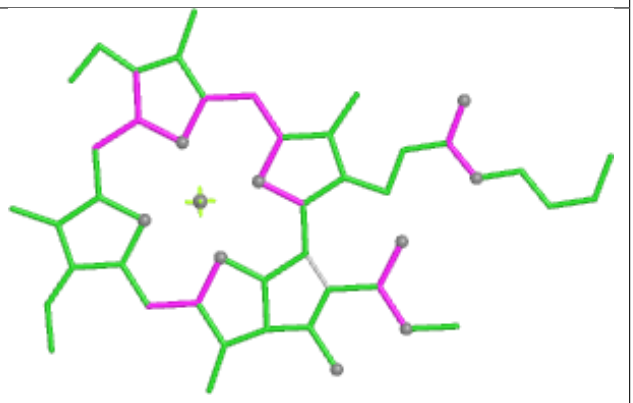

Torsions


Rings

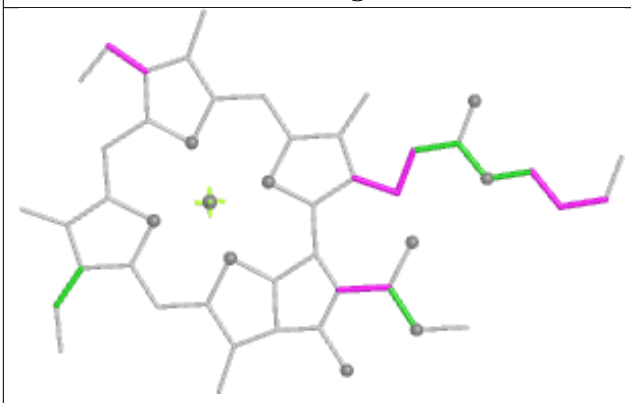
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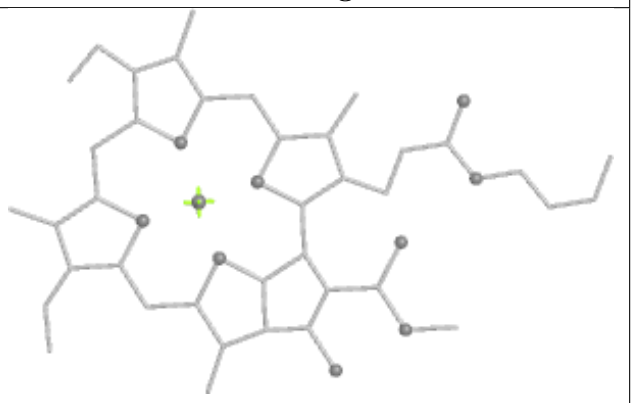
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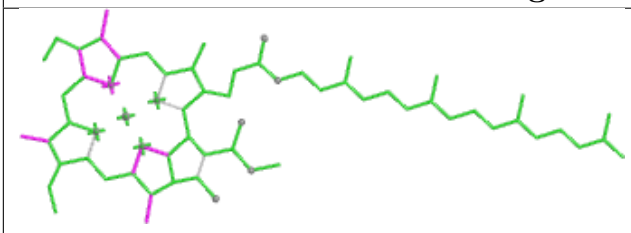


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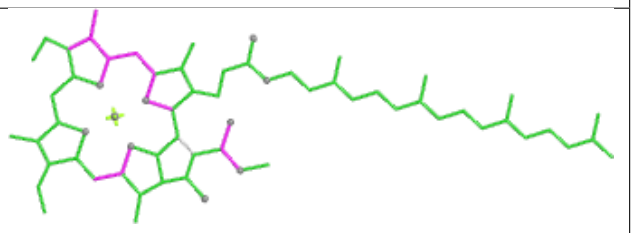


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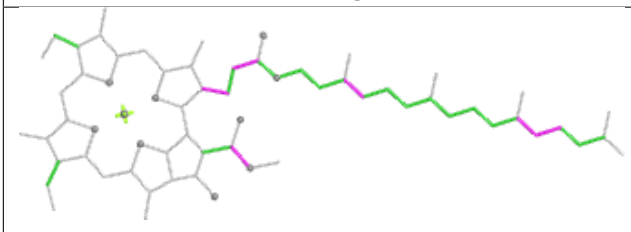
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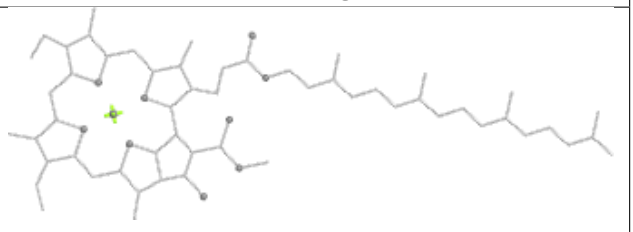
Bond lengths



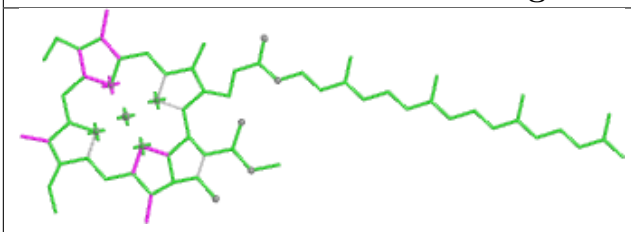
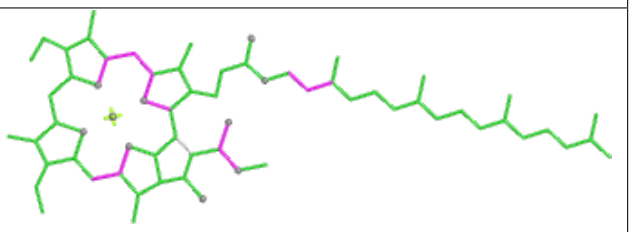
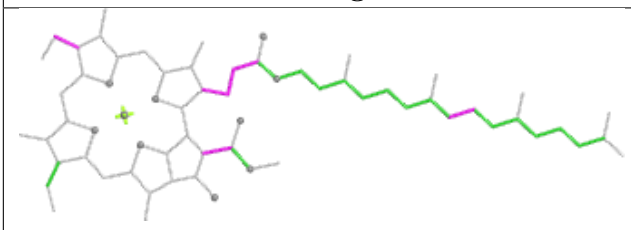
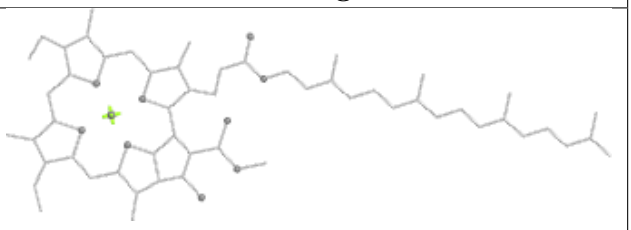
Bond angles

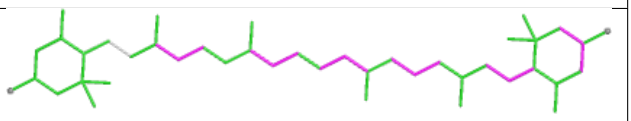
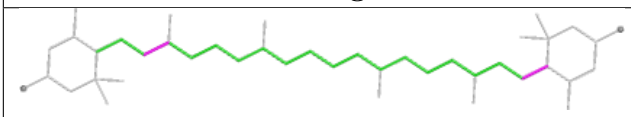
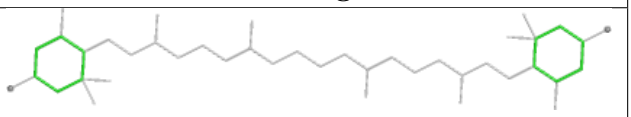


Torsions

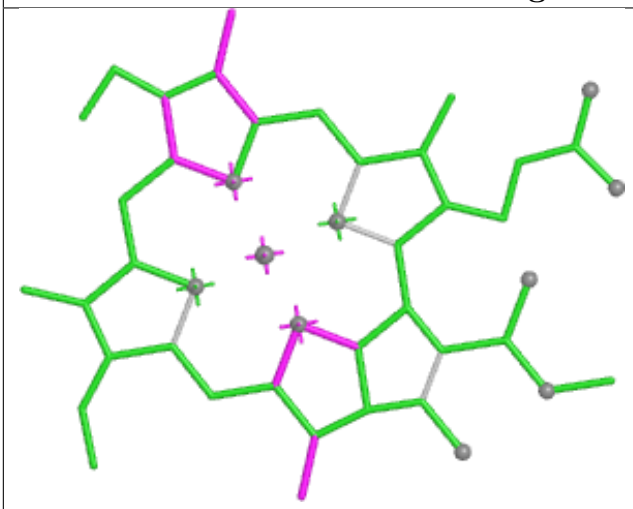


Rings

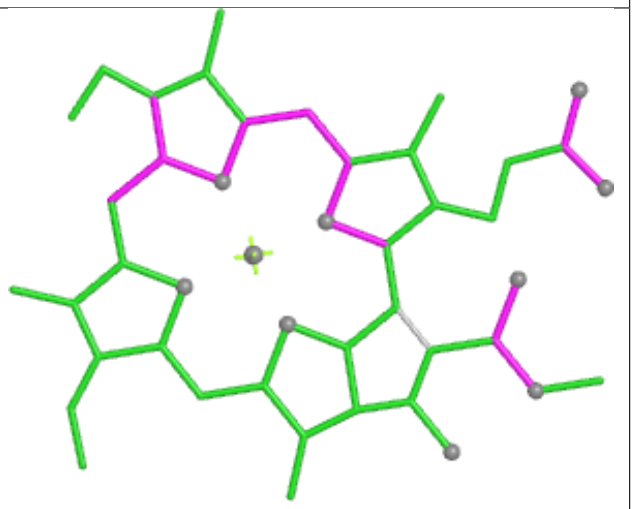
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

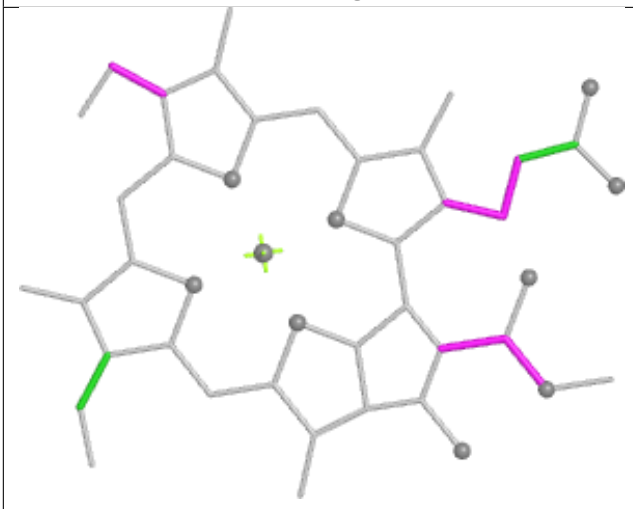
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Bond lengths



Bond angles

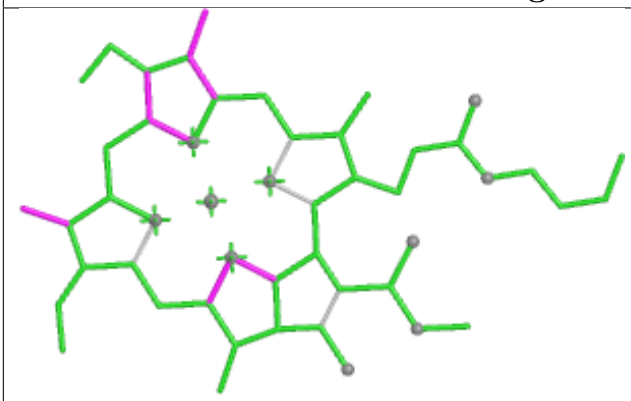


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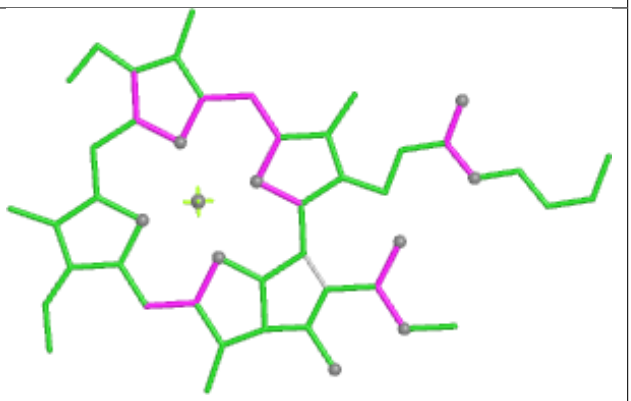


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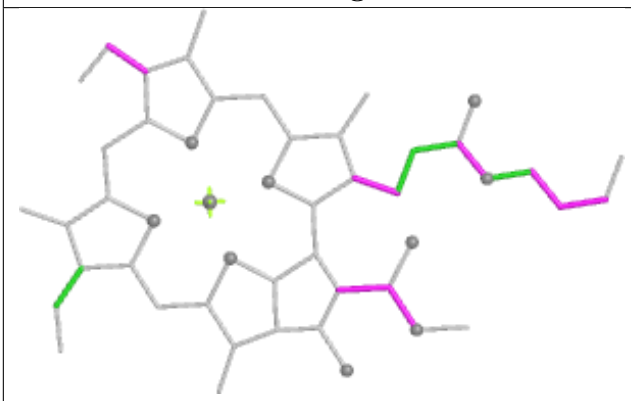
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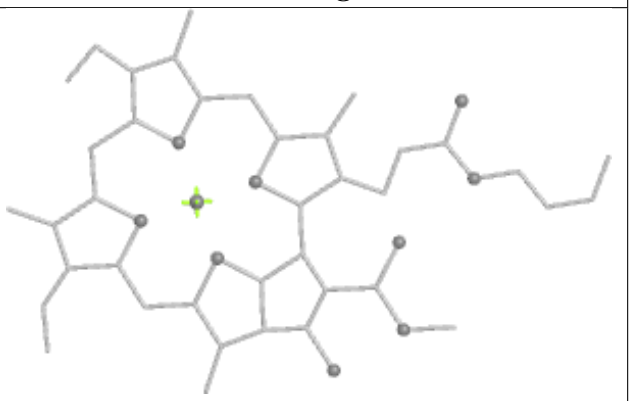
Bond lengths



Bond angles

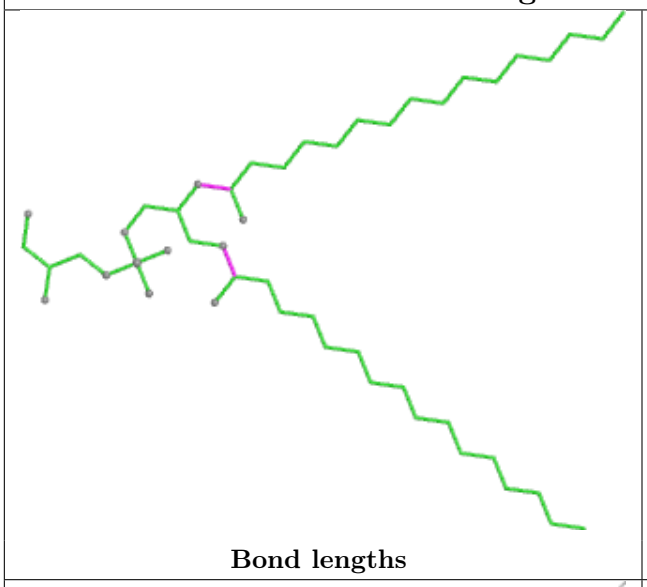


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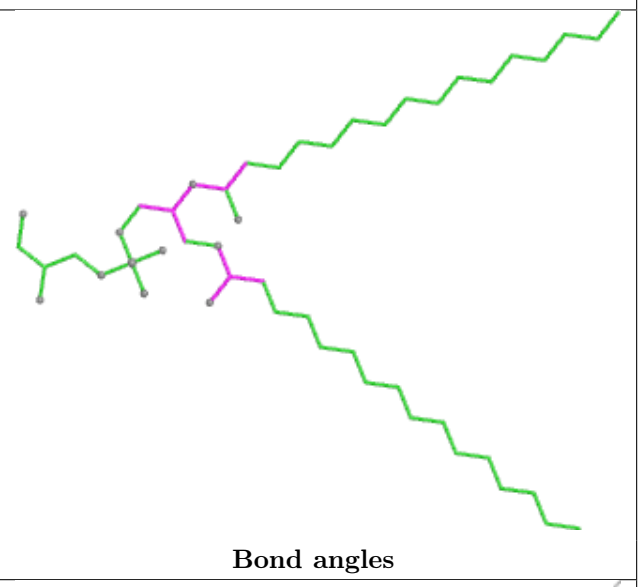


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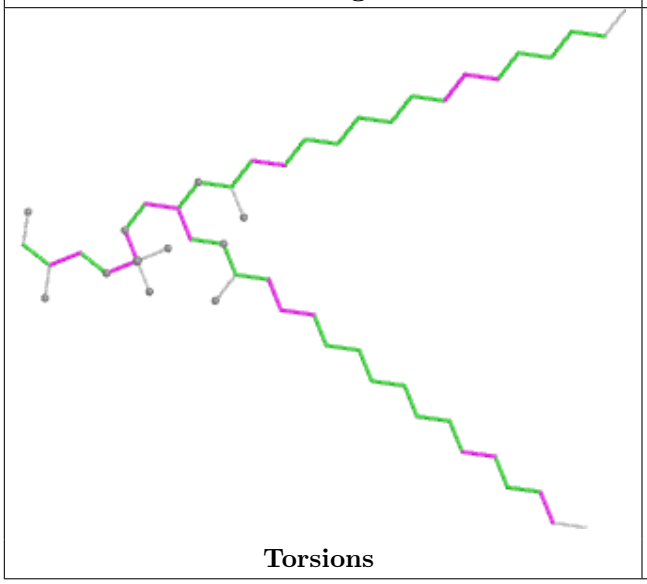
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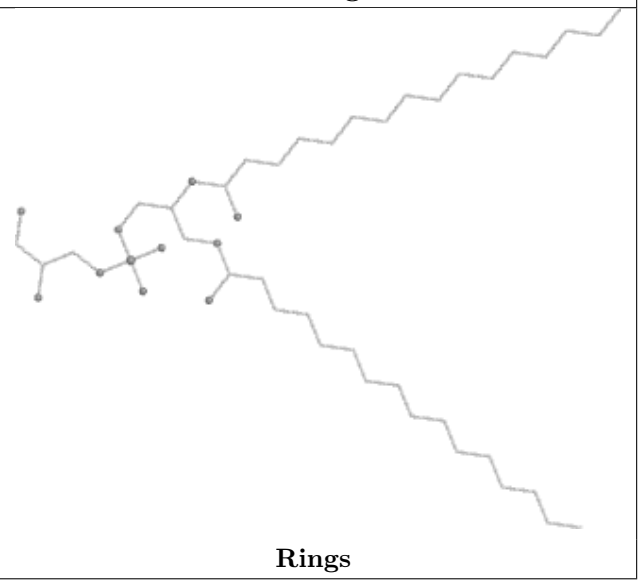
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Bond angles

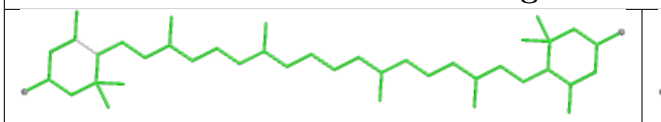


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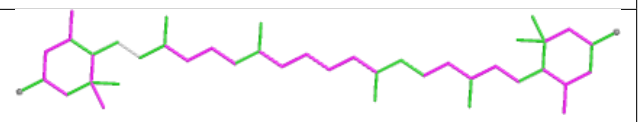


Rings

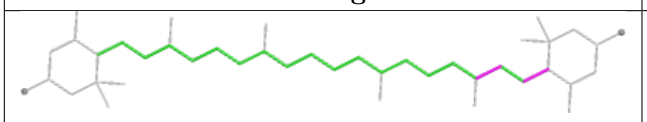
Ligand LUT 9 1621



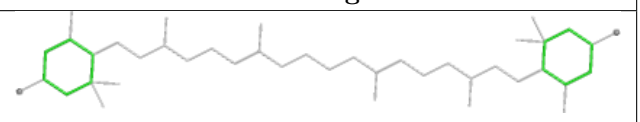
Bond lengths



Bond angles

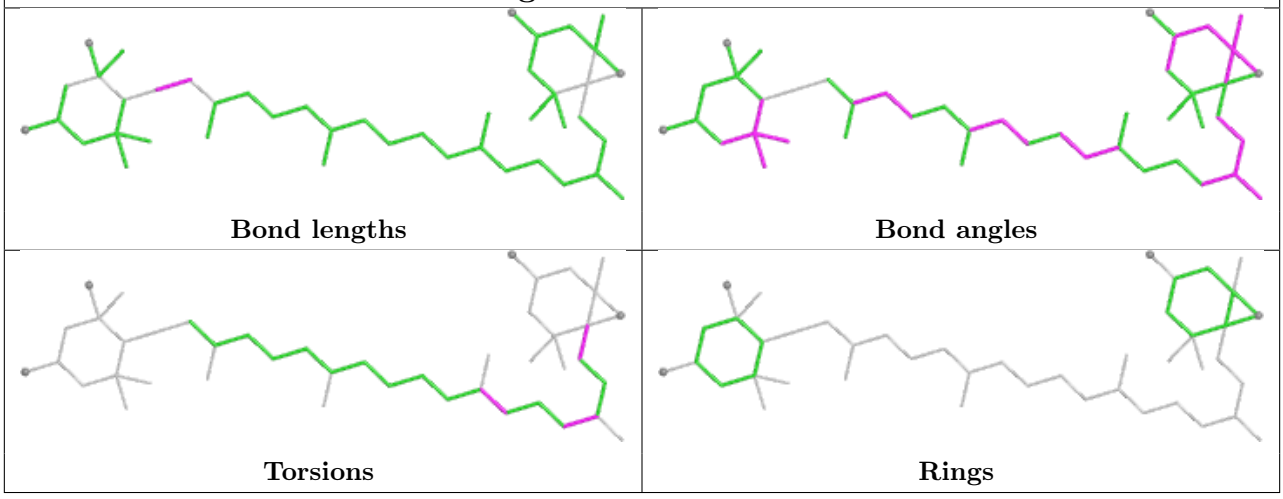


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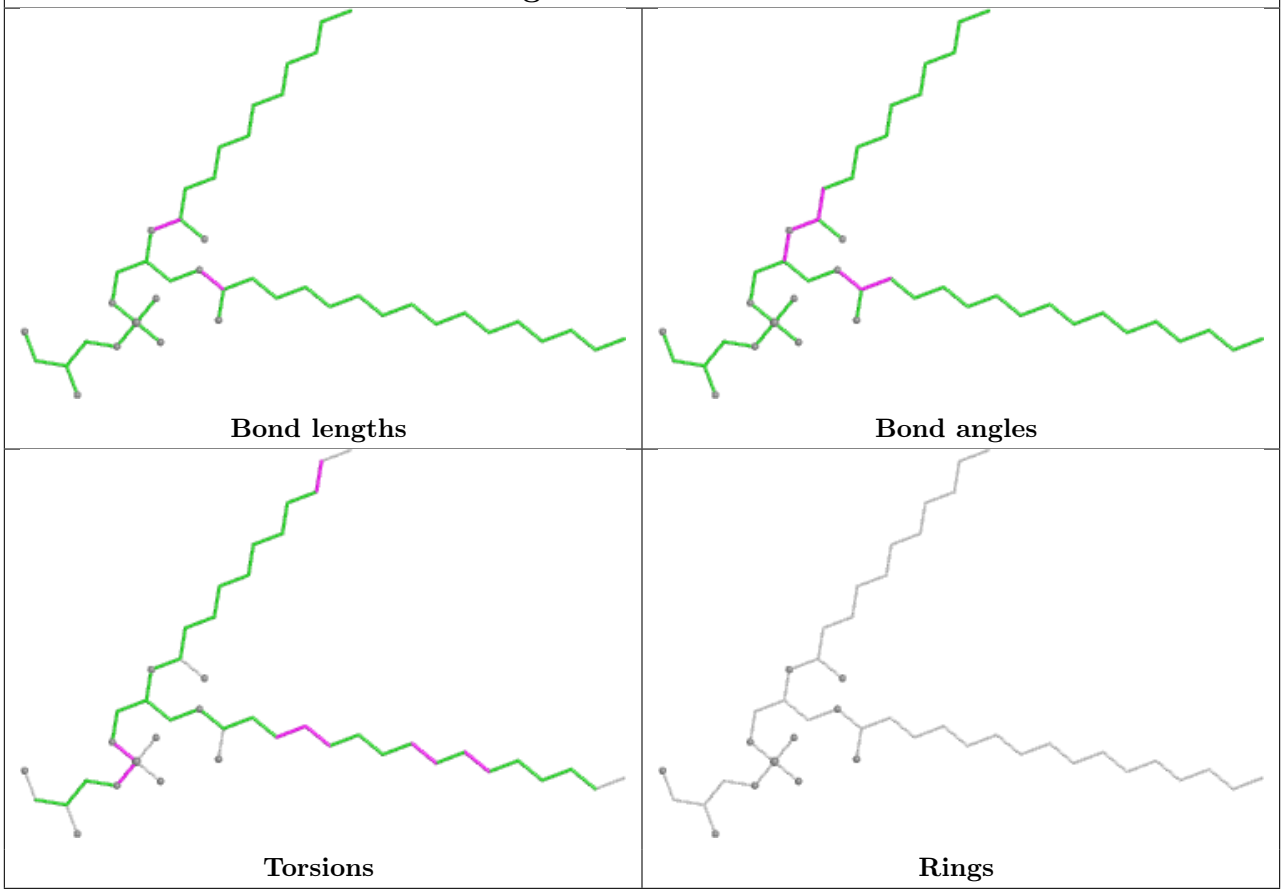


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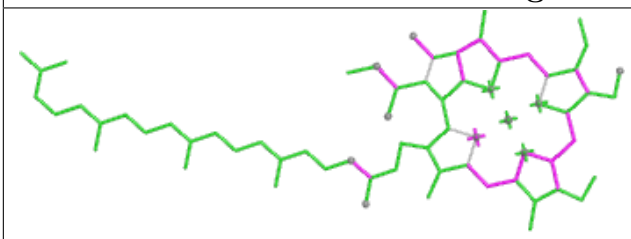
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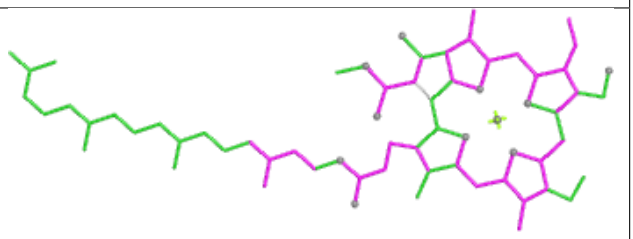
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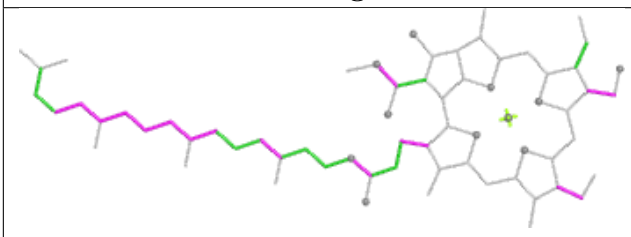
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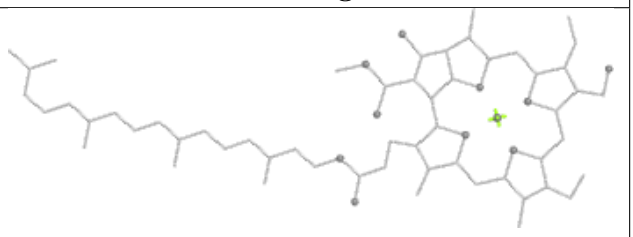
Bond lengths



Bond angles

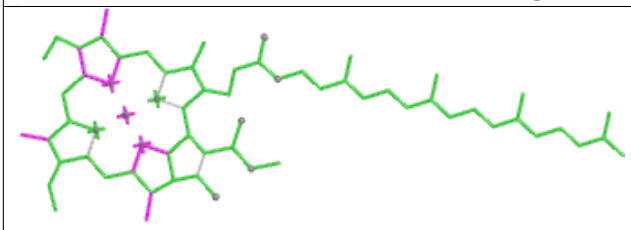


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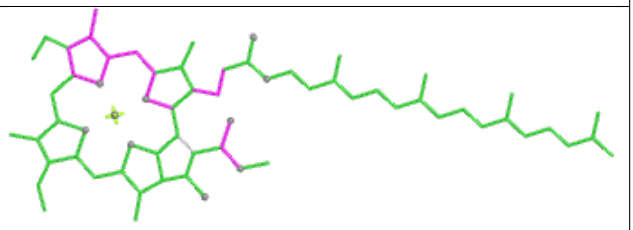


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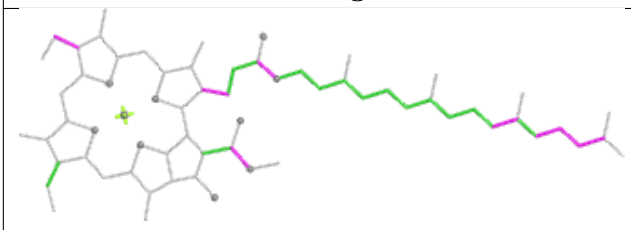
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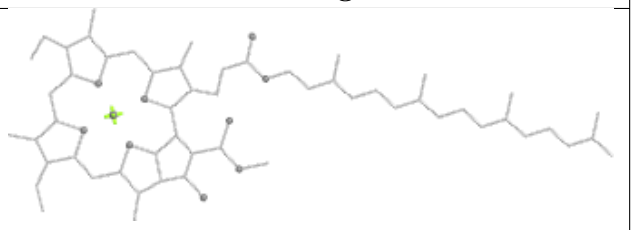
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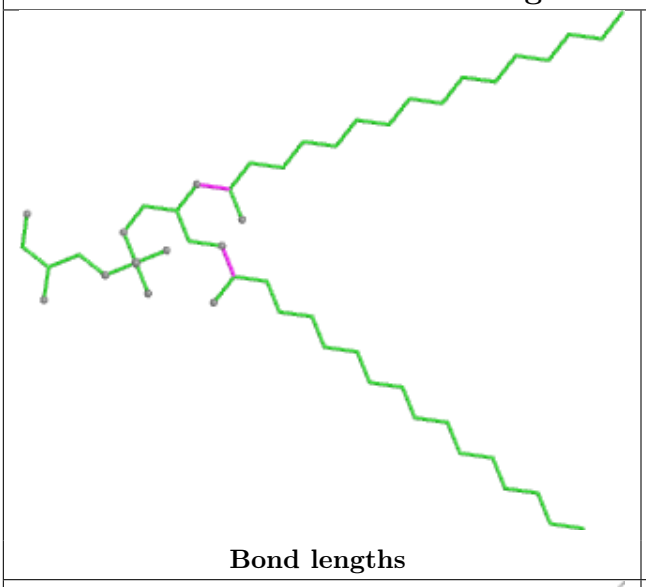


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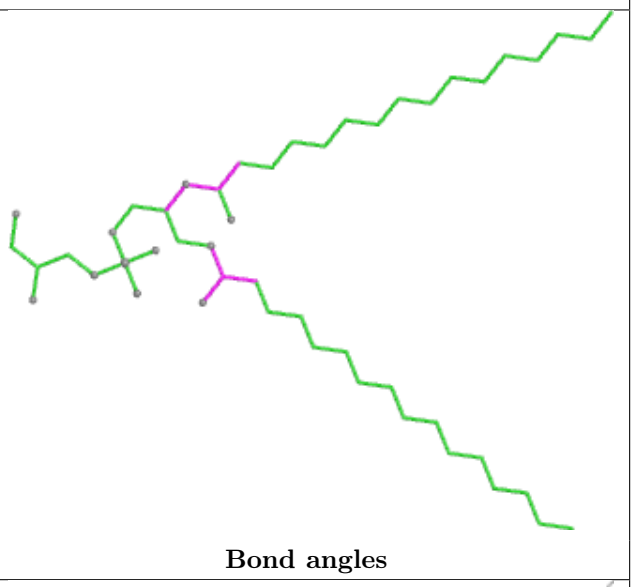


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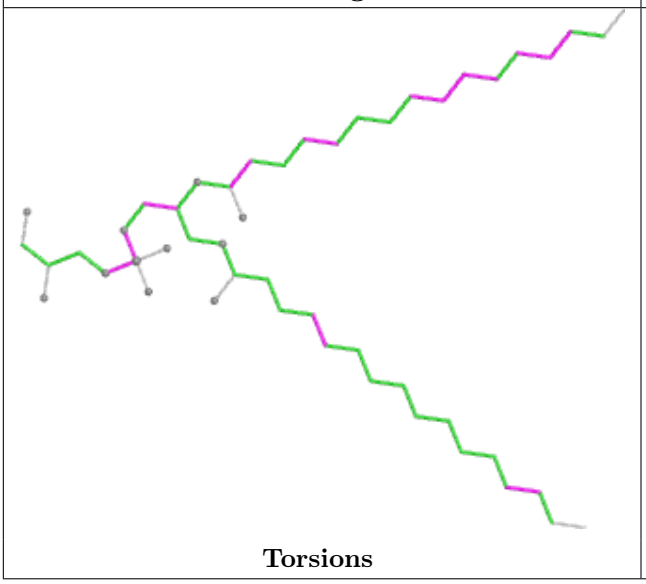
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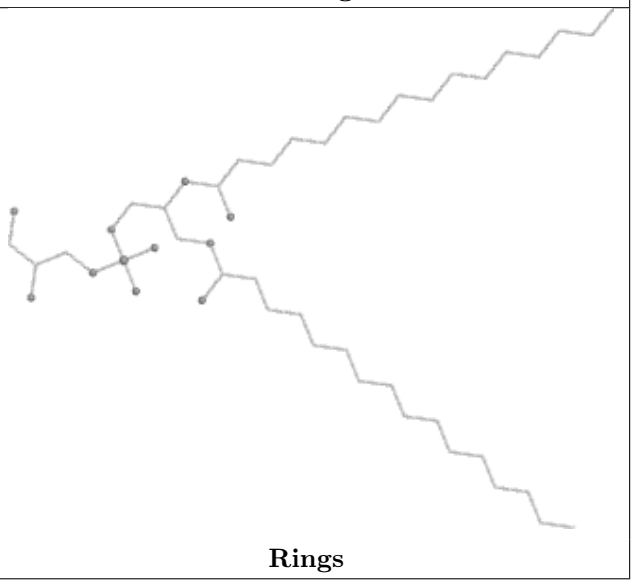
Bond lengths



Bond angles

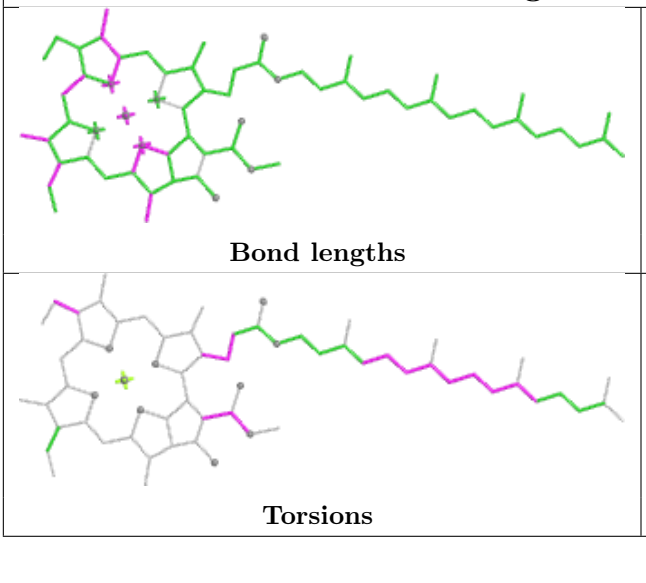


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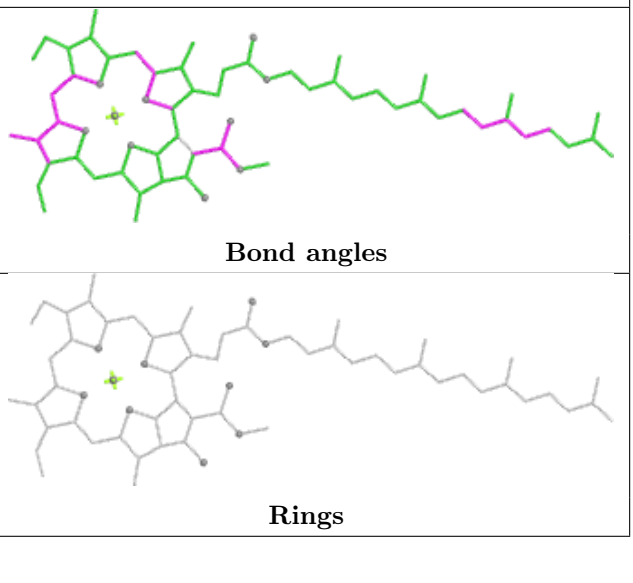


Rings

Ligand CLA C 502



Bond lengths

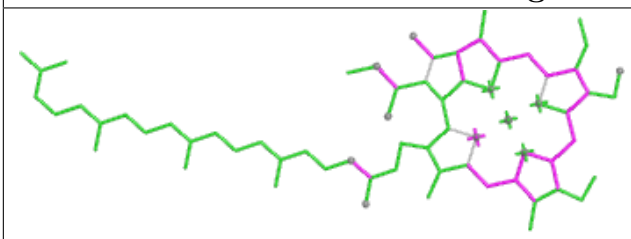


Bond angles

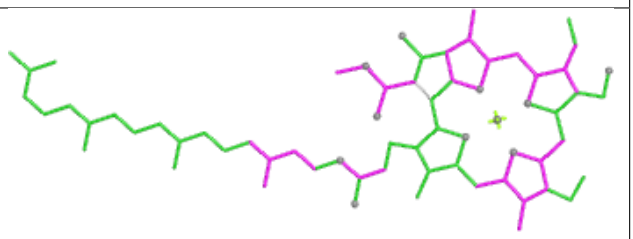
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Rings

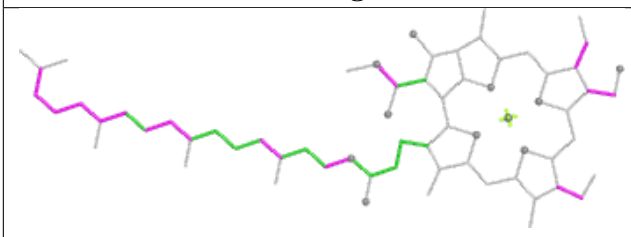
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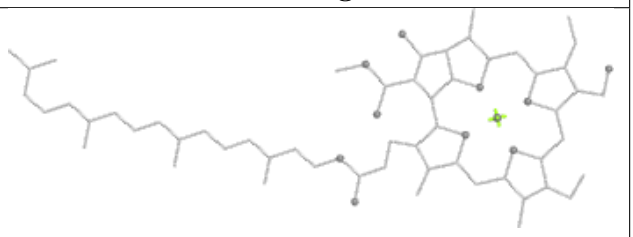
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Bond angles

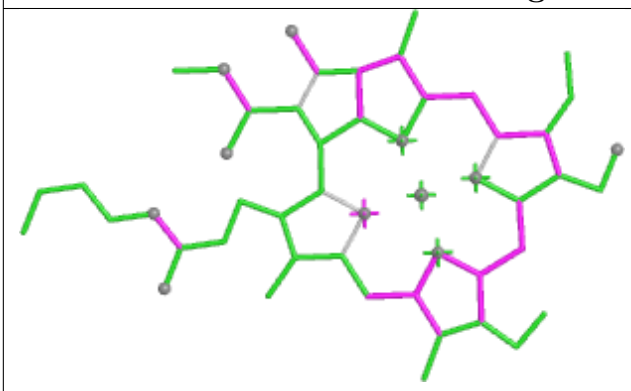


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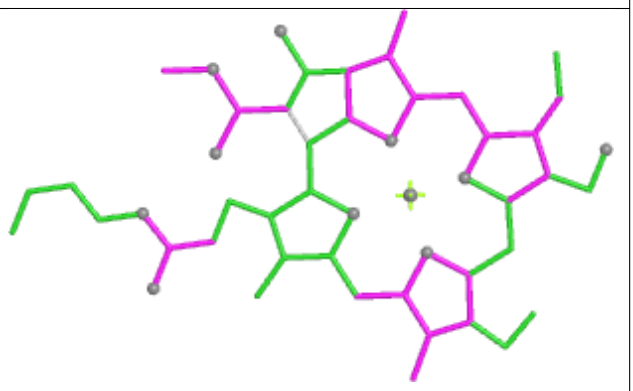


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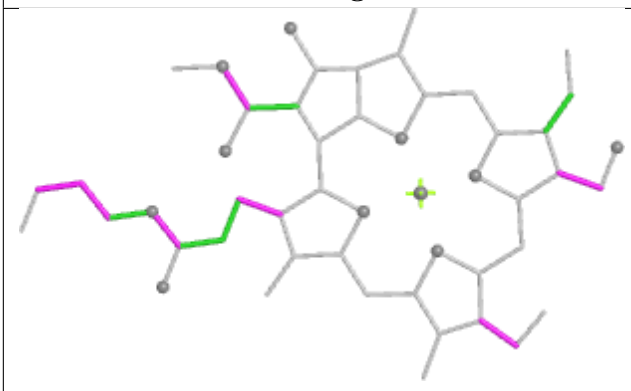
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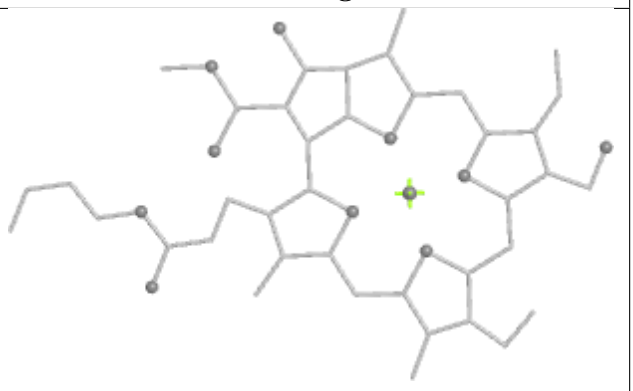
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Bond angles

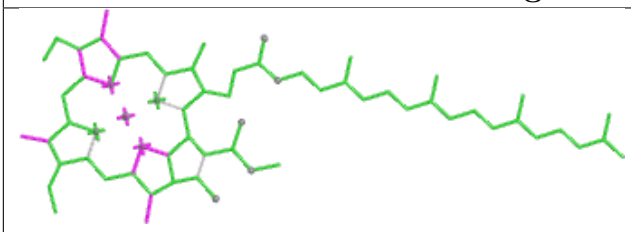


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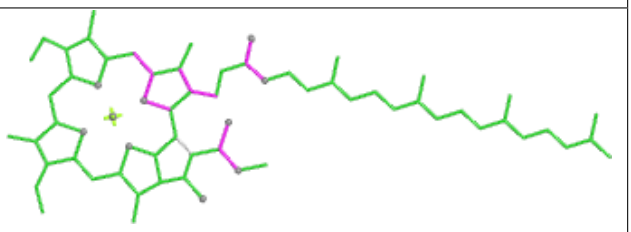


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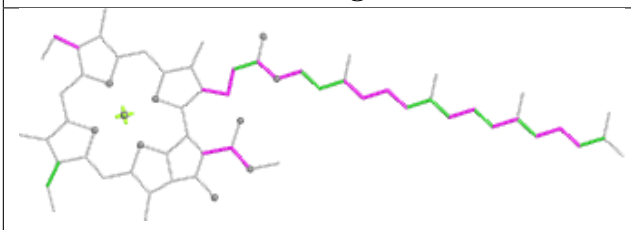
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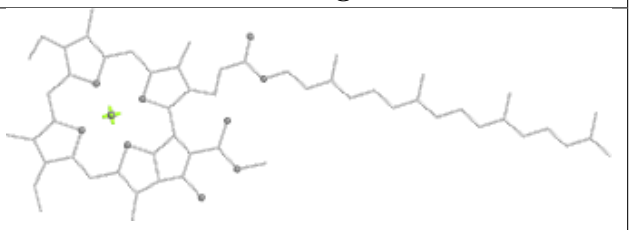
Bond lengths



Bond angles

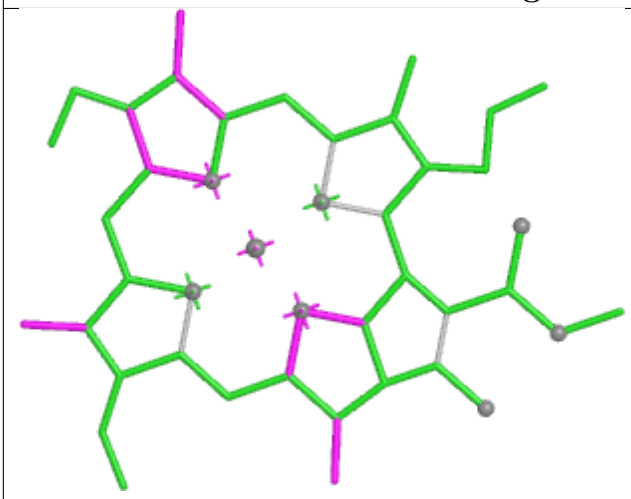


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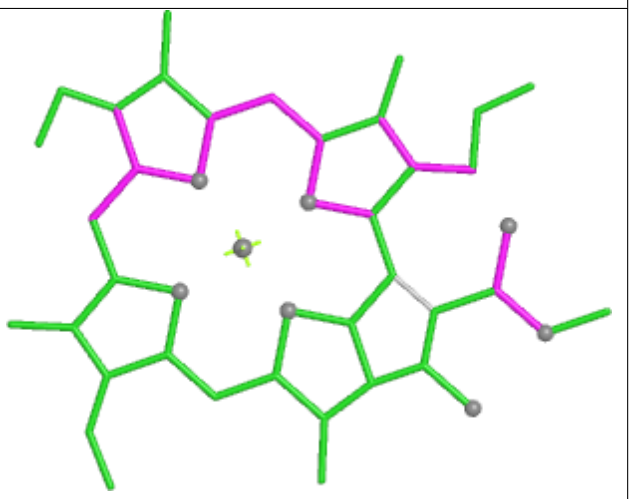


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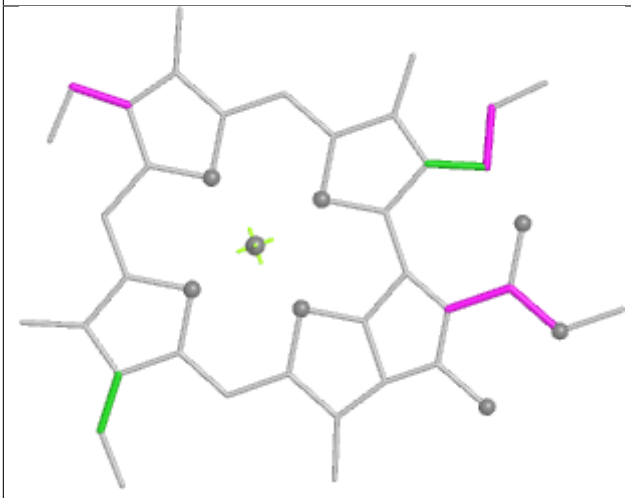
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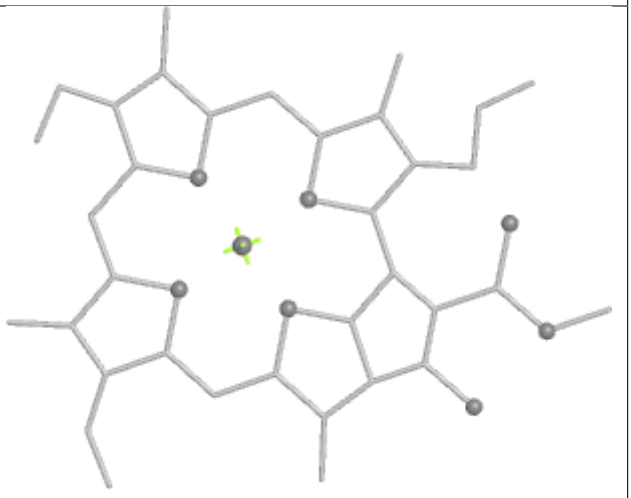
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Bond angles

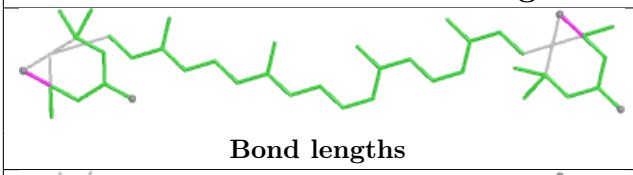


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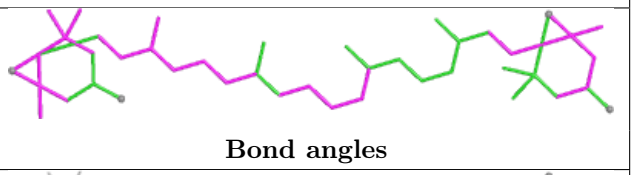


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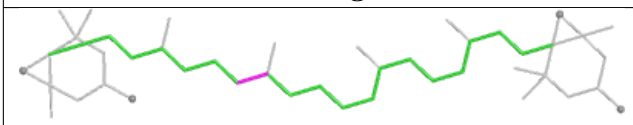
Ligand XAT 6 1622



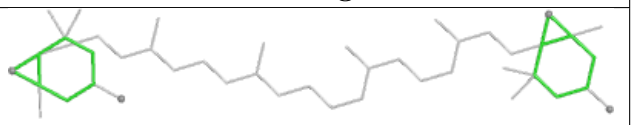
Bond lengths



Bond angles

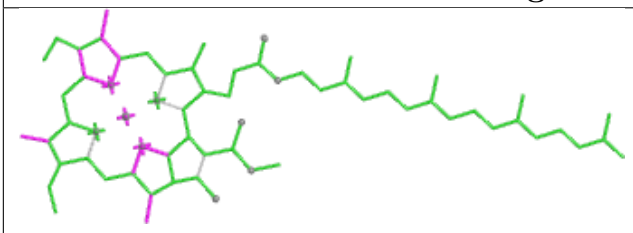


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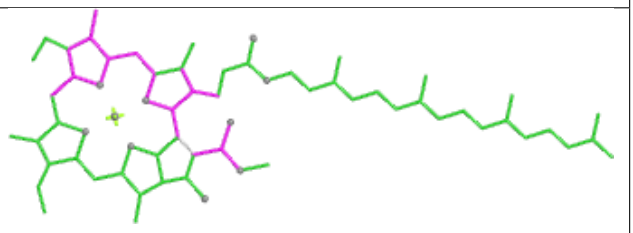


Rings

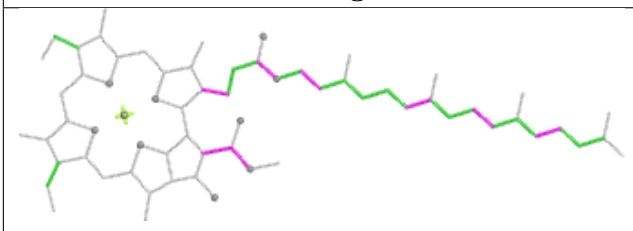
Ligand CLA b 603



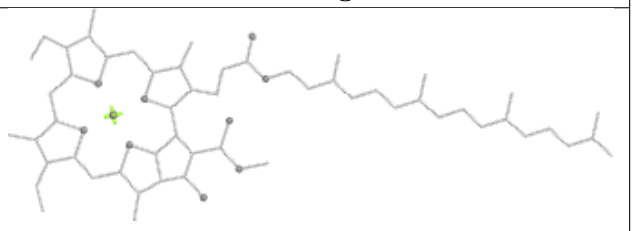
Bond lengths



Bond angles

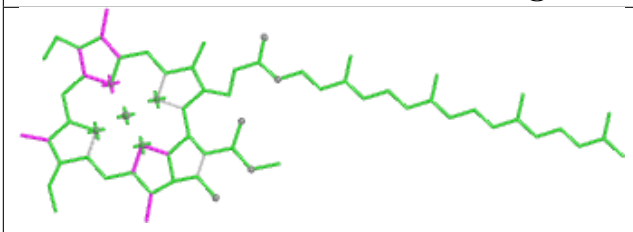


Torsions

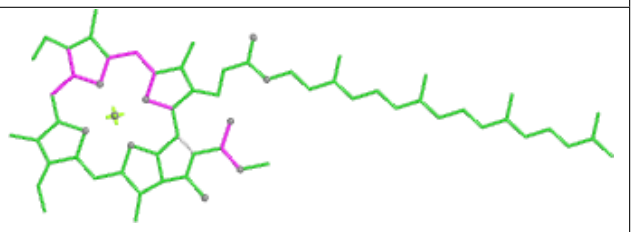


Rings

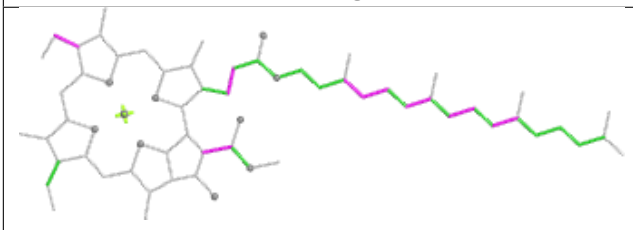
Ligand CLA 1 602



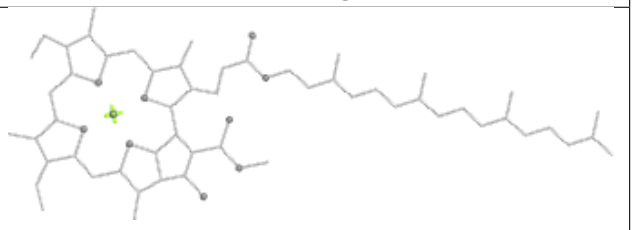
Bond lengths



Bond angles

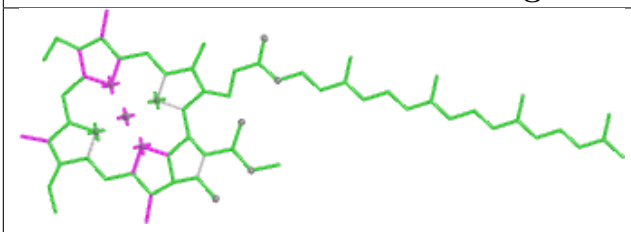


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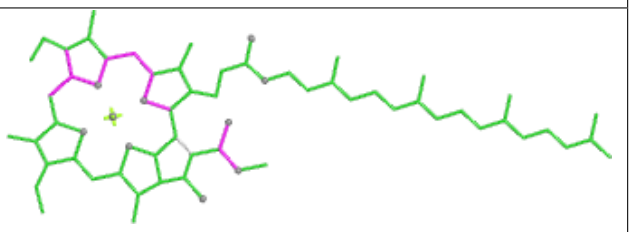


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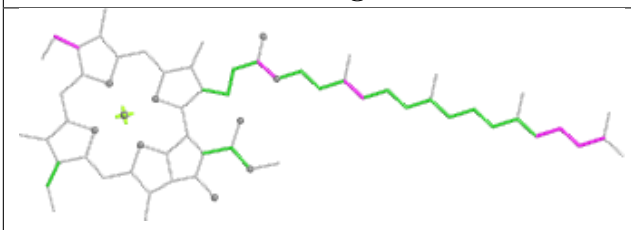
Ligand CLA Y 611



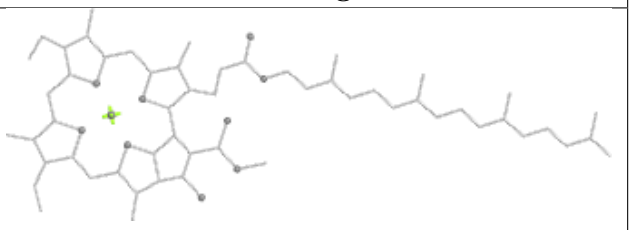
Bond lengths



Bond angles

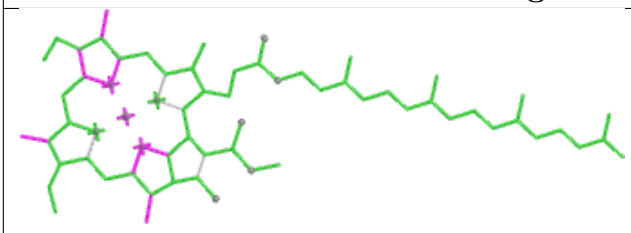


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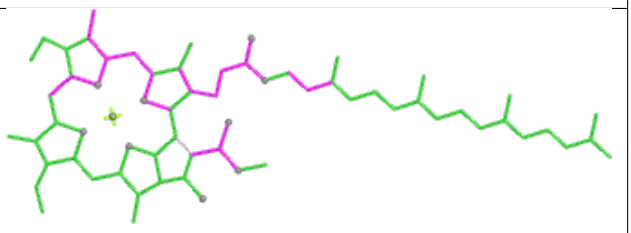


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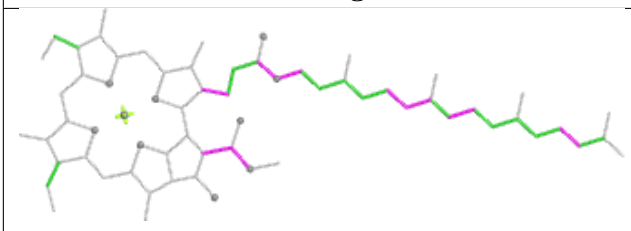
Ligand CLA b 605



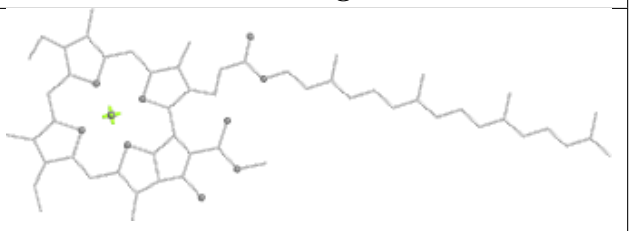
Bond lengths



Bond angles

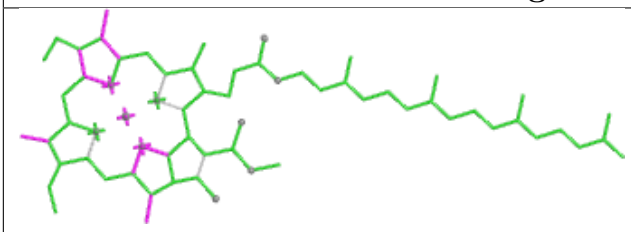


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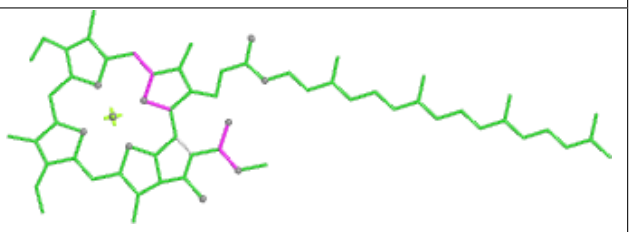


Rings

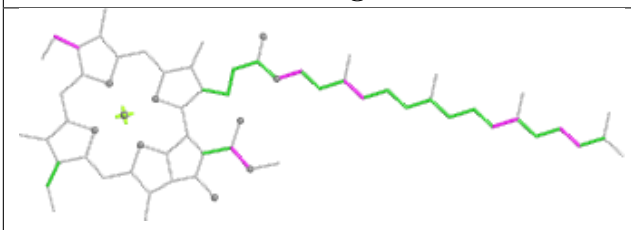
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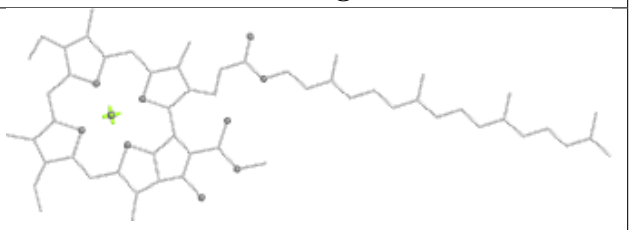
Bond lengths



Bond angles

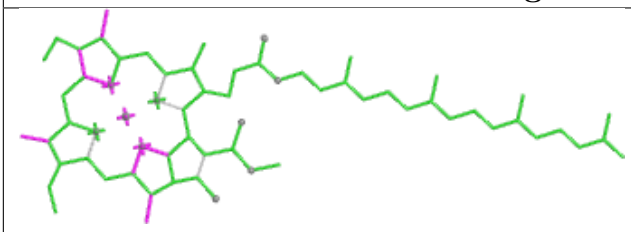


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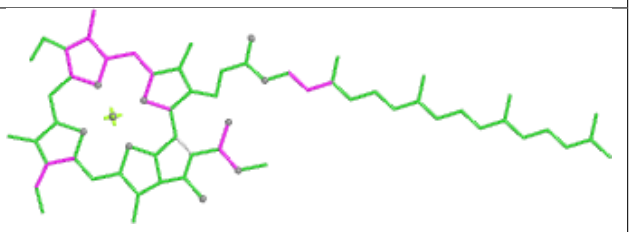


Rings

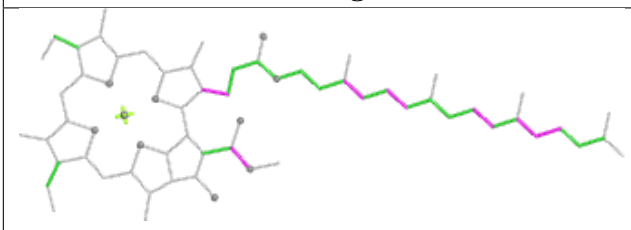
Ligand CLA B 612



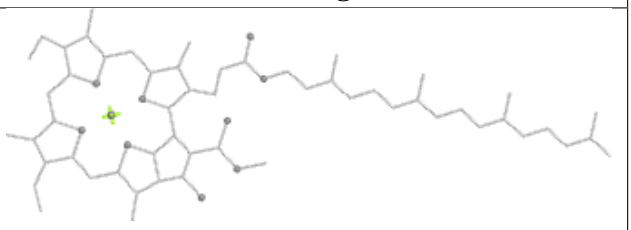
Bond lengths



Bond angles

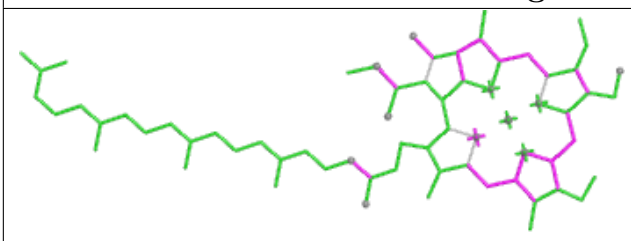


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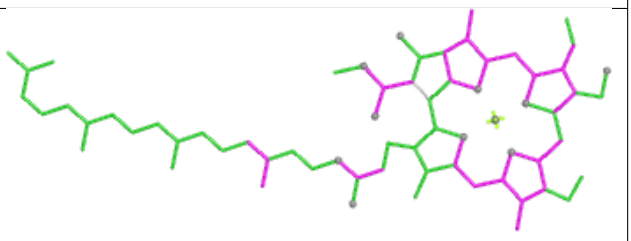


Rings

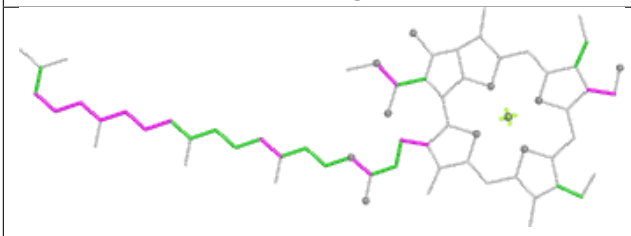
Ligand CHL 7 609



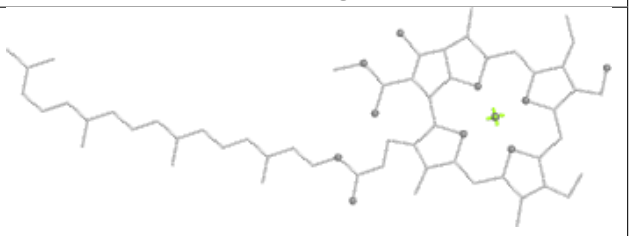
Bond lengths



Bond angles

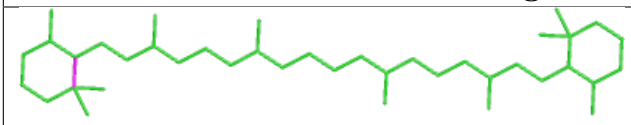


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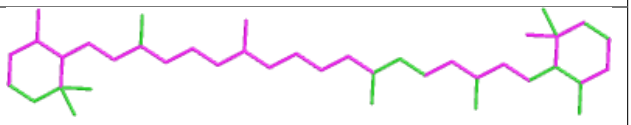


Rings

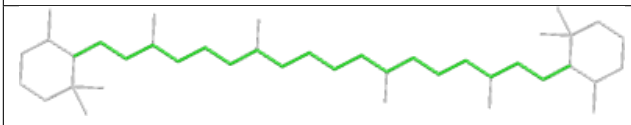
Ligand BCR B 619



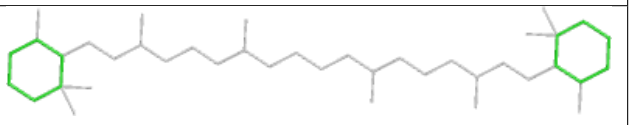
Bond lengths



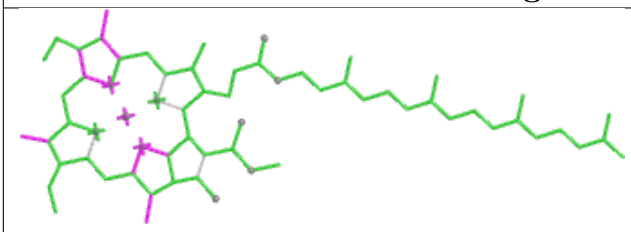
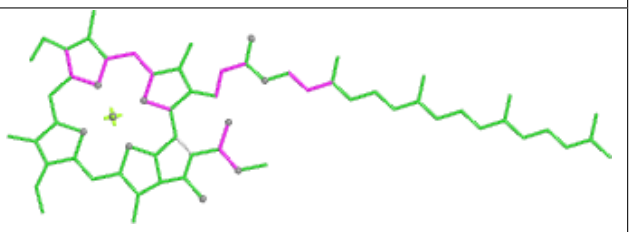
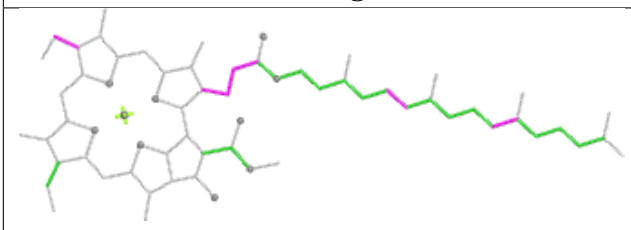
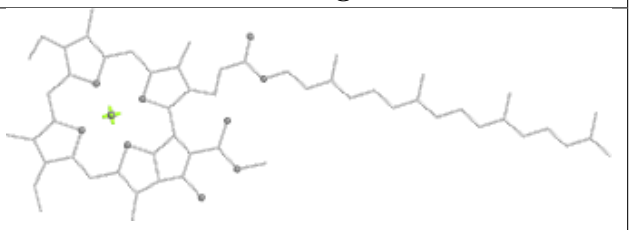
Bond angles

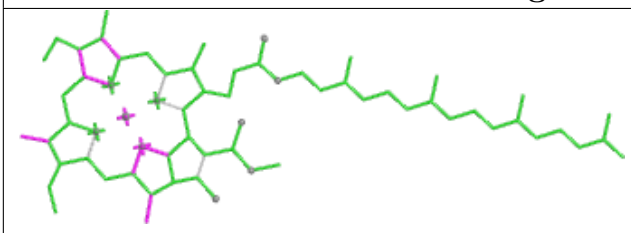
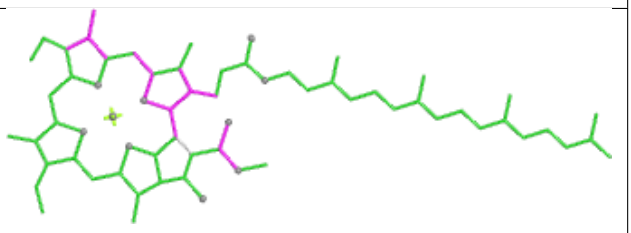
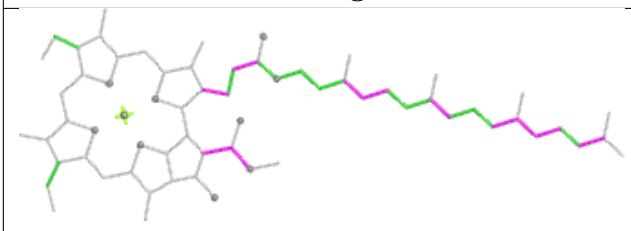
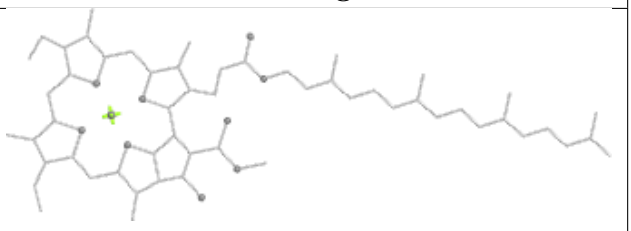


Torsions

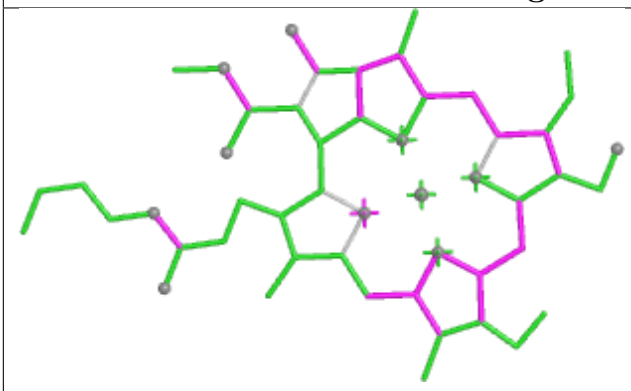


Rings

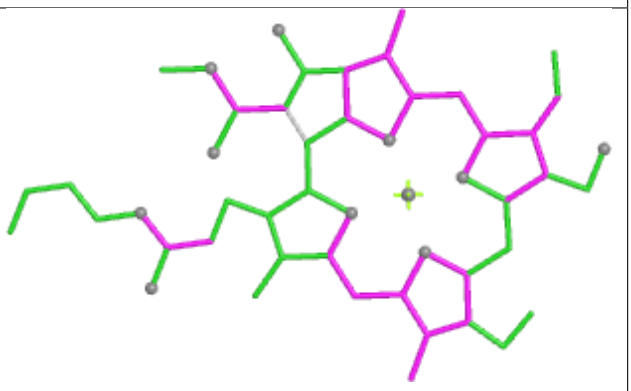
Ligand CLA N 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

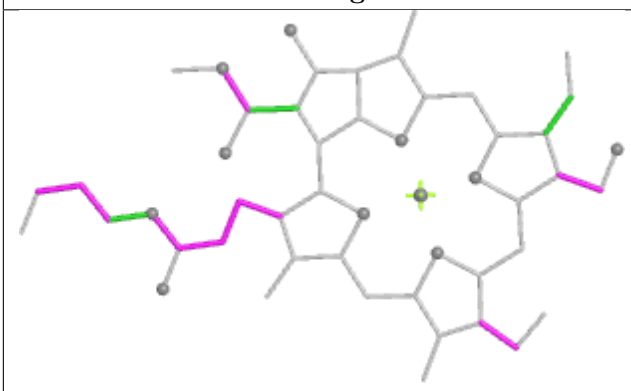
Ligand CHL 5 608



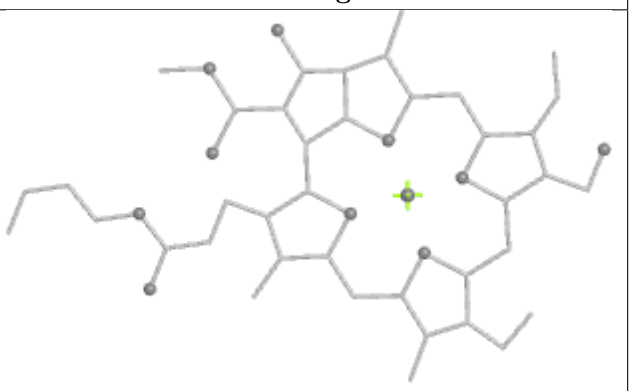
Bond lengths



Bond angles

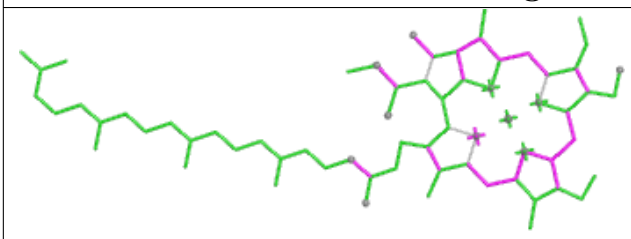


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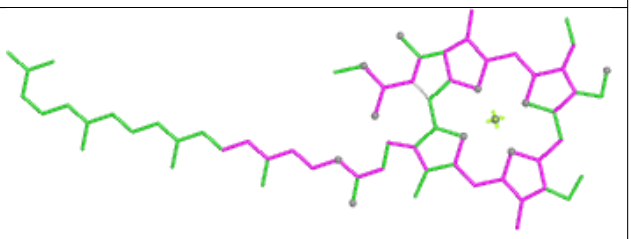


Rings

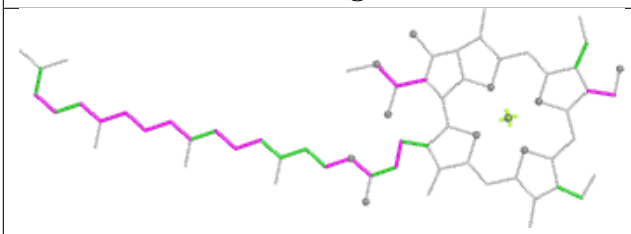
Ligand CHL Y 607



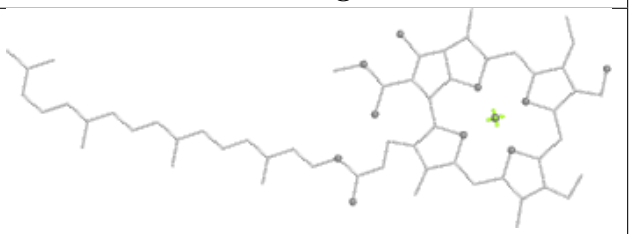
Bond lengths



Bond angles

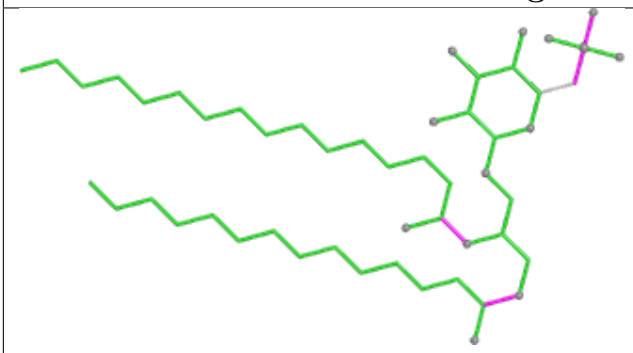


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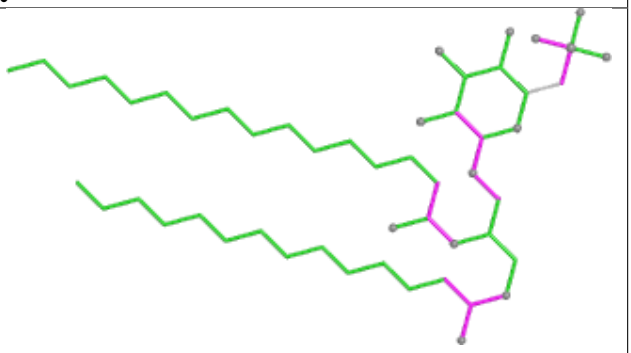


Rings

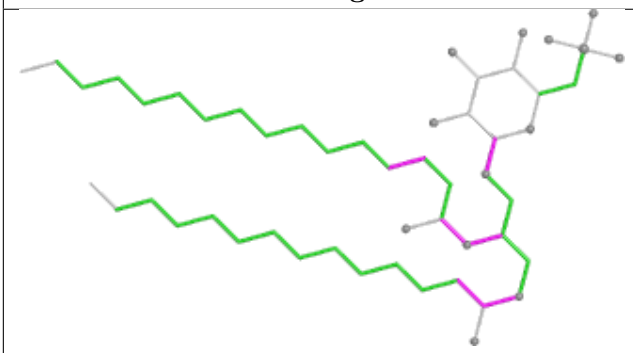
Ligand SQD d 413



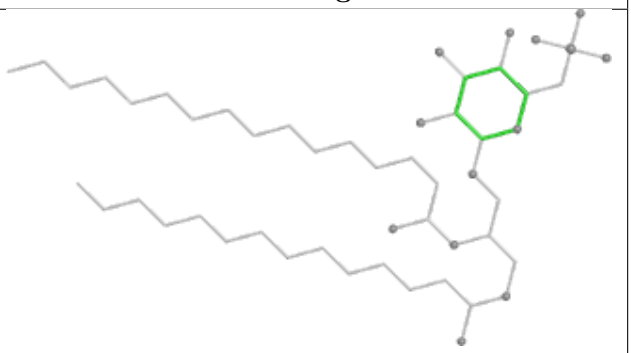
Bond lengths



Bond angles

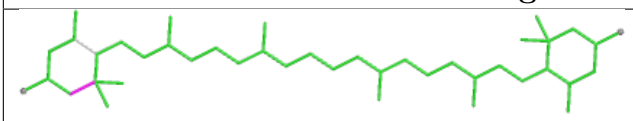


Torsions

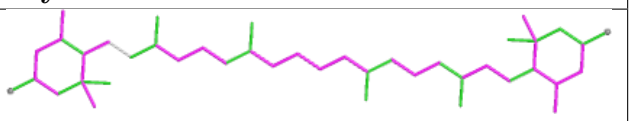


Rings

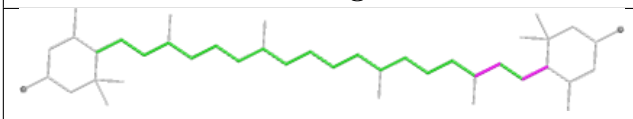
Ligand LUT y 1621



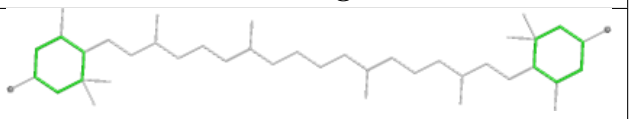
Bond lengths



Bond angles

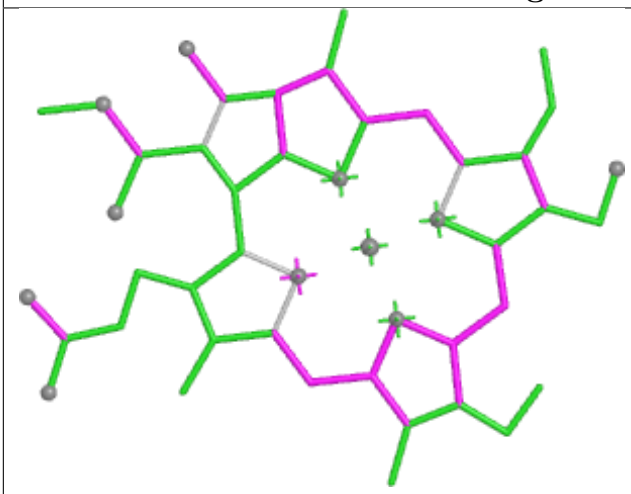


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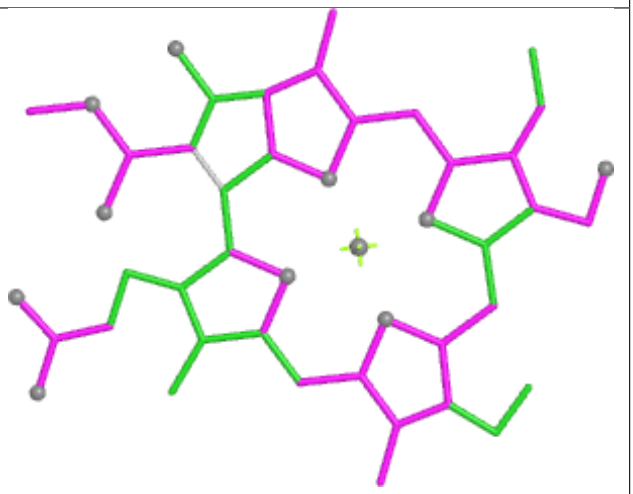


Rings

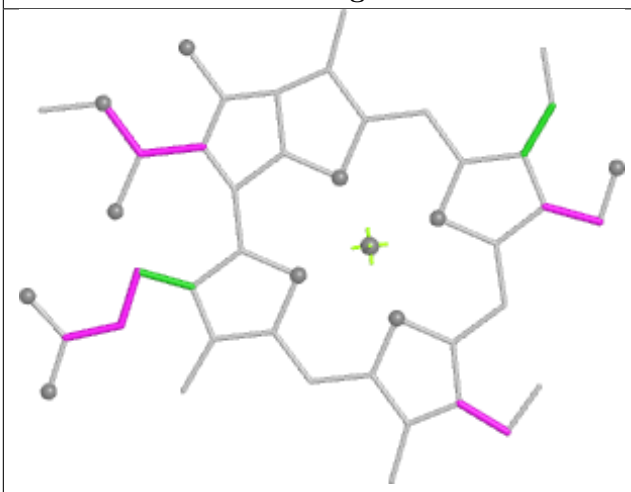
Ligand CHL S 601



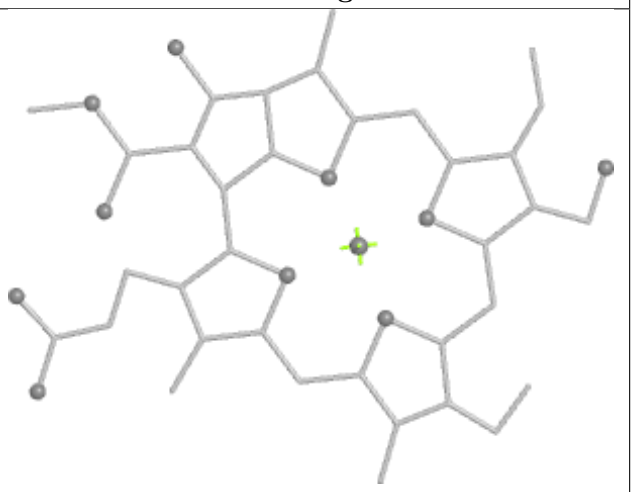
Bond lengths



Bond angles

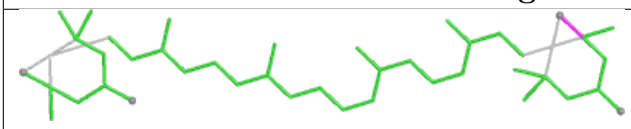


Torsions

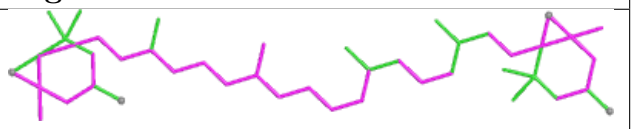


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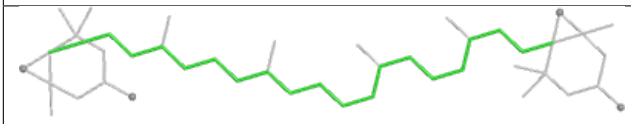
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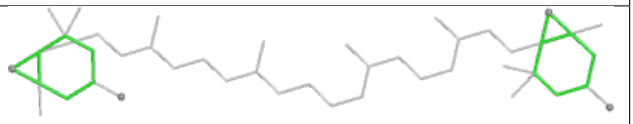
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Bond angles

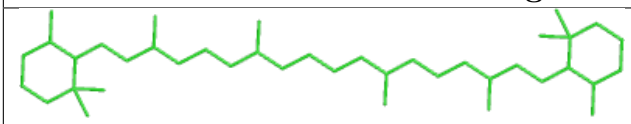


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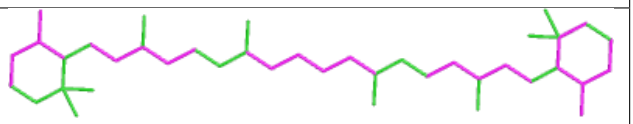


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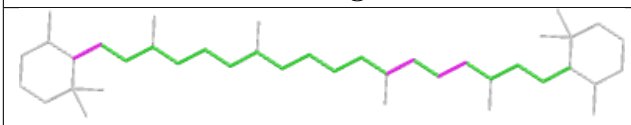
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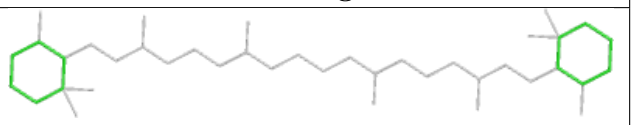
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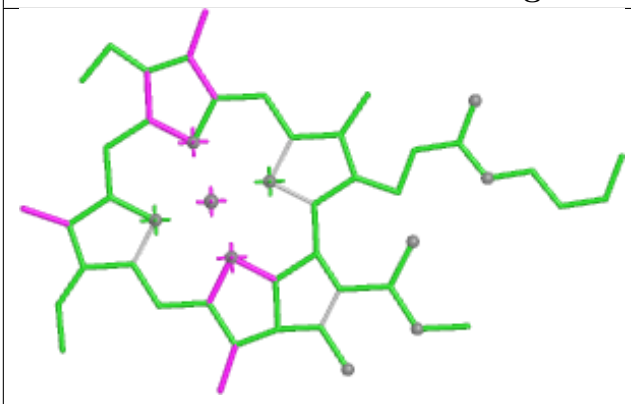


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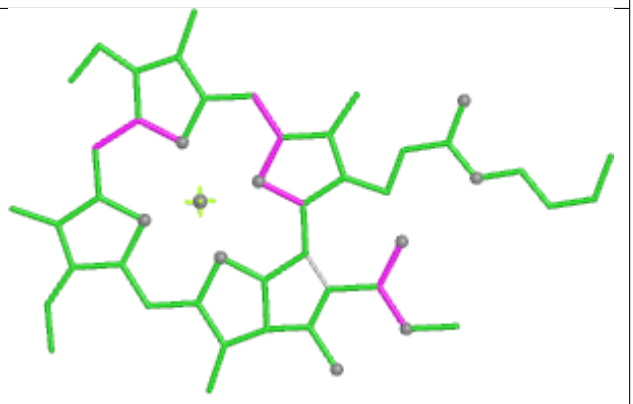


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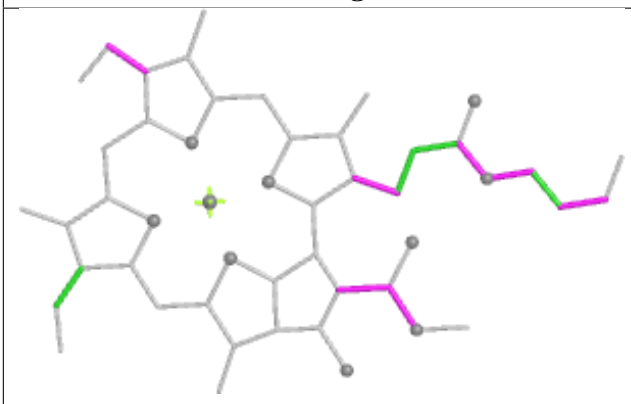
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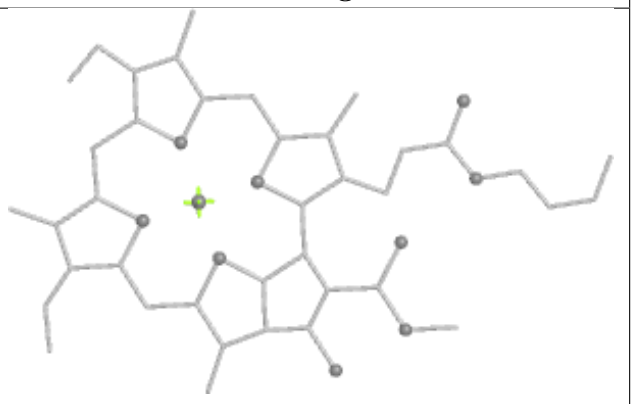
Bond lengths



Bond angles

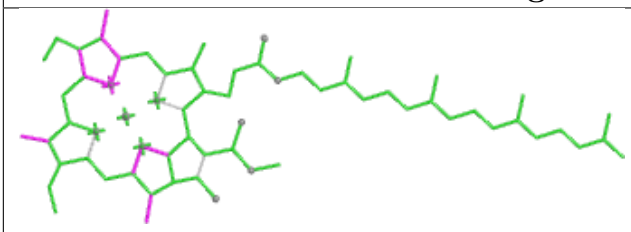


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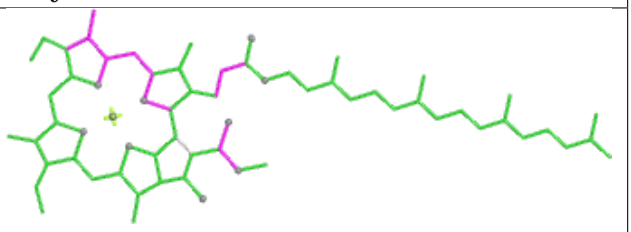


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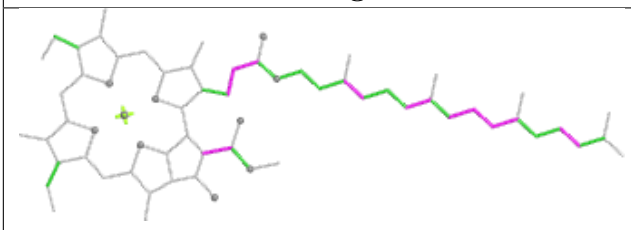
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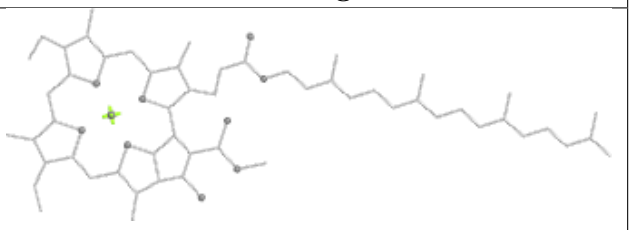
Bond lengths



Bond angles



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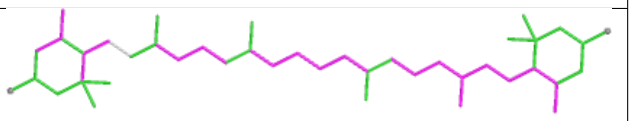


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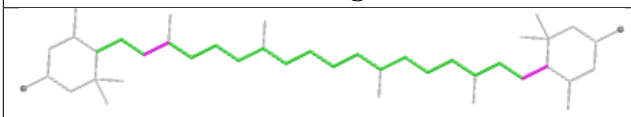
Ligand LUT 8 1620



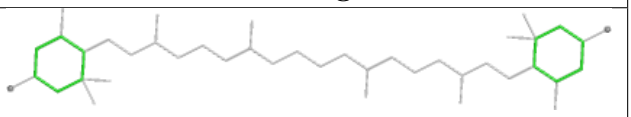
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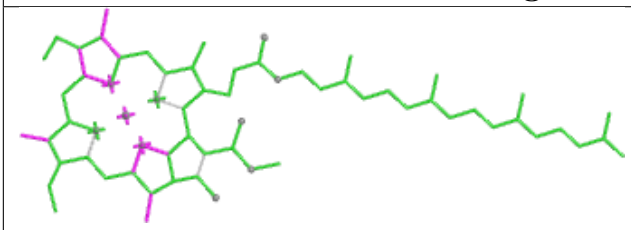


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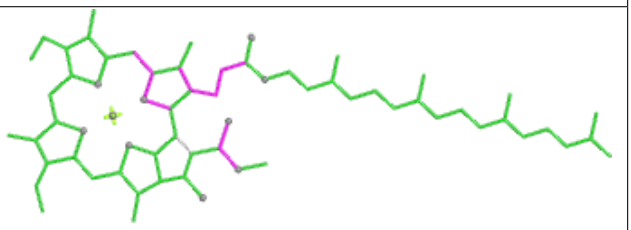


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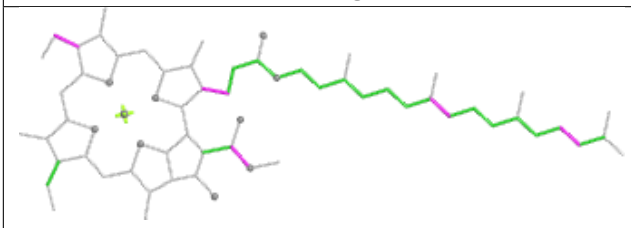
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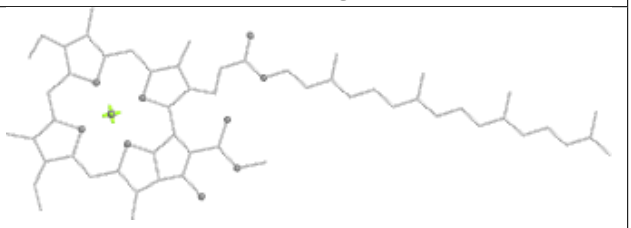
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Bond angles

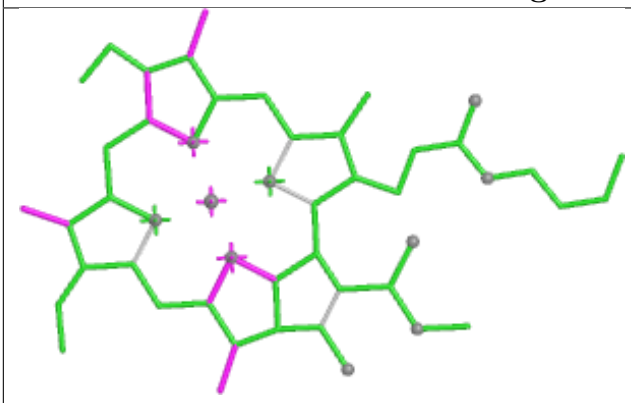


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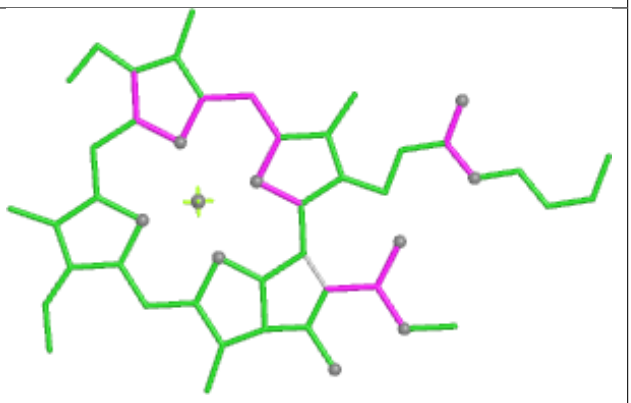


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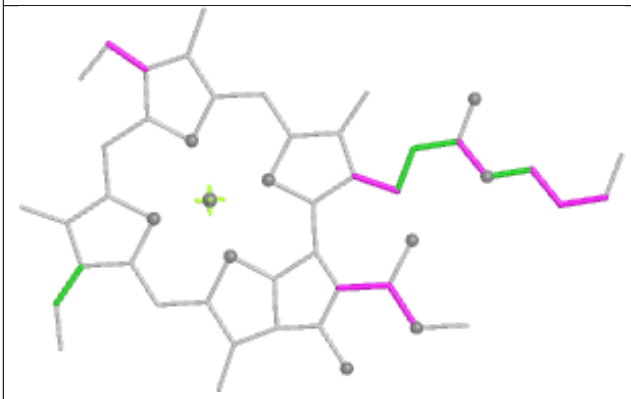
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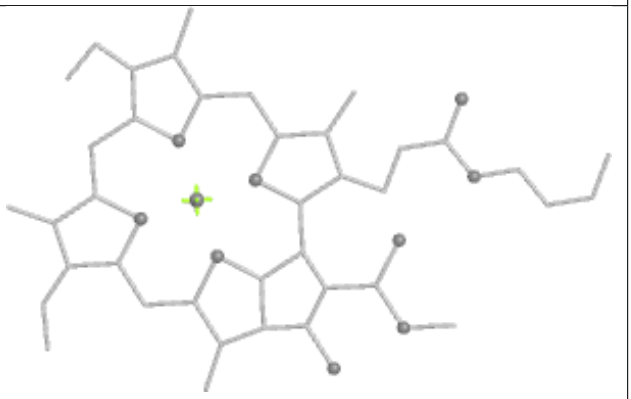
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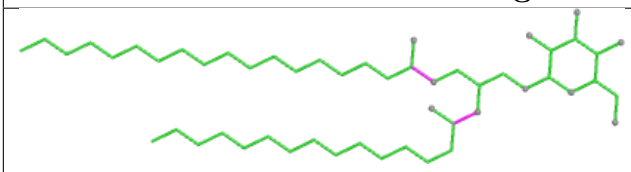


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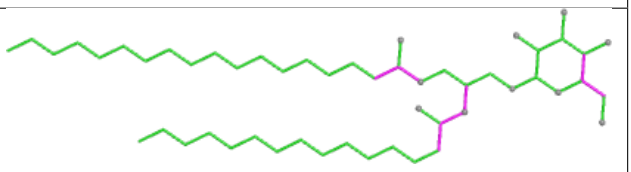


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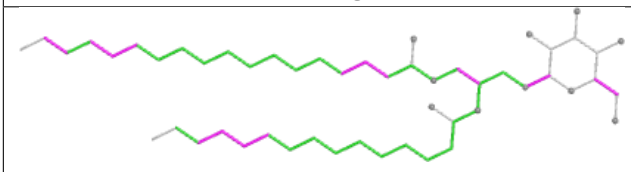
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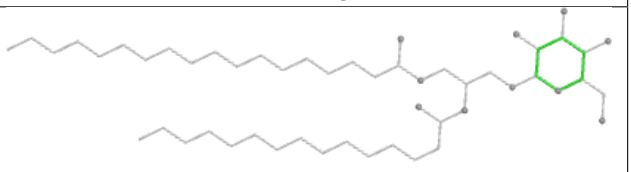
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Bond angles

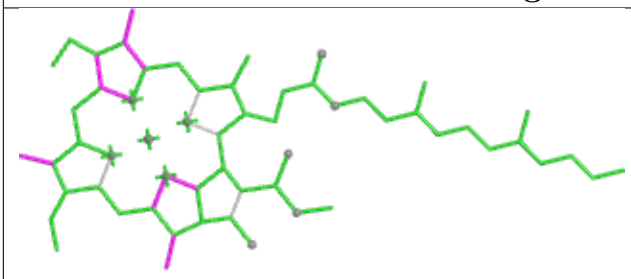


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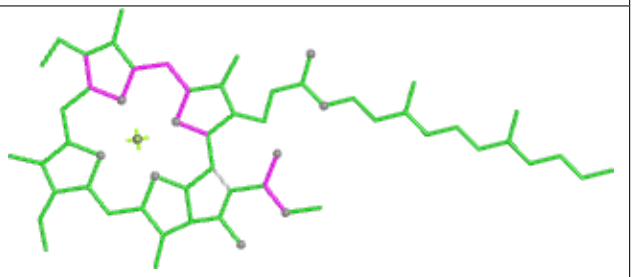


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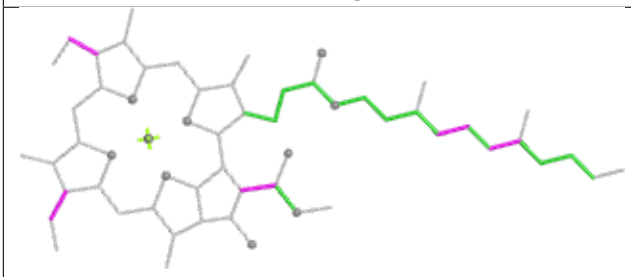
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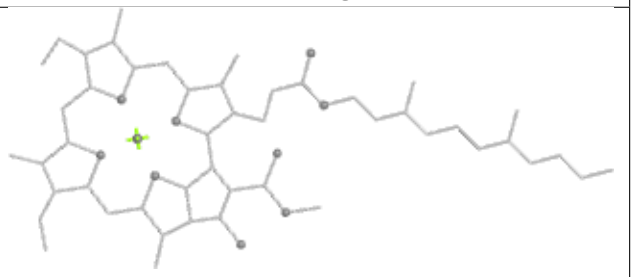
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Bond angles



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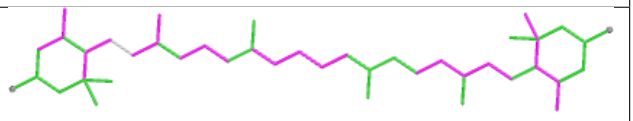


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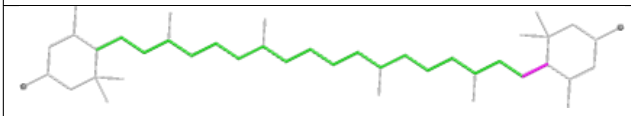
Ligand LUT 2 1620



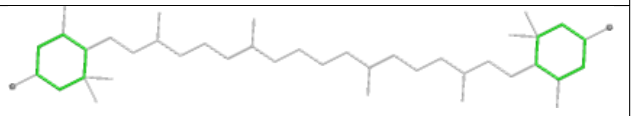
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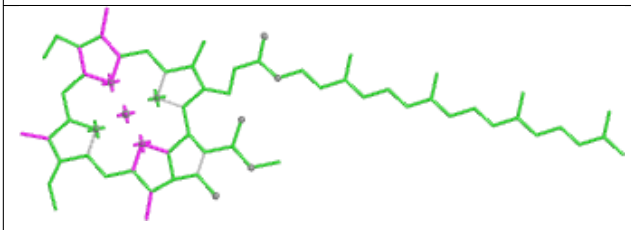


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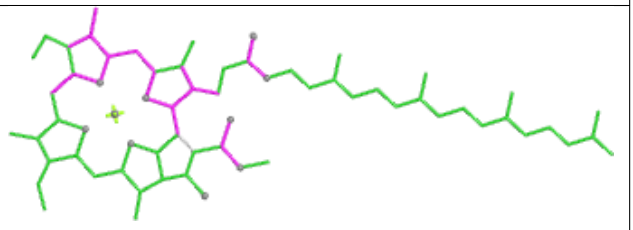


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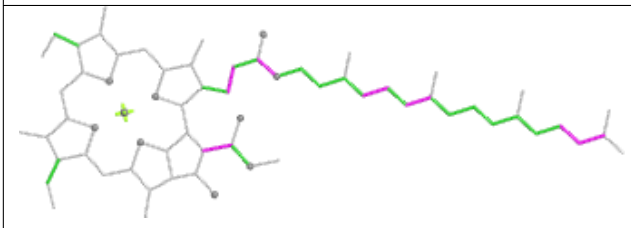
Ligand CLA b 617



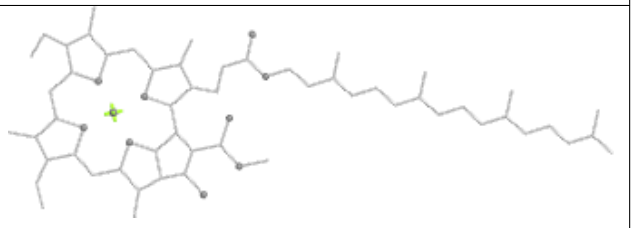
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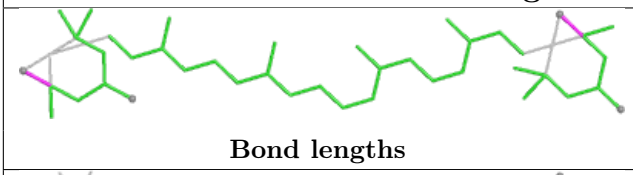


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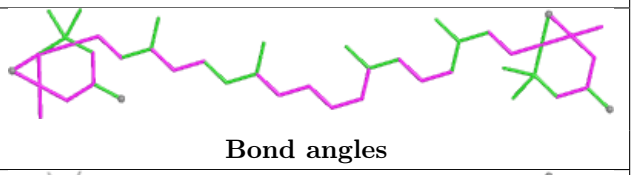


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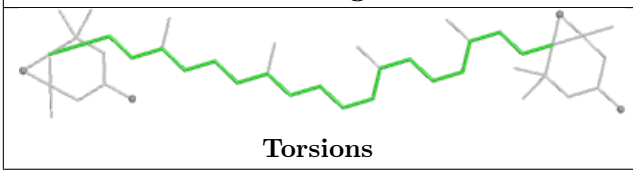
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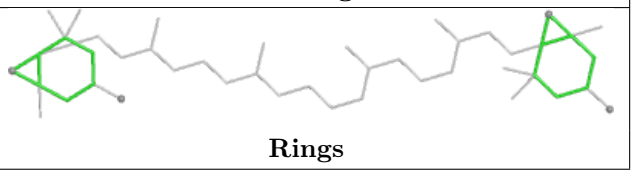
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Bond angles

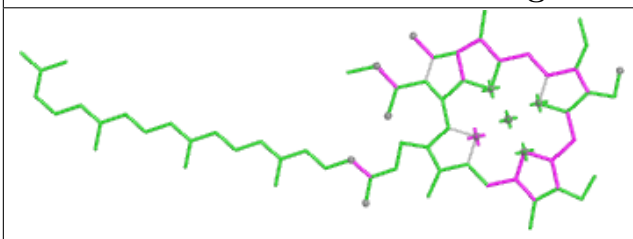


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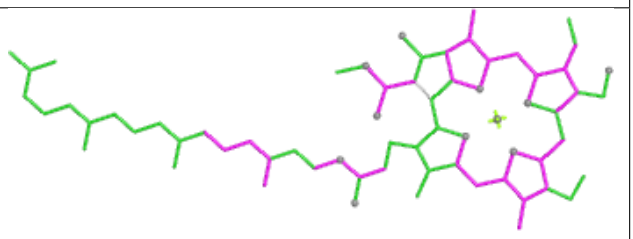


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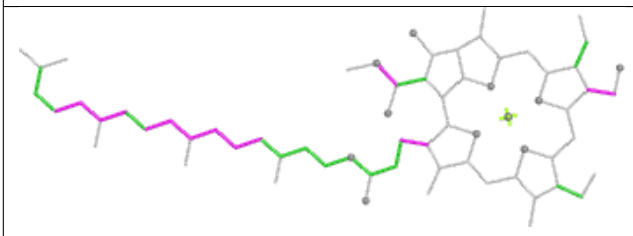
Ligand CHL 4 601



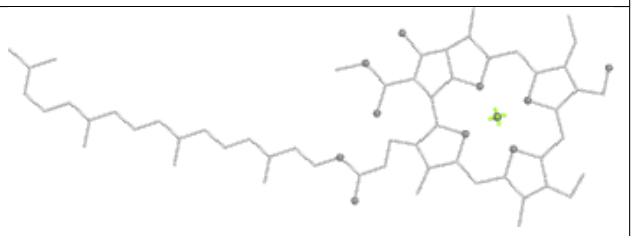
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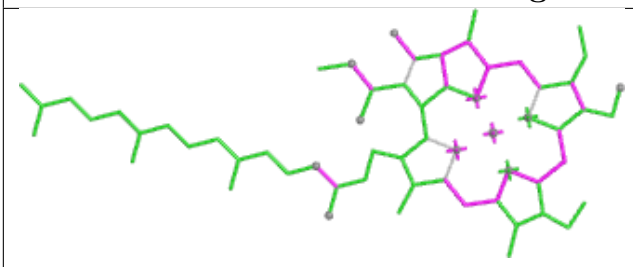


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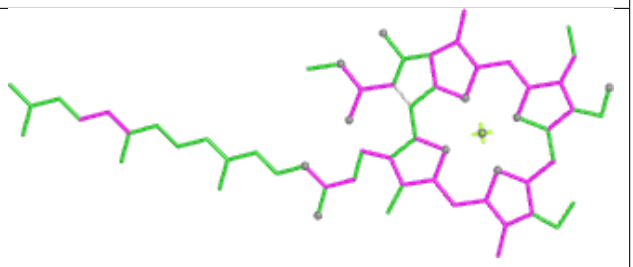


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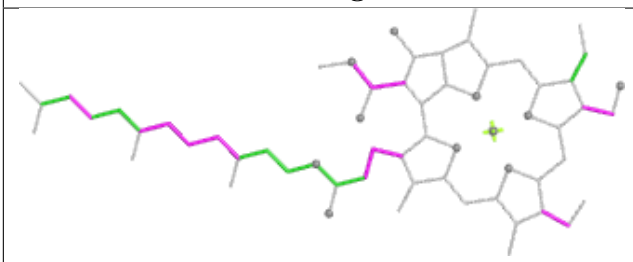
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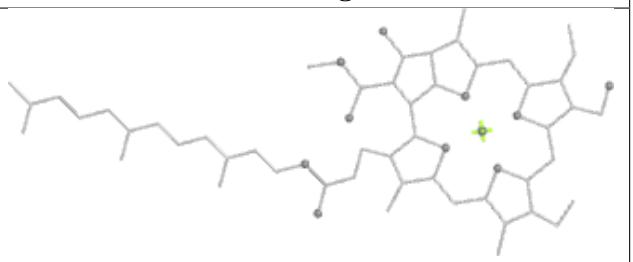
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Bond angles

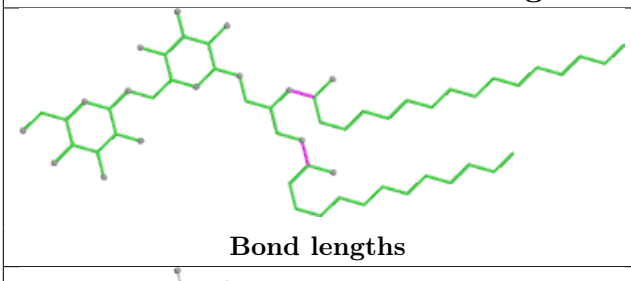


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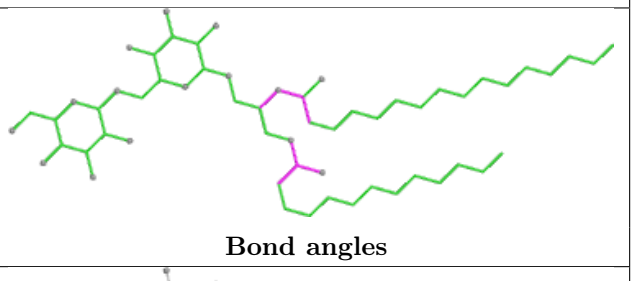


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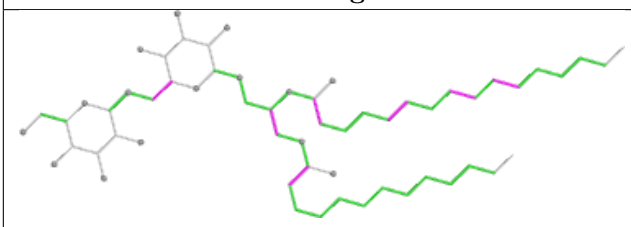
Ligand DGD c 520



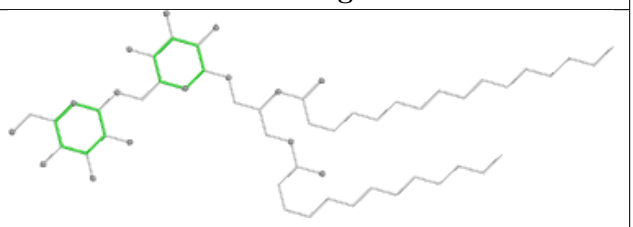
Bond lengths



Bond angles

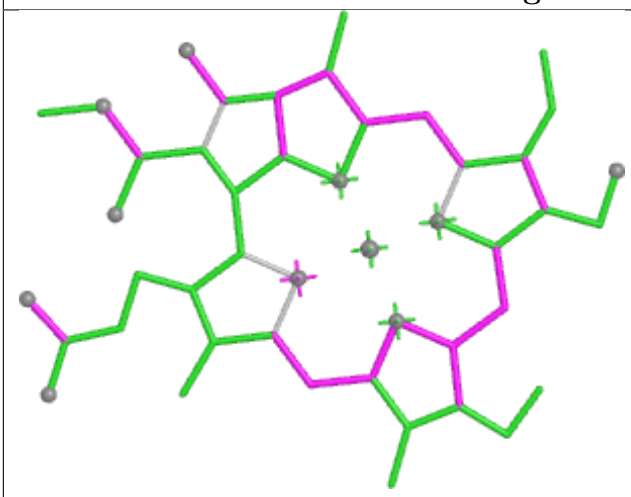


Torsions

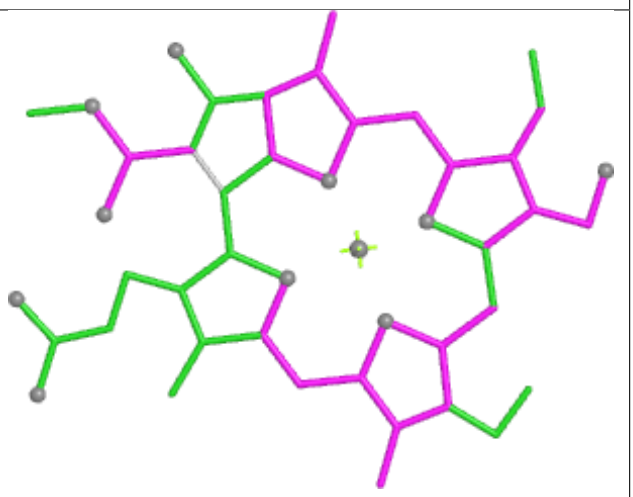


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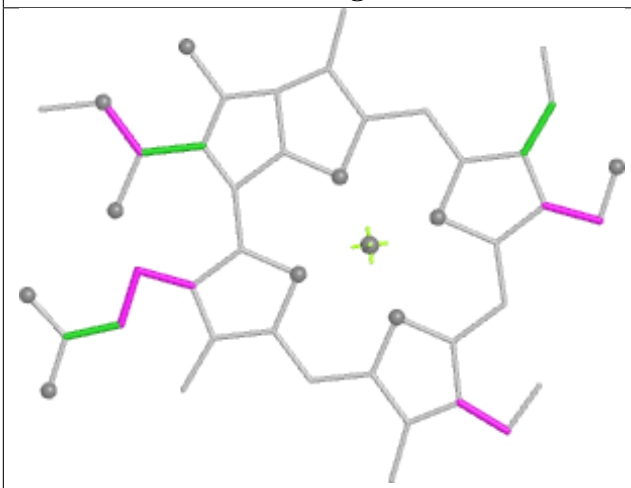
Ligand CHL Y 605



Bond lengths



Bond angles

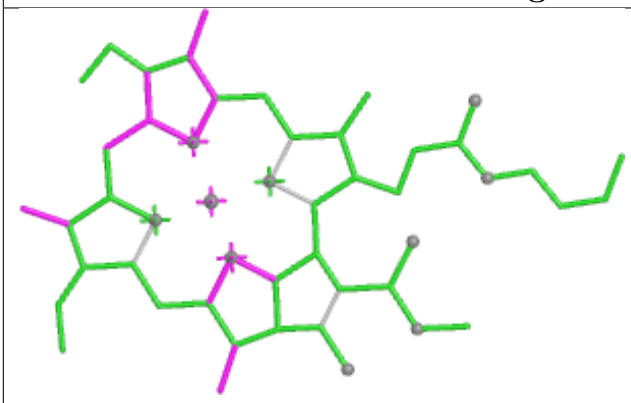


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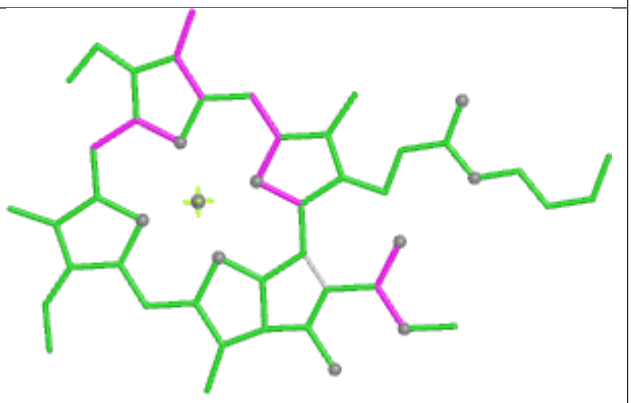


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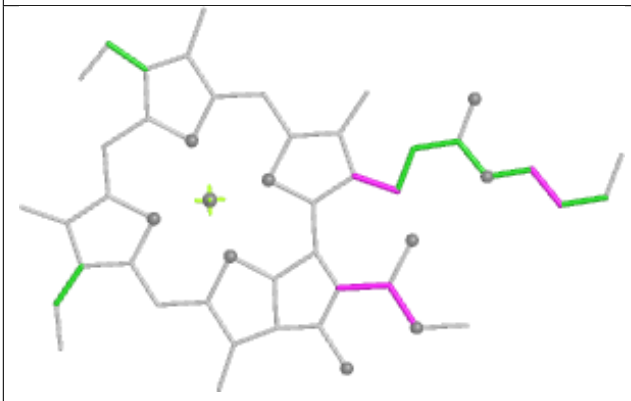
Ligand CLA a 407



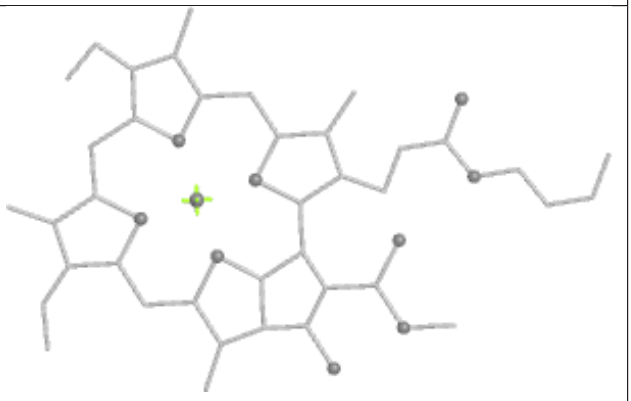
Bond lengths



Bond angles



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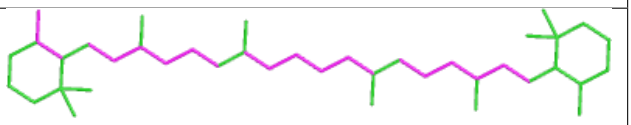


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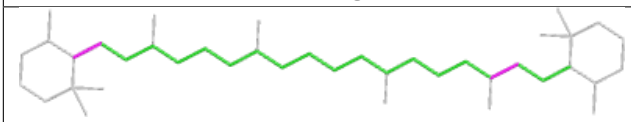
Ligand BCR C 514



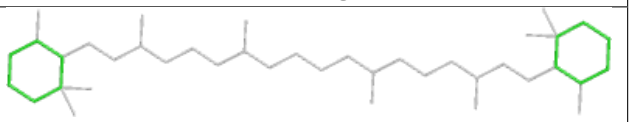
Bond lengths



Bond angles

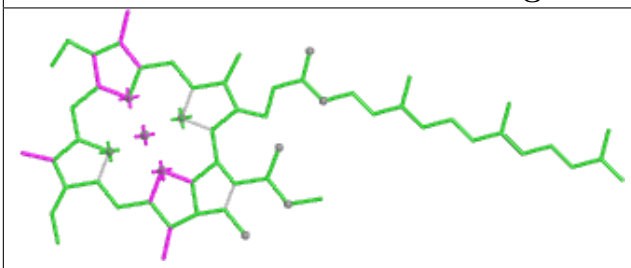


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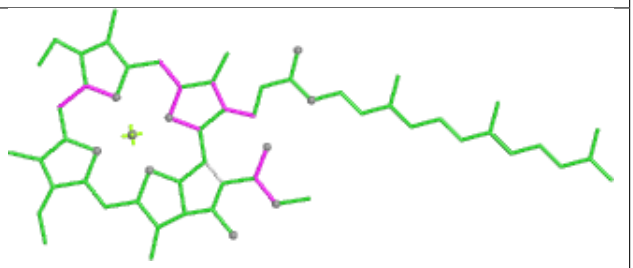


Rings

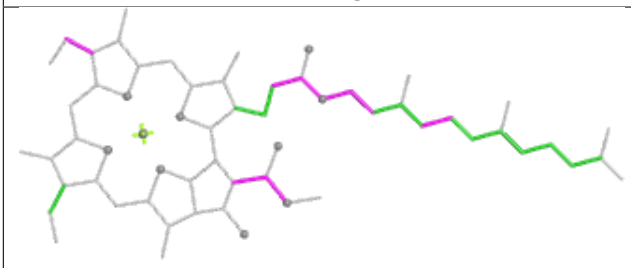
Ligand CLA R 603



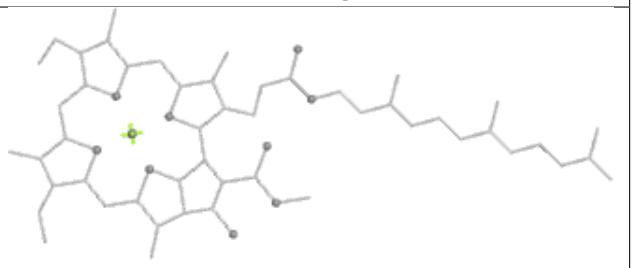
Bond lengths



Bond angles

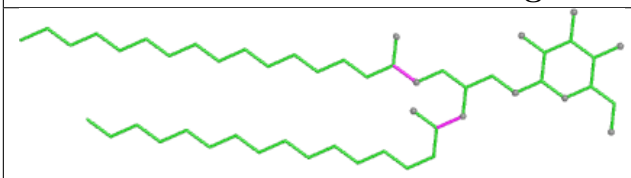


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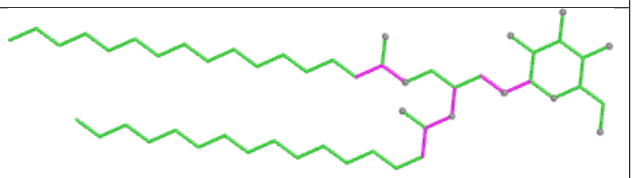


Rings

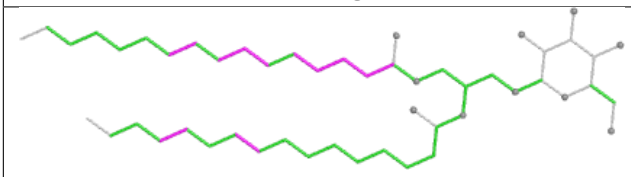
Ligand LMG c 521



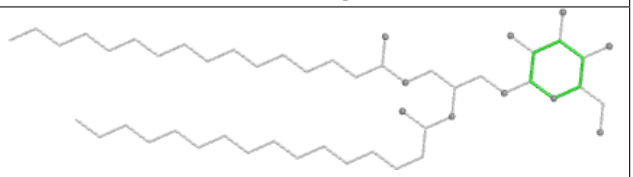
Bond lengths



Bond angles

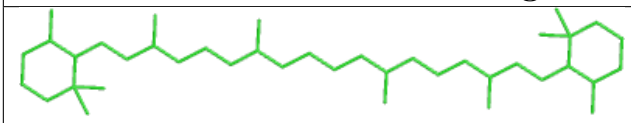


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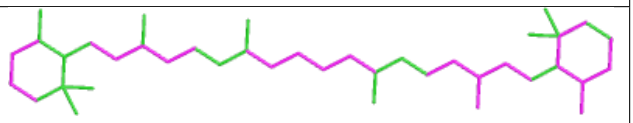


Rings

Ligand BCR H 101



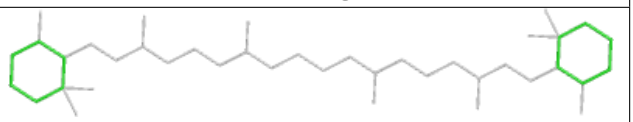
Bond lengths



Bond angles

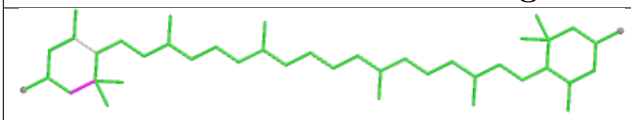


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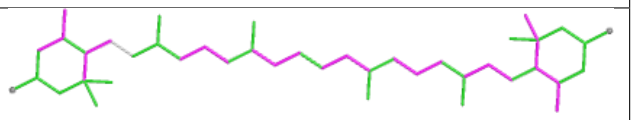


Rings

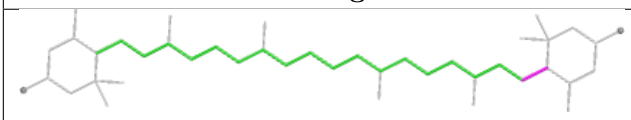
Ligand LUT 1 1620



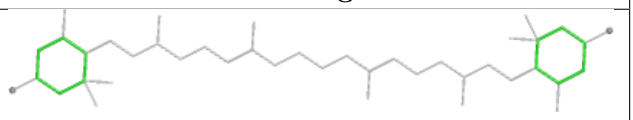
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Bond angles

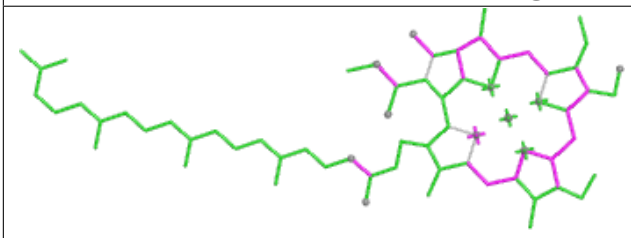


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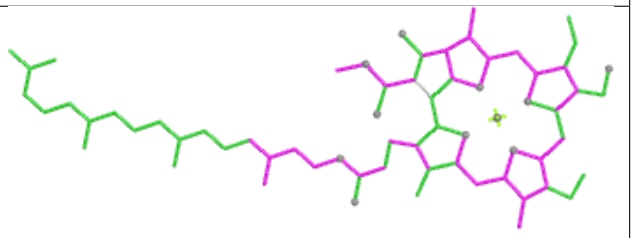


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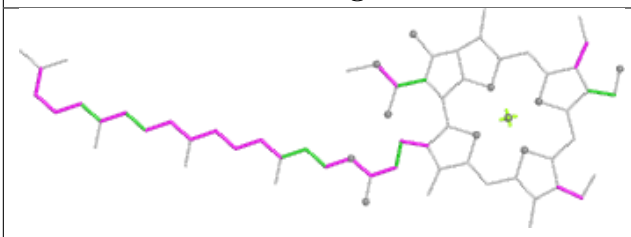
Ligand CHL 3 607



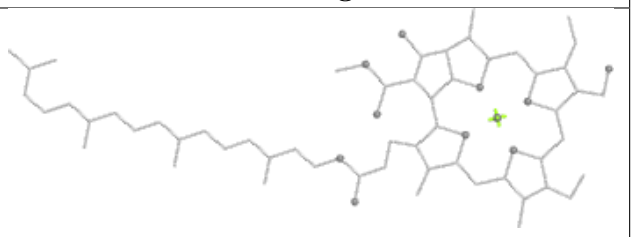
Bond lengths



Bond angles

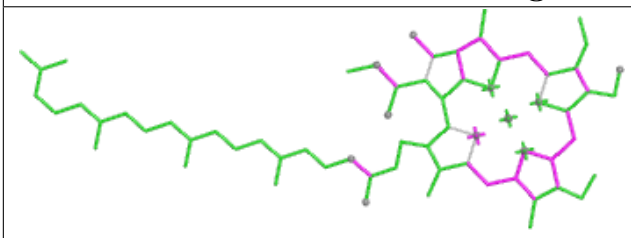


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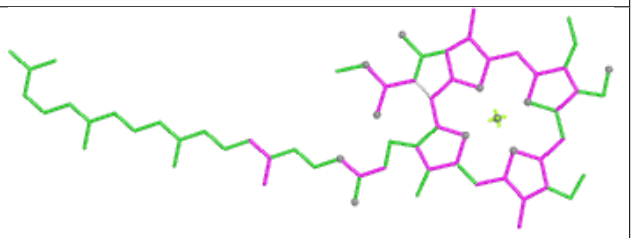


Rings

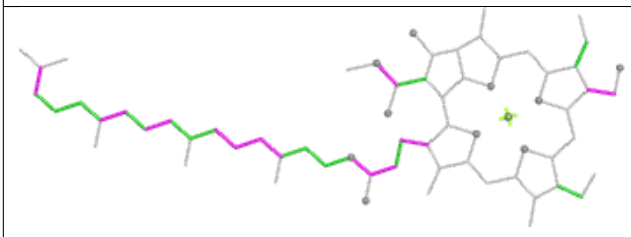
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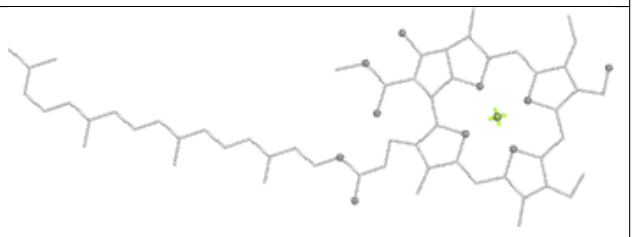
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Bond angles

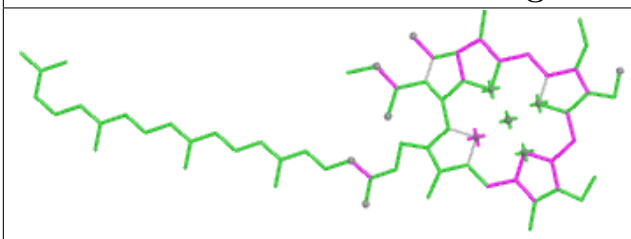


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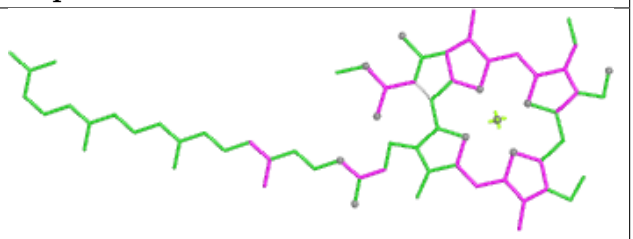


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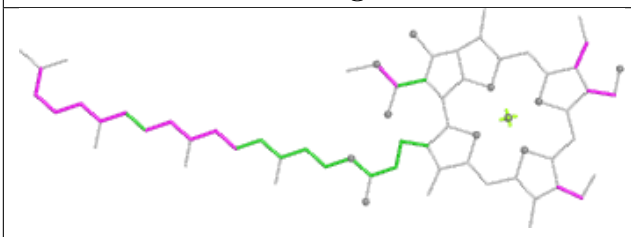
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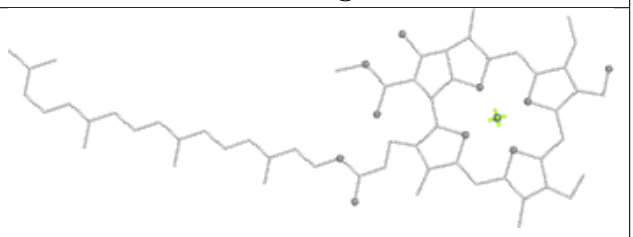
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Bond angles

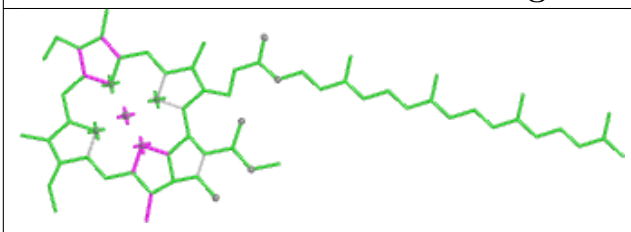


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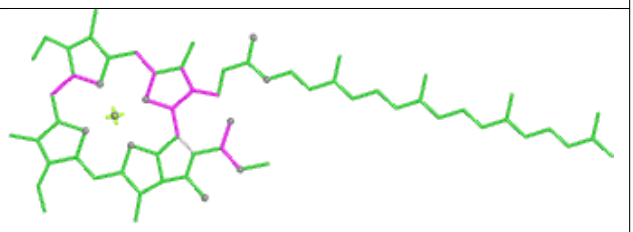


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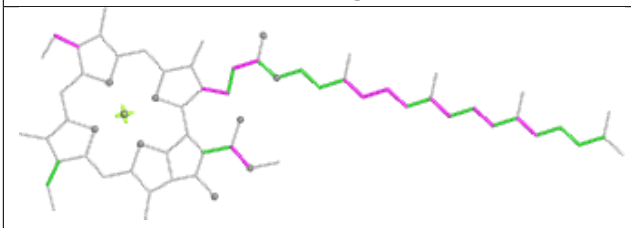
Ligand CLA 8 603



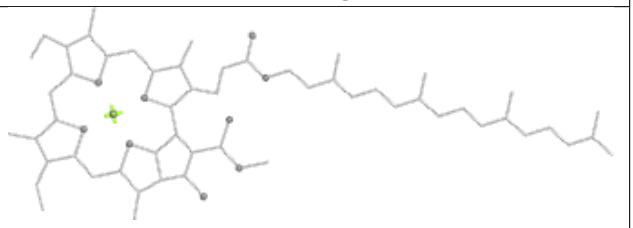
Bond lengths



Bond angles

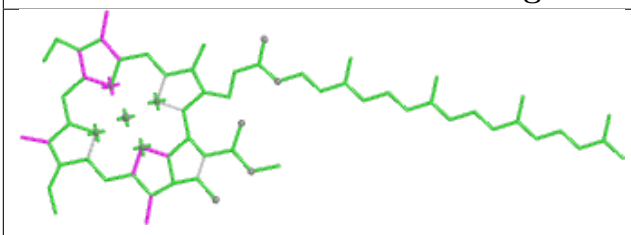


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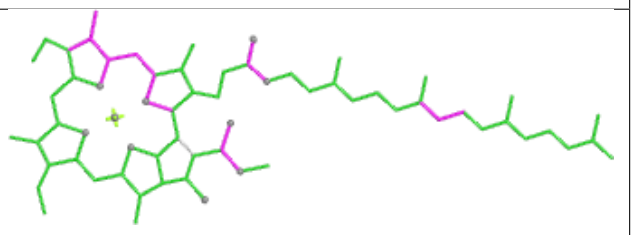


Rings

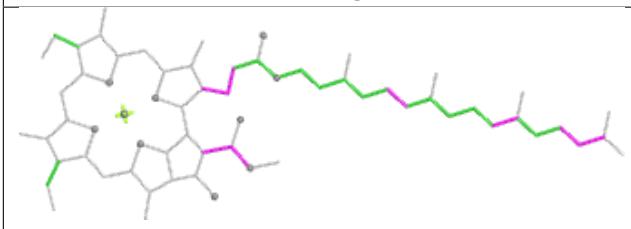
Ligand CLA Y 610



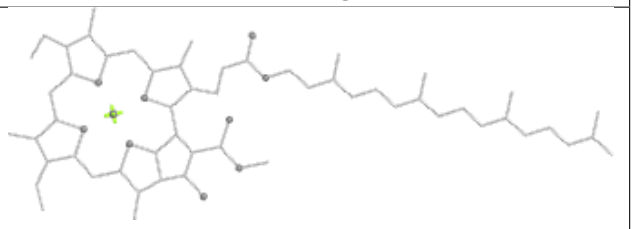
Bond lengths



Bond angles

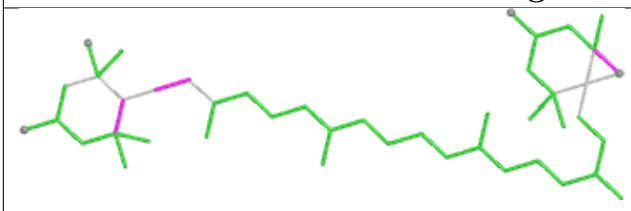


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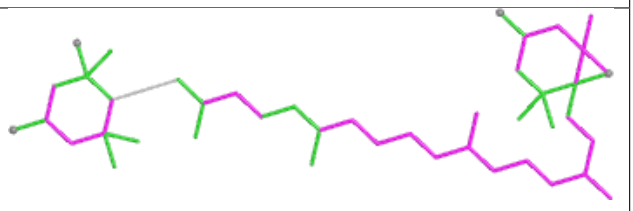


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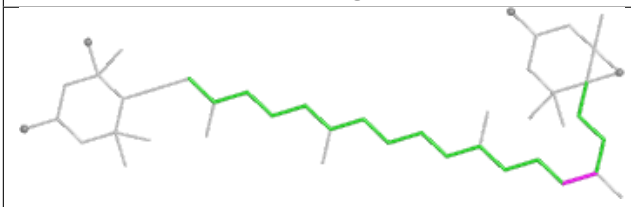
Ligand NEX r 623



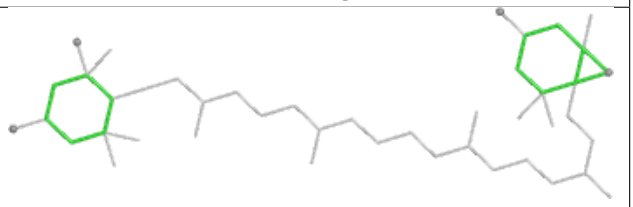
Bond lengths



Bond angles

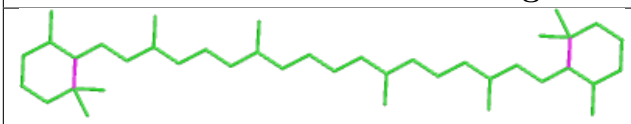


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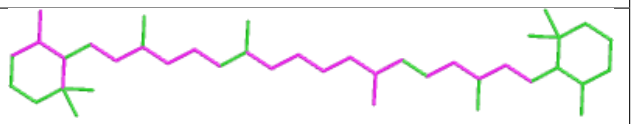


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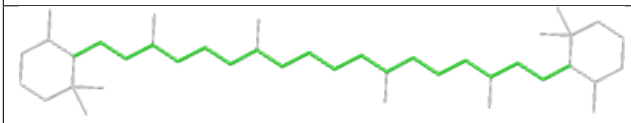
Ligand BCR C 517



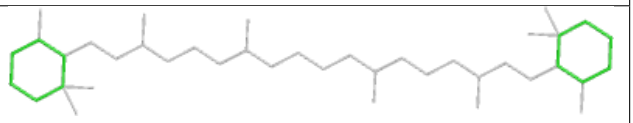
Bond lengths



Bond angles

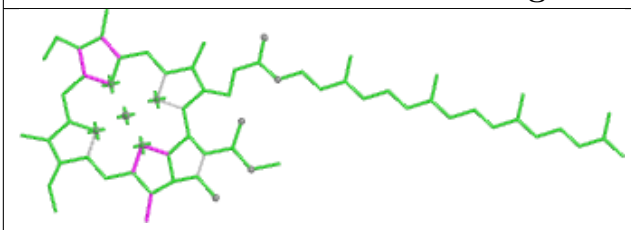


Torsions

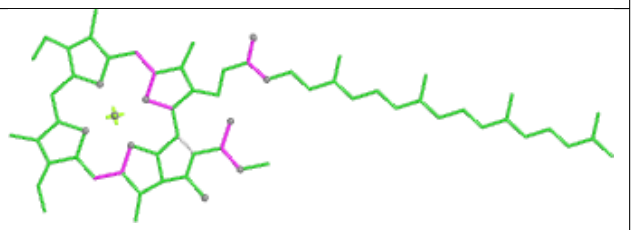


Rings

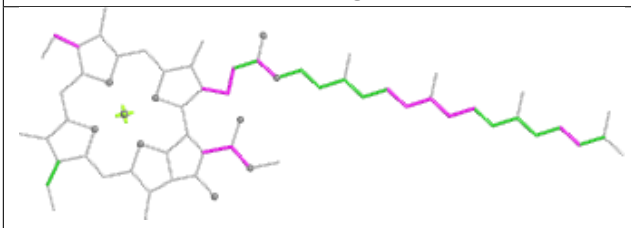
Ligand CLA 8 613



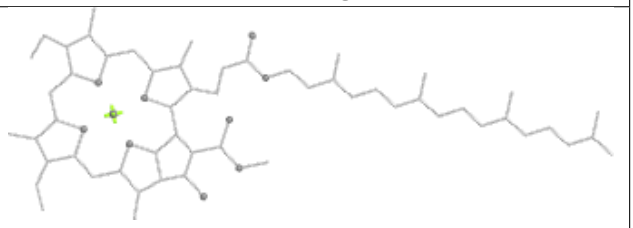
Bond lengths



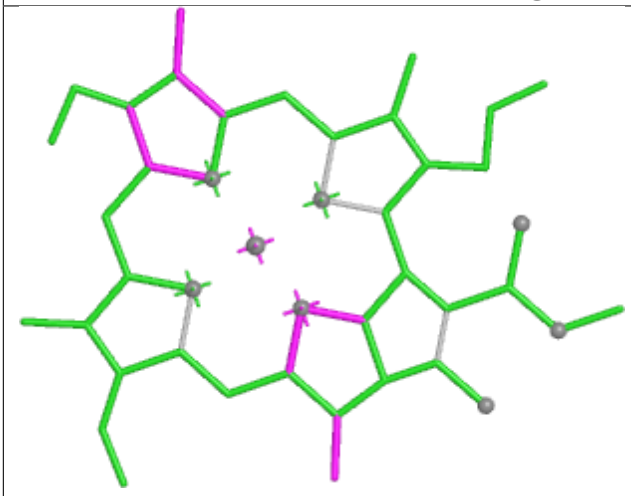
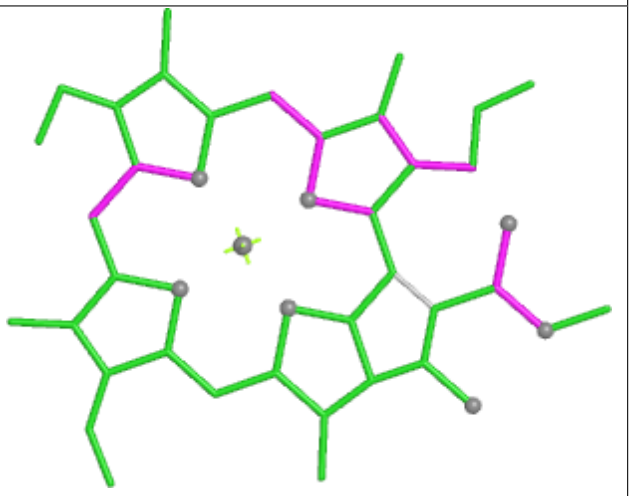
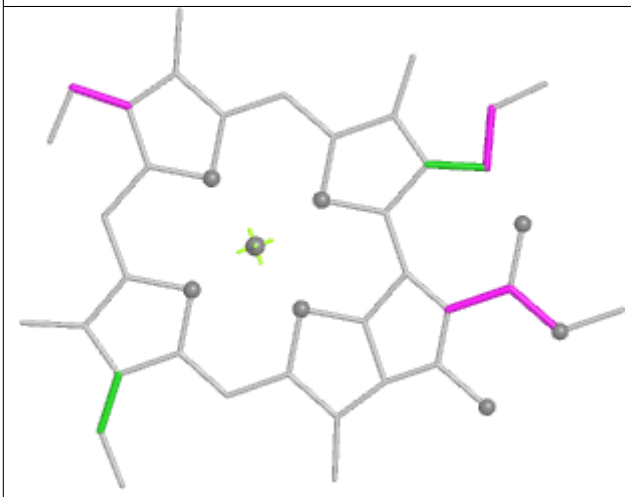
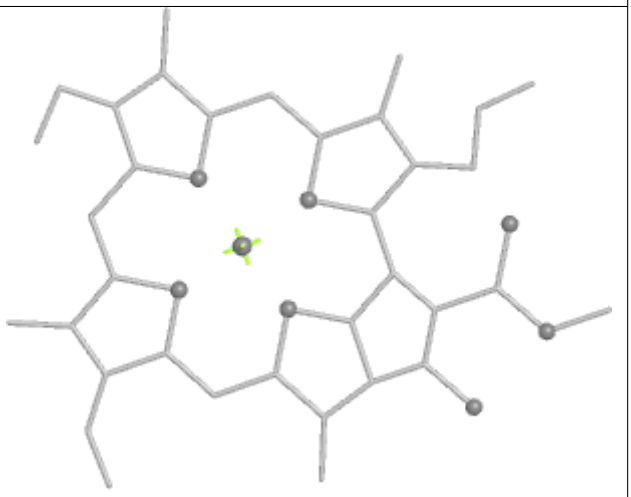
Bond angles

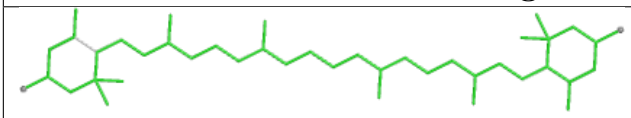
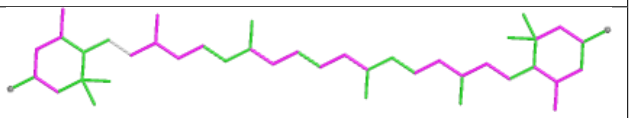
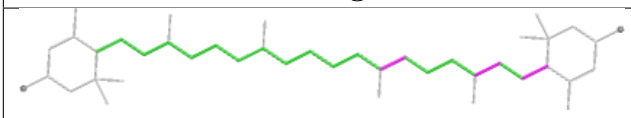
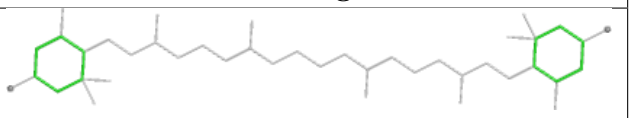


Torsions

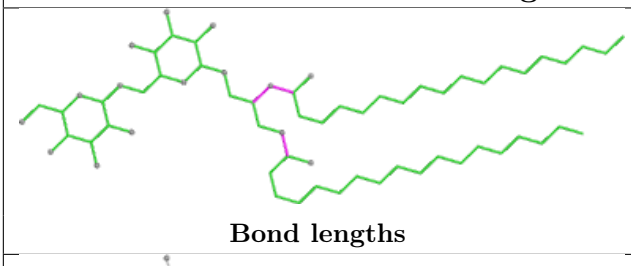


Rings

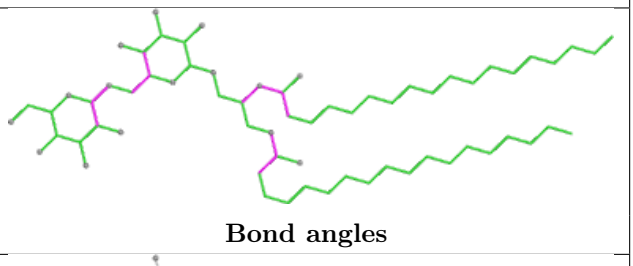
Ligand CLA 2 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 2 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

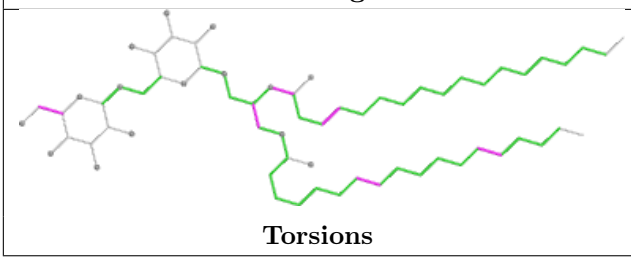
Ligand DGD C 524



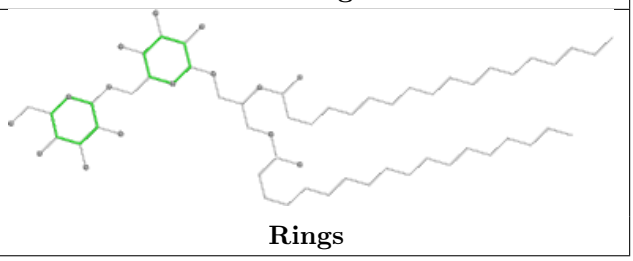
Bond lengths



Bond angles



Torsions



Rings

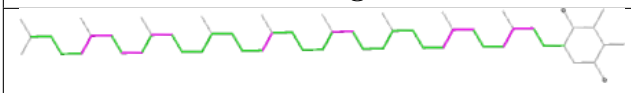
Ligand PL9 D 405



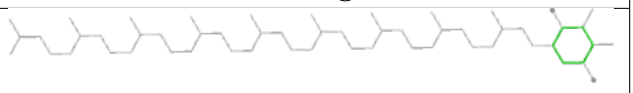
Bond lengths



Bond angles

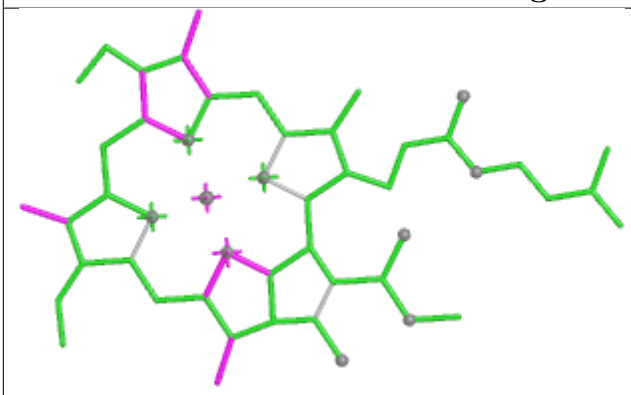


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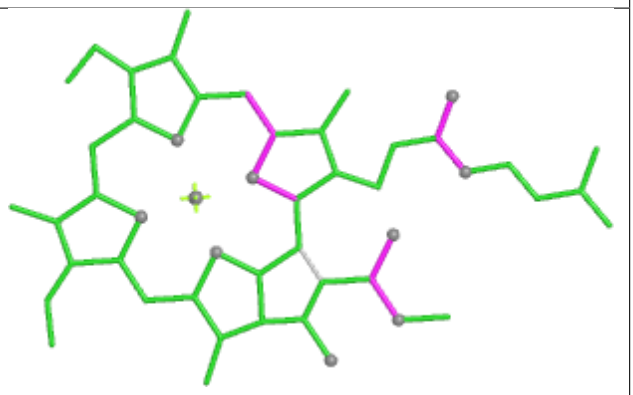


Rings

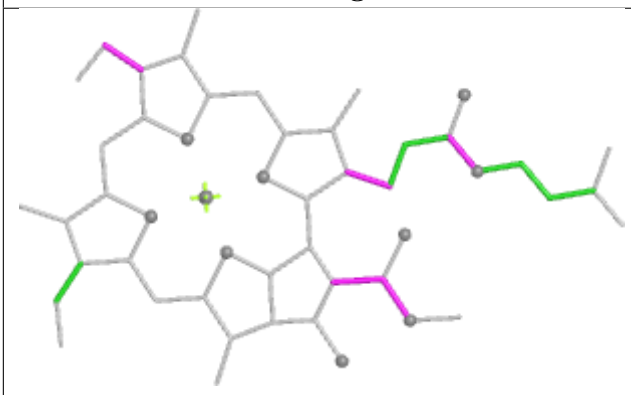
Ligand CLA s 605



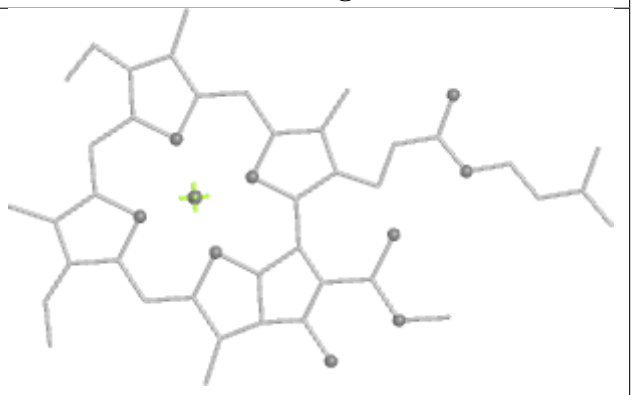
Bond lengths



Bond angles

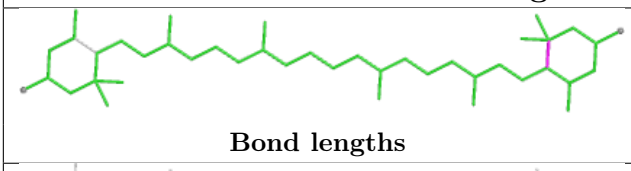


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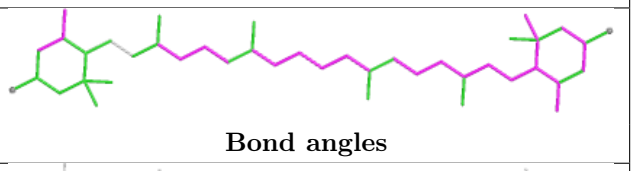


Rings

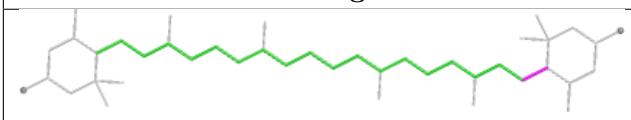
Ligand LUT r 620



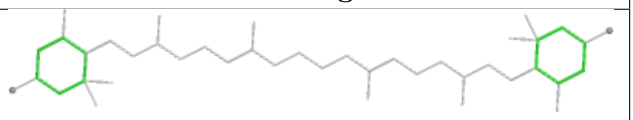
Bond lengths



Bond angles

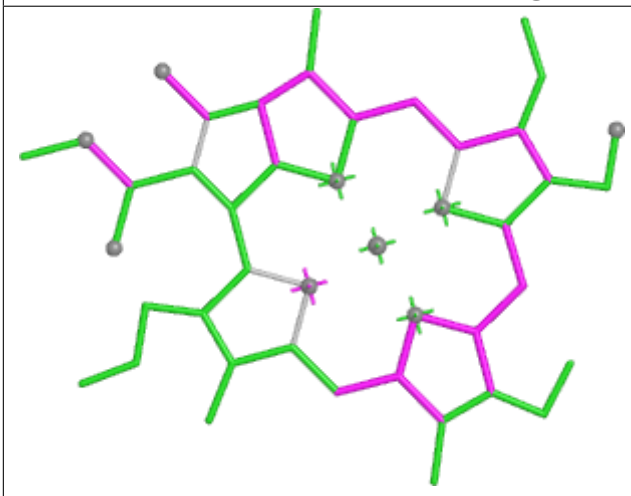


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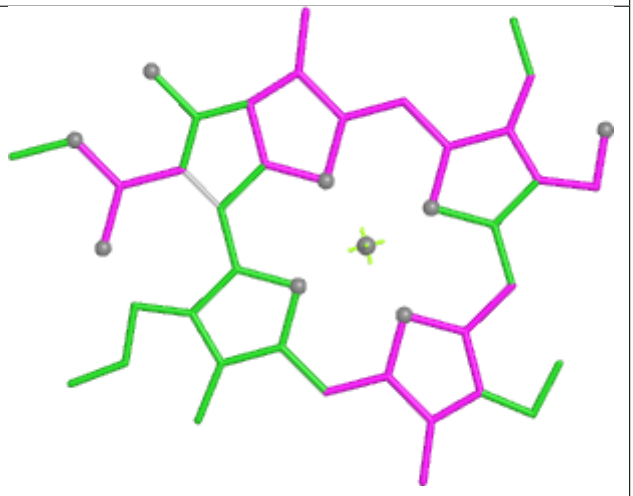


Rings

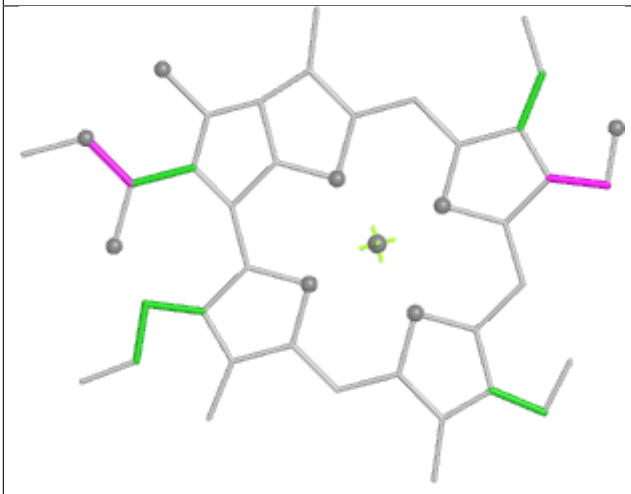
Ligand CHL 4 608



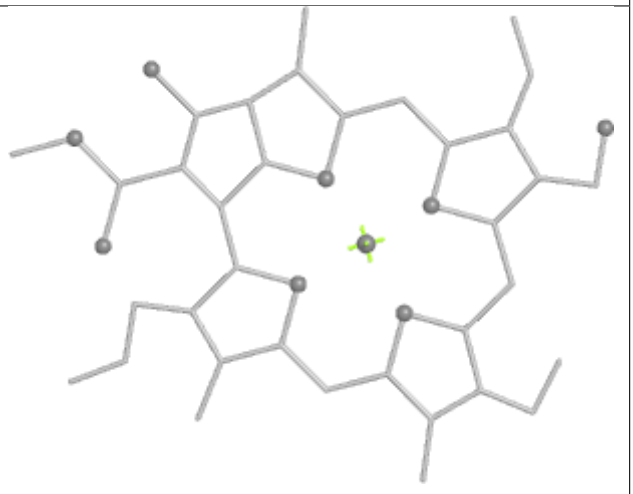
Bond lengths



Bond angles

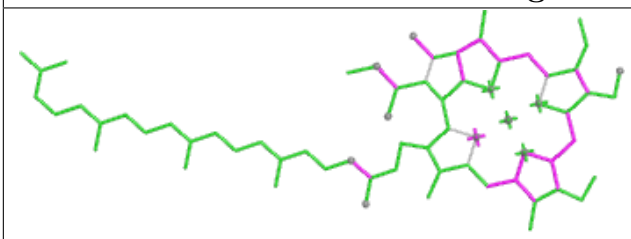


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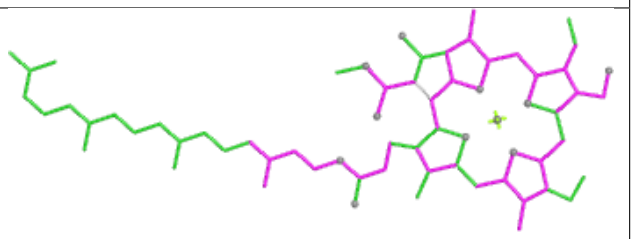


Rings

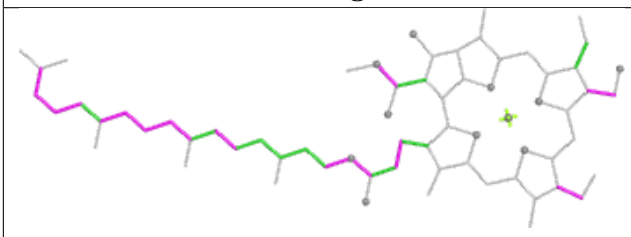
Ligand CHL 1 607



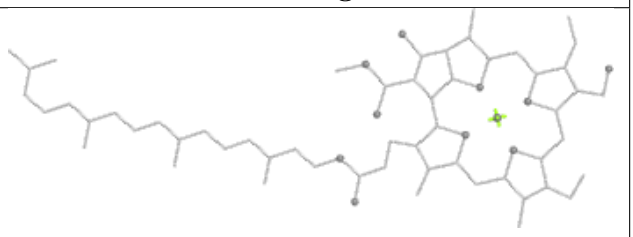
Bond lengths



Bond angles

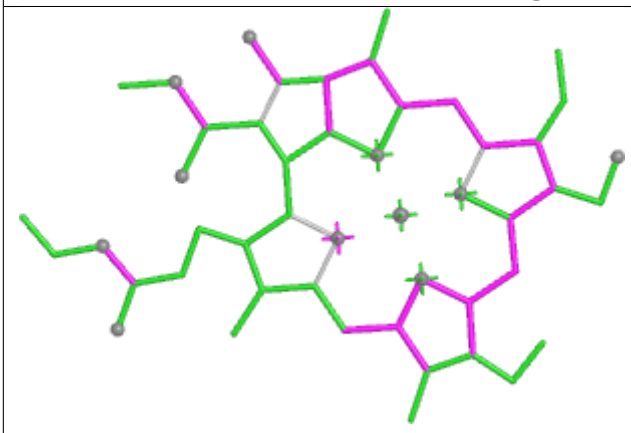


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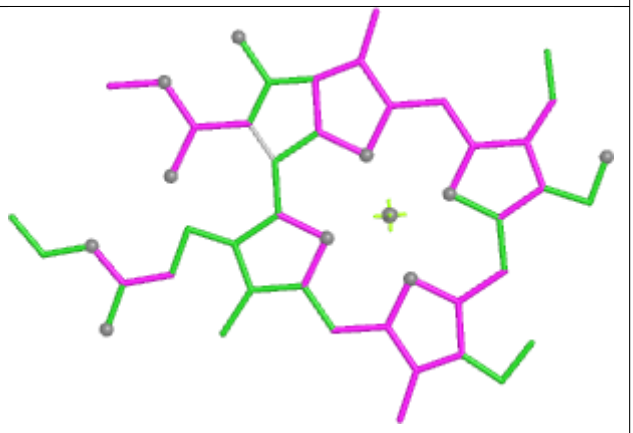


Rings

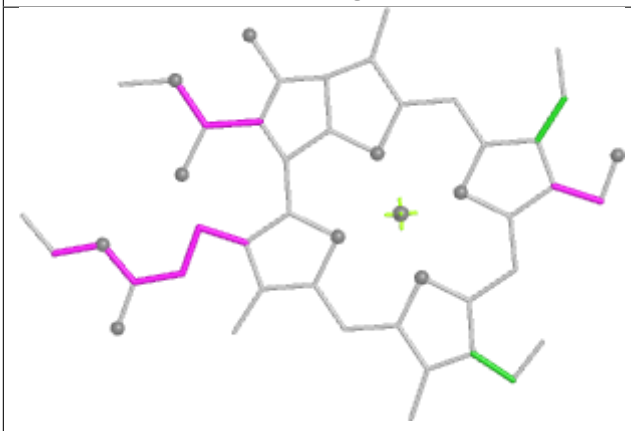
Ligand CHL 4 605



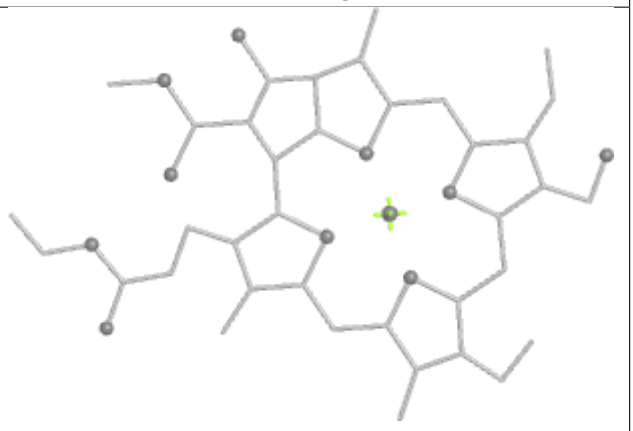
Bond lengths



Bond angles

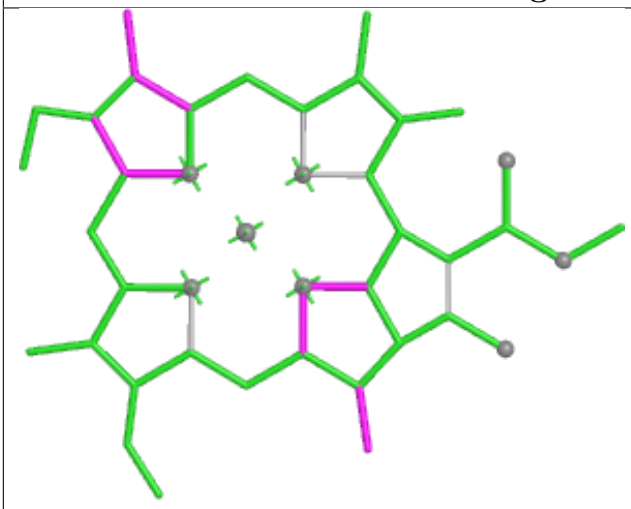


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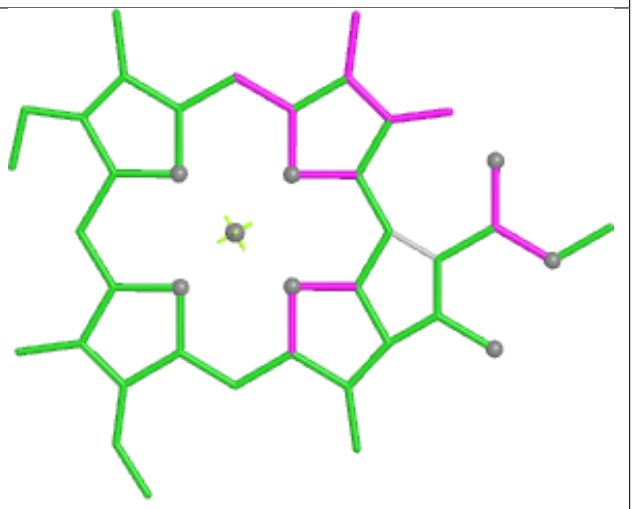


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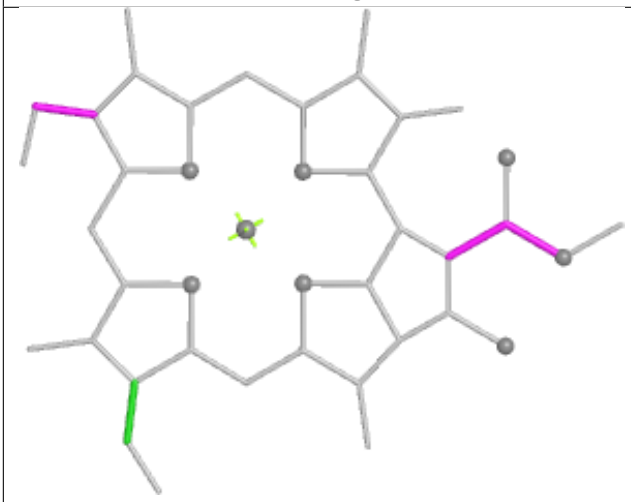
Ligand CLA s 609



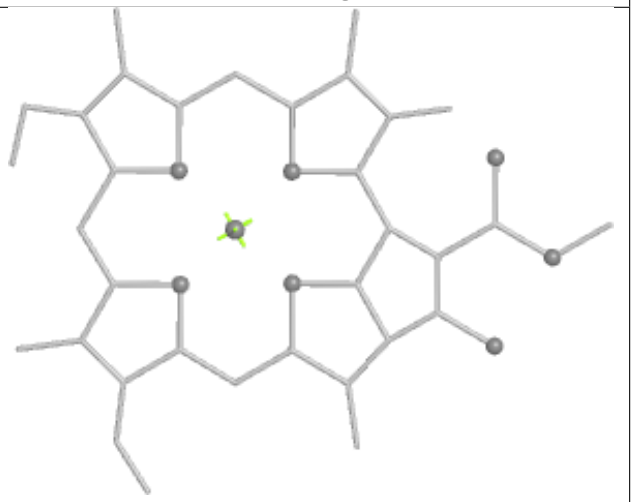
Bond lengths



Bond angles

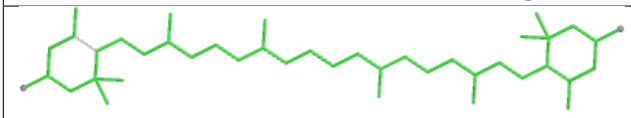


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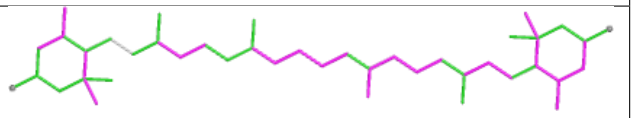


Rings

Ligand LUT 5 1621



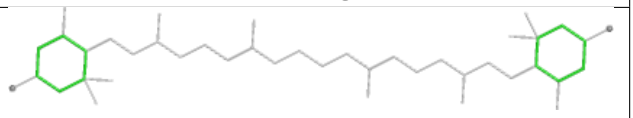
Bond lengths



Bond angles

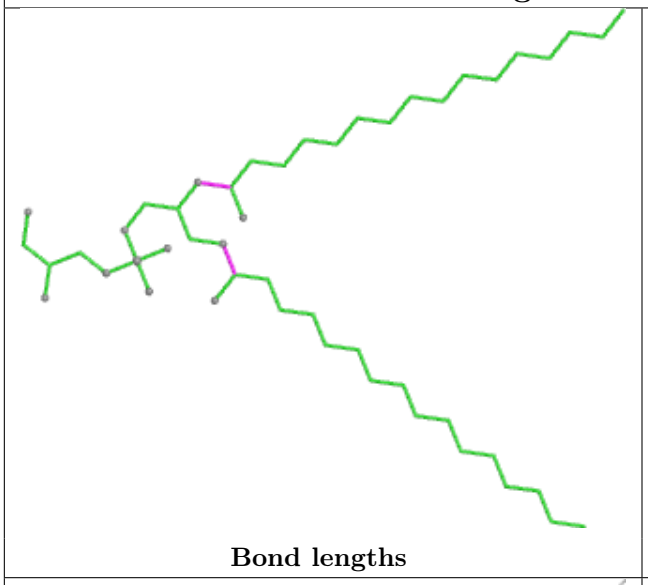


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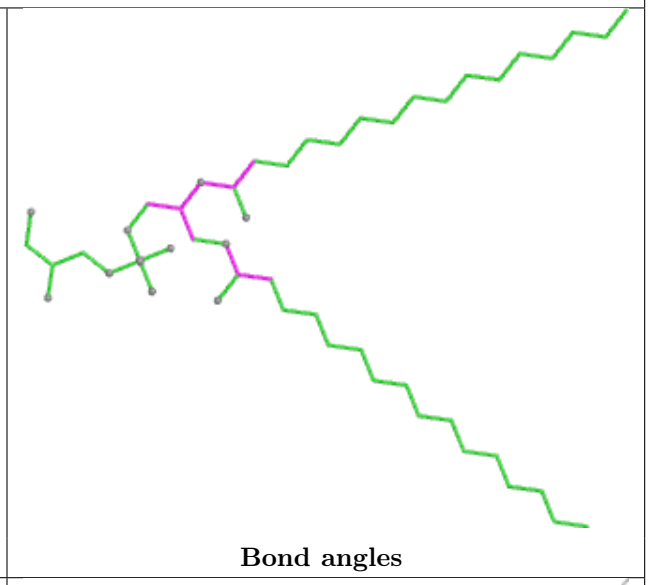


Rings

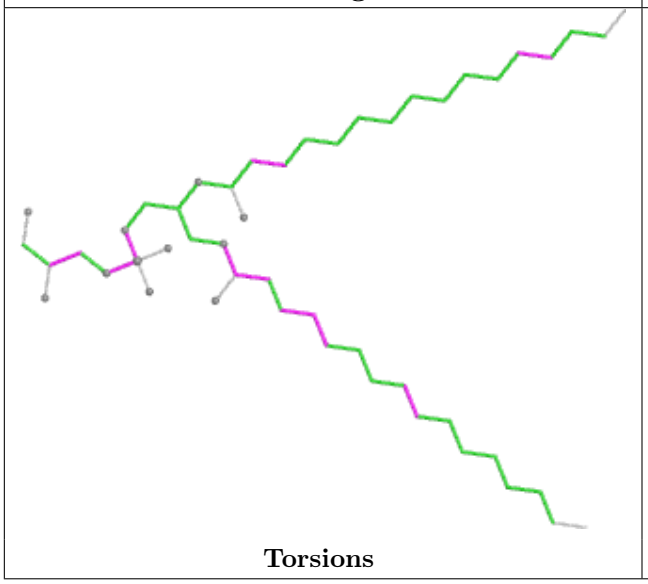
Ligand LHG G 2630



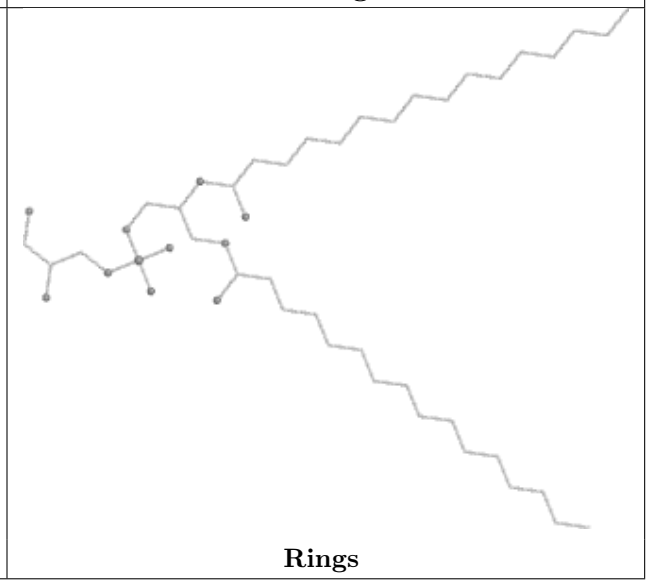
Bond lengths



Bond angles

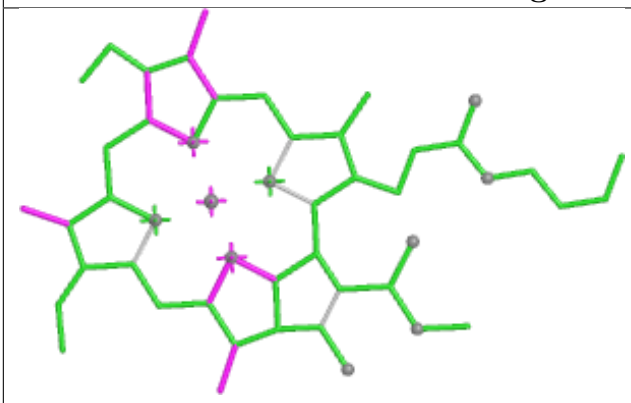


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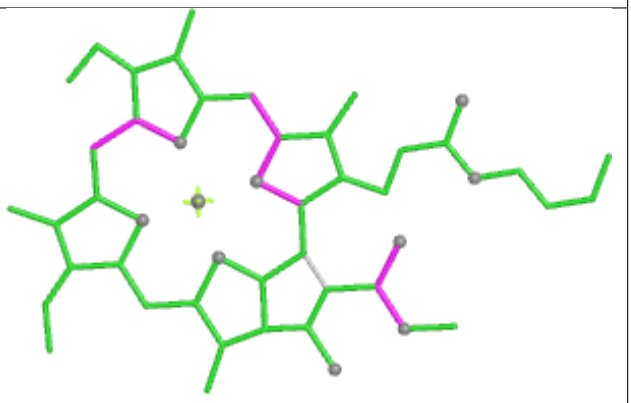


Rings

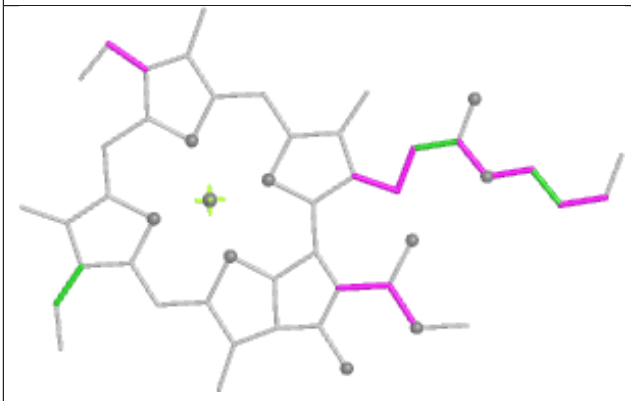
Ligand CLA r 611



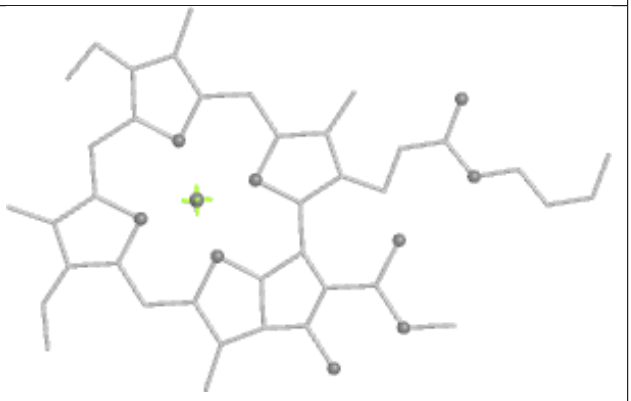
Bond lengths



Bond angles

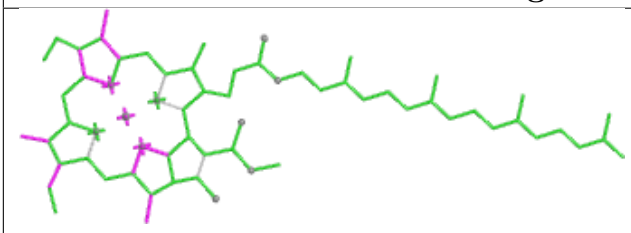


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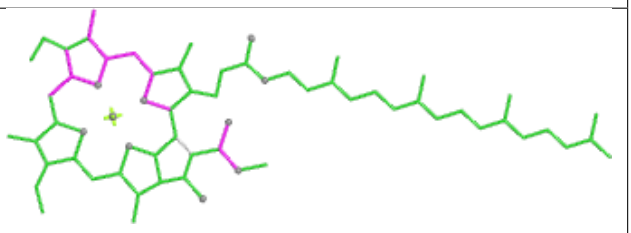


Rings

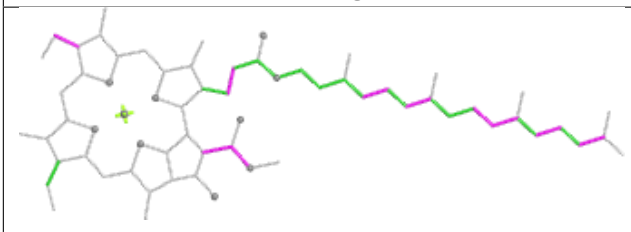
Ligand CLA b 615



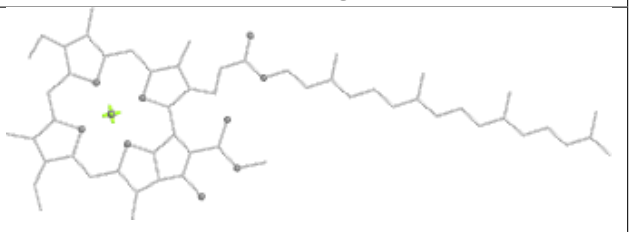
Bond lengths



Bond angles

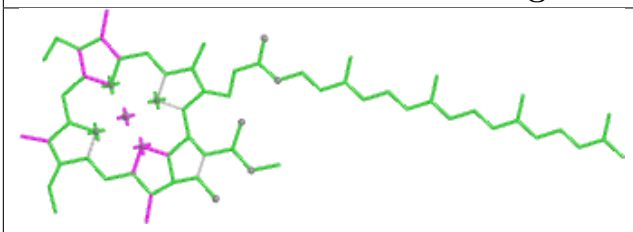


Torsions

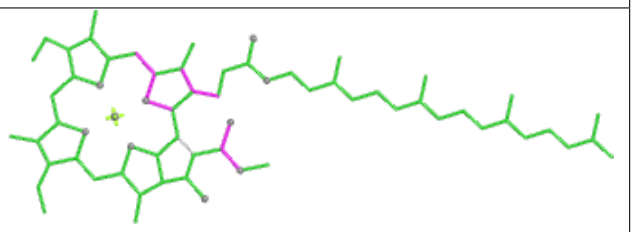


Rings

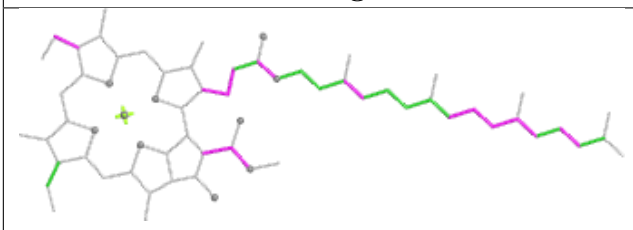
Ligand CLA 1 603



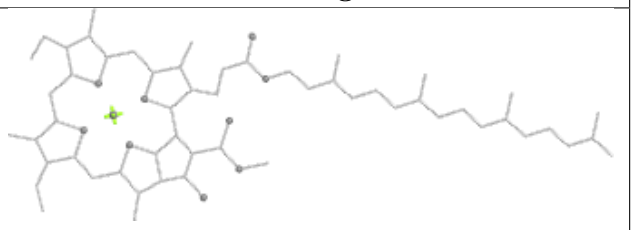
Bond lengths



Bond angles

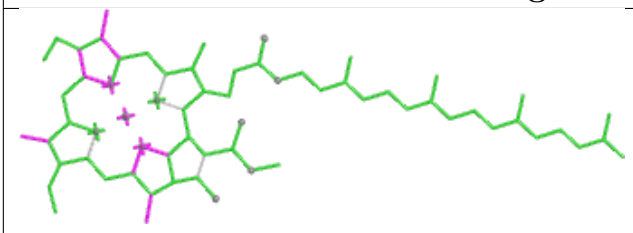


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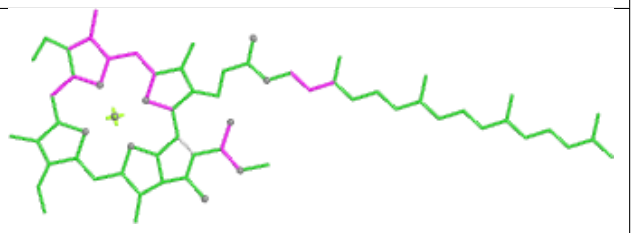


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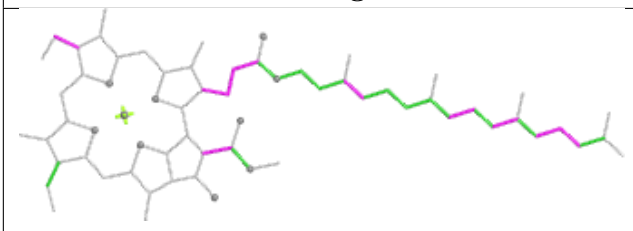
Ligand CLA 2 602



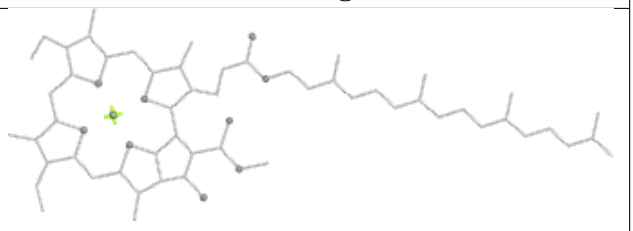
Bond lengths



Bond angles

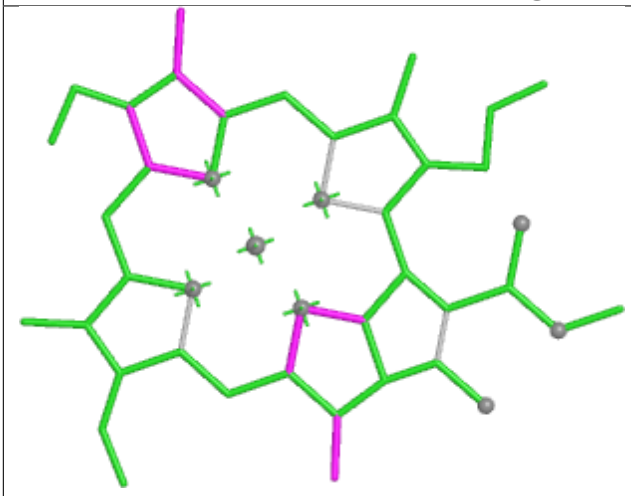


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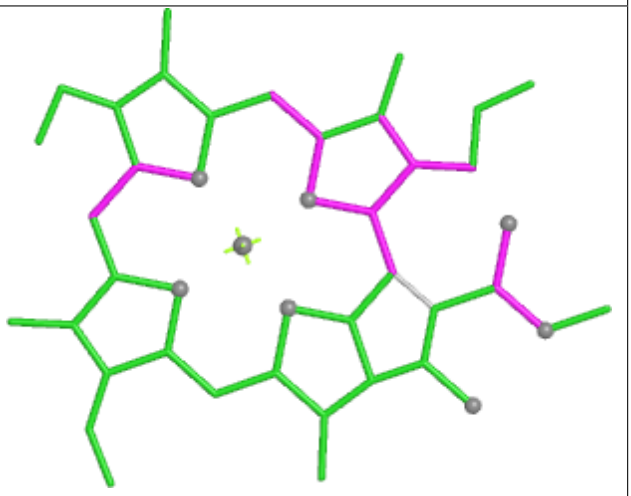


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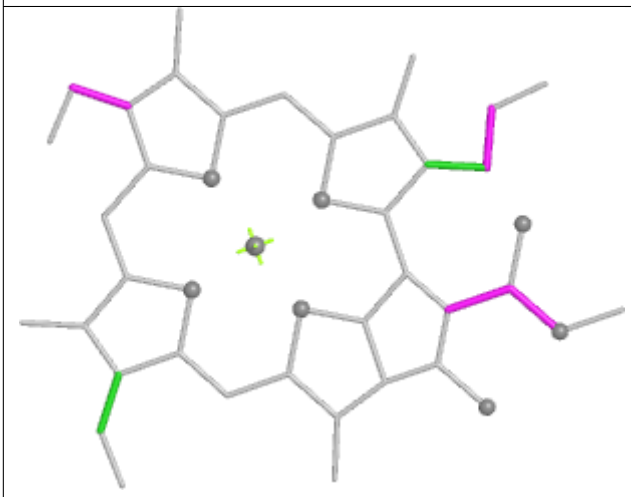
Ligand CLA 9 612



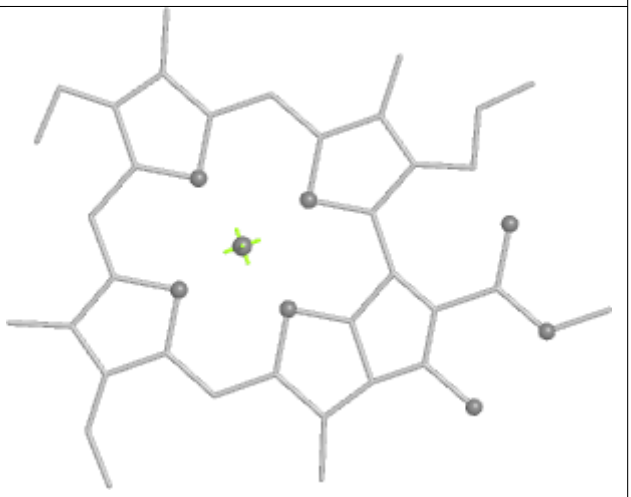
Bond lengths



Bond angles

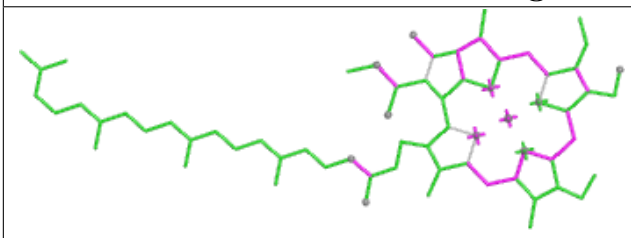


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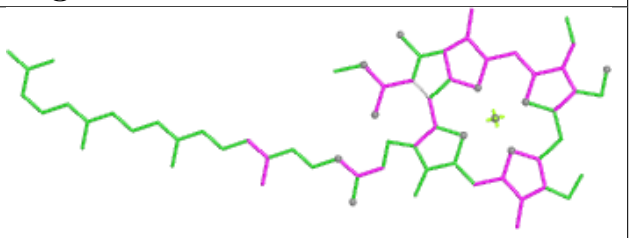


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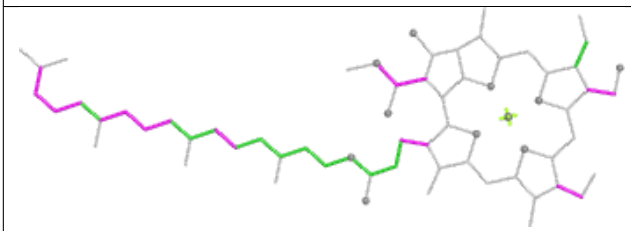
Ligand CHL g 609



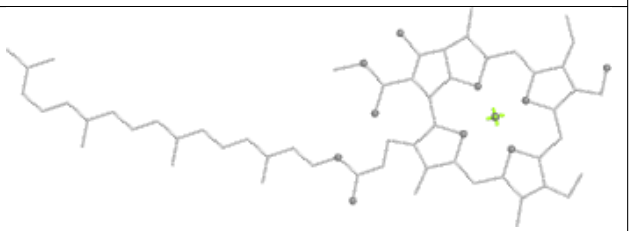
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Bond angles

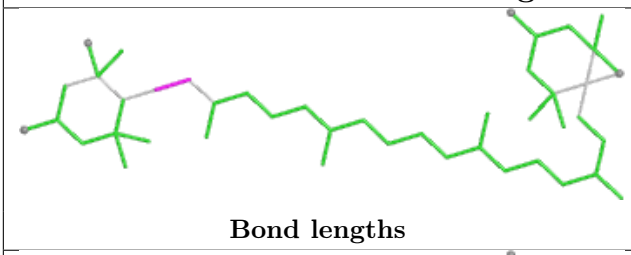


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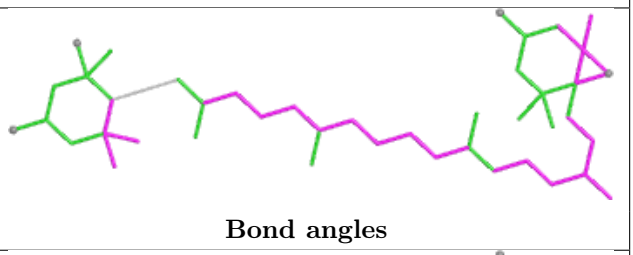


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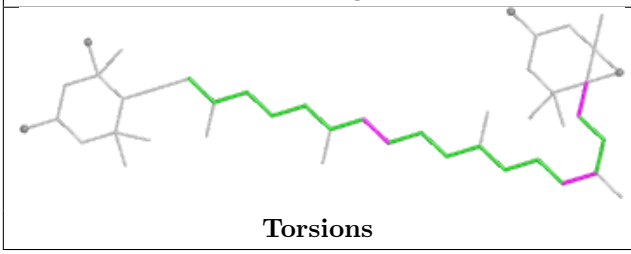
Ligand NEX 5 1623



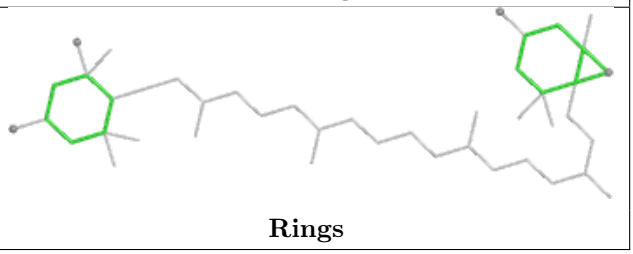
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Bond angles

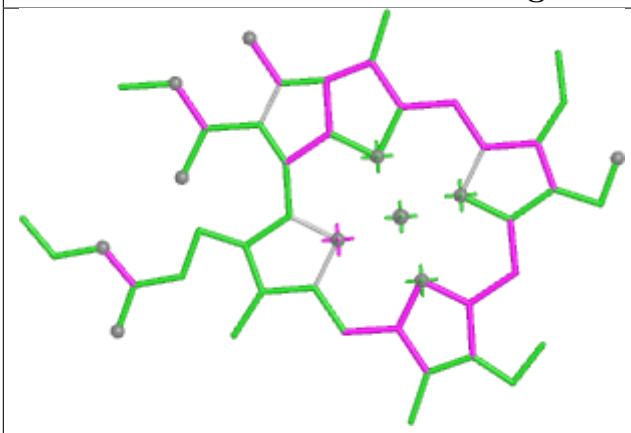


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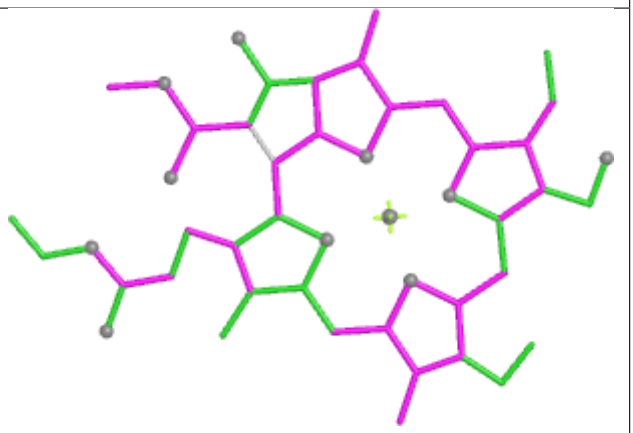


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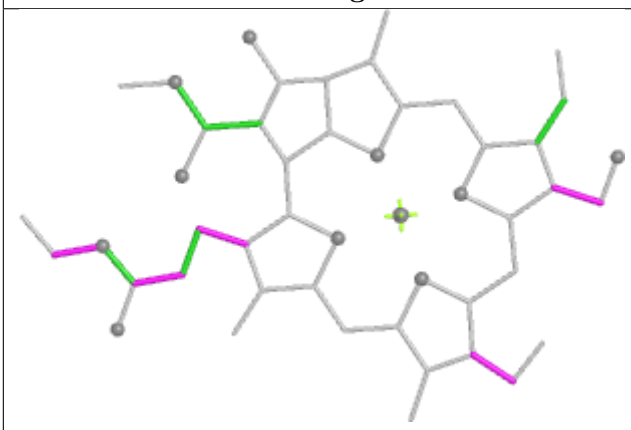
Ligand CHL 9 605



Bond lengths



Bond angles

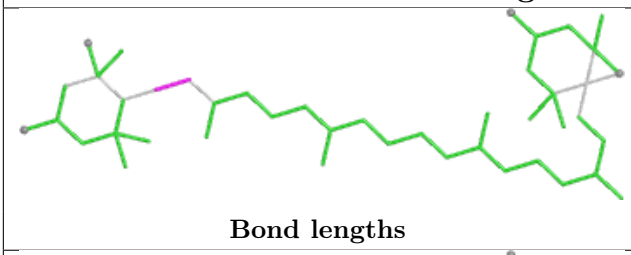


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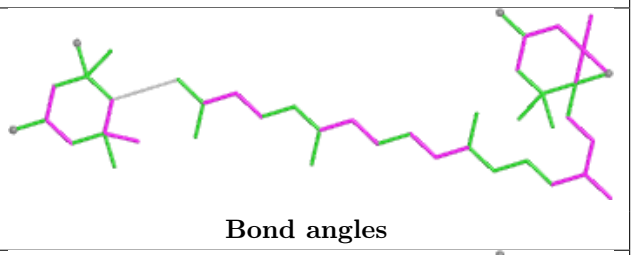


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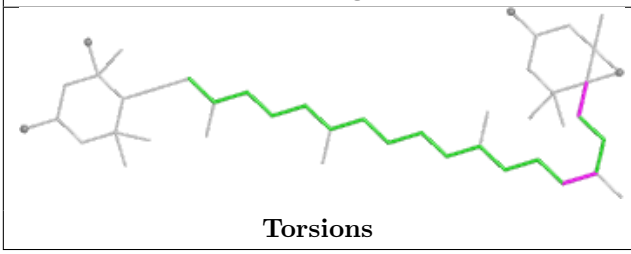
Ligand NEX 8 1623



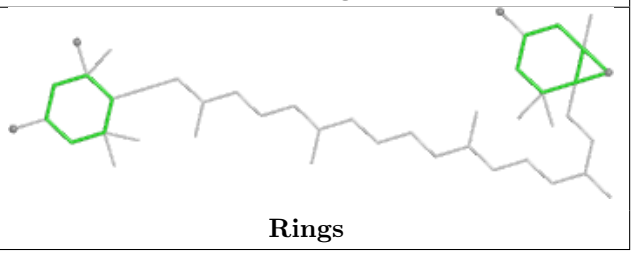
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Bond angles

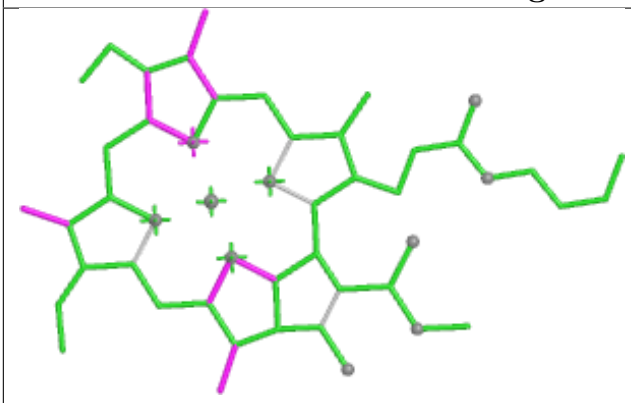


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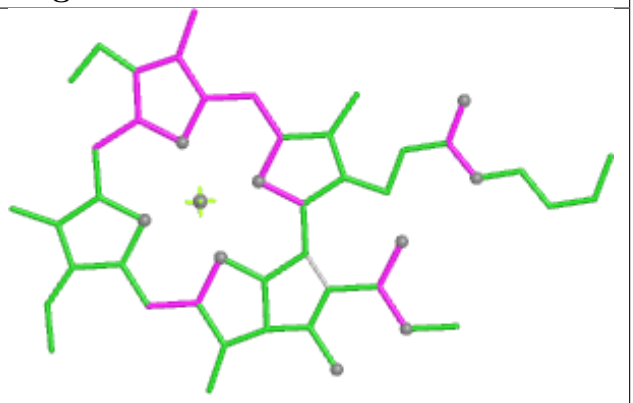


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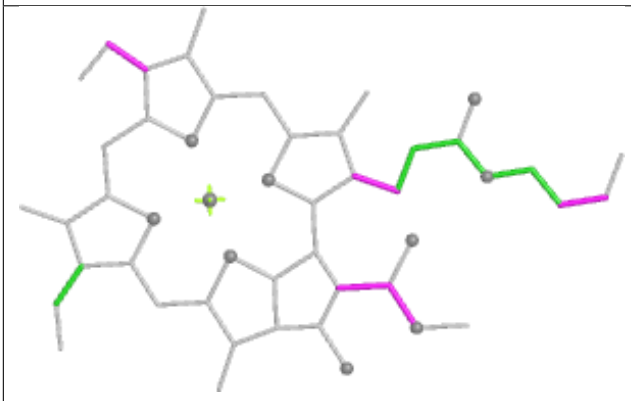
Ligand CLA g 604



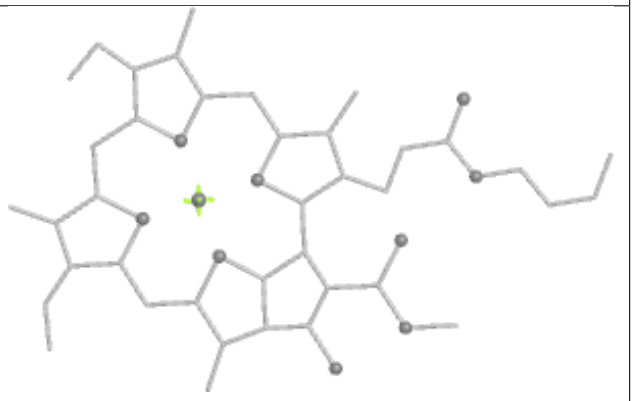
Bond lengths



Bond angles

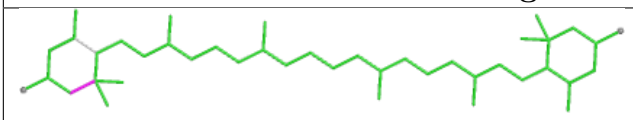


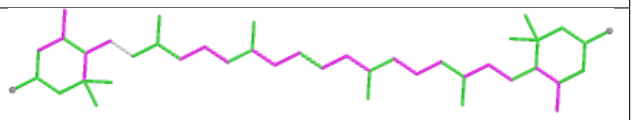
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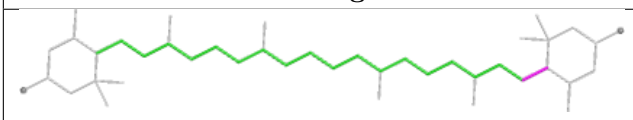


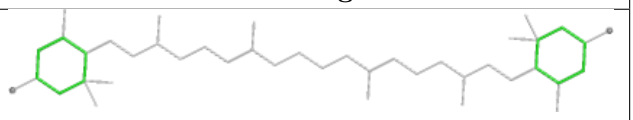
Rings

Ligand LUT 7 1620

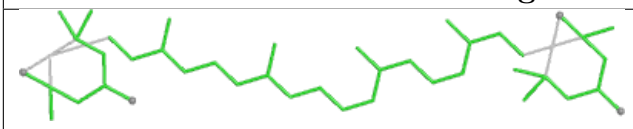

Bond lengths

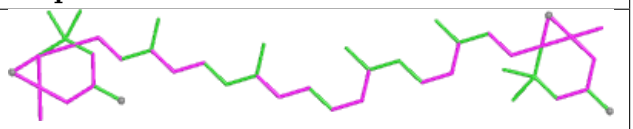

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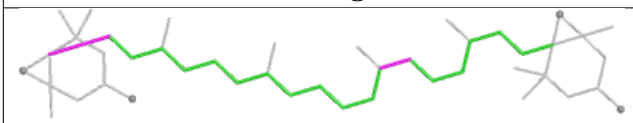

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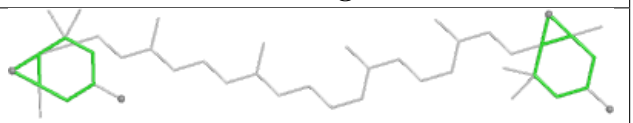

Rings

Ligand XAT q 1622


Bond lengths

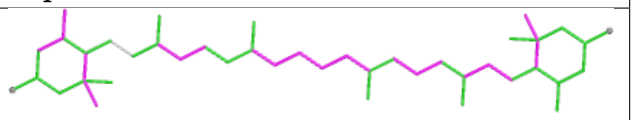

Bond angles

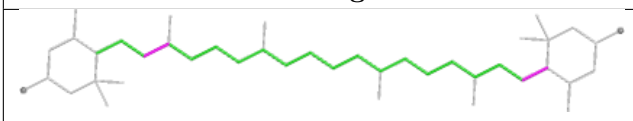

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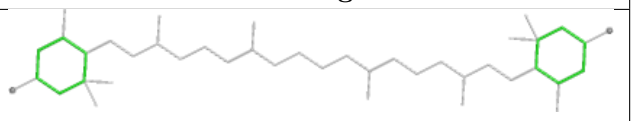

Rings

Ligand LUT p 1621


Bond lengths

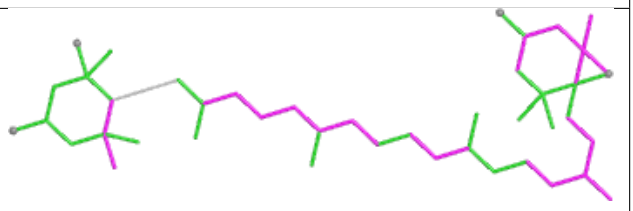

Bond angles

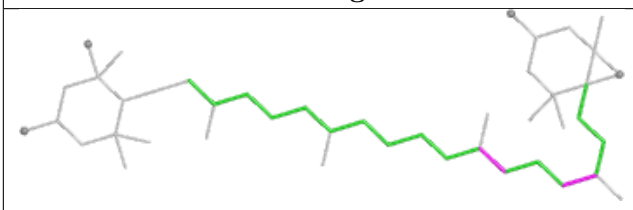

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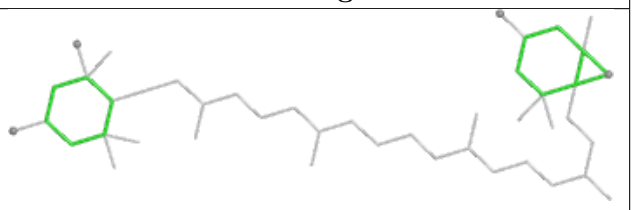

Rings

Ligand NEX 2 1623

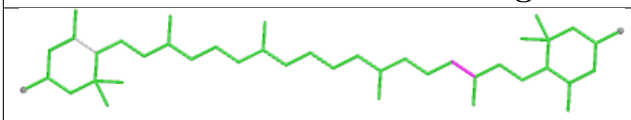

Bond lengths


Bond angles

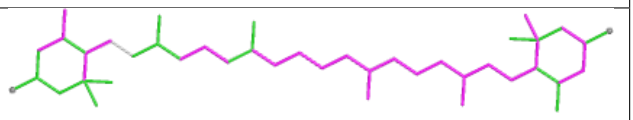

Torsions


Rings

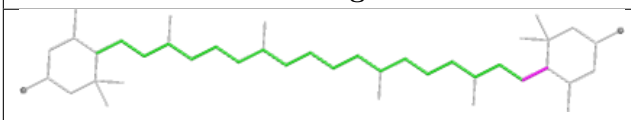
Ligand LUT Y 1620



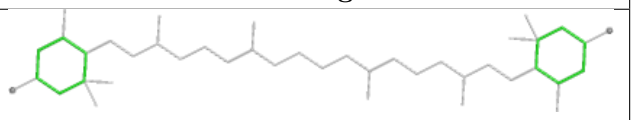
Bond lengths



Bond angles

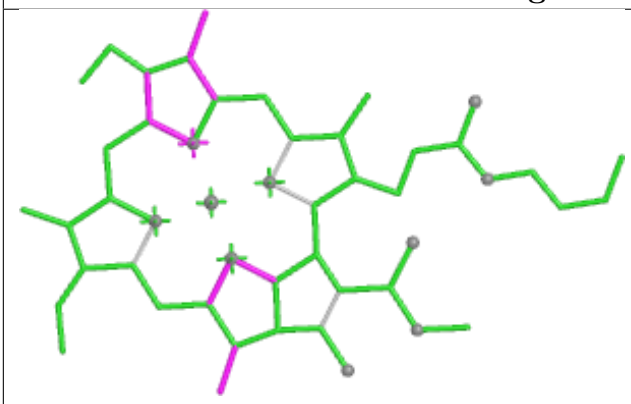


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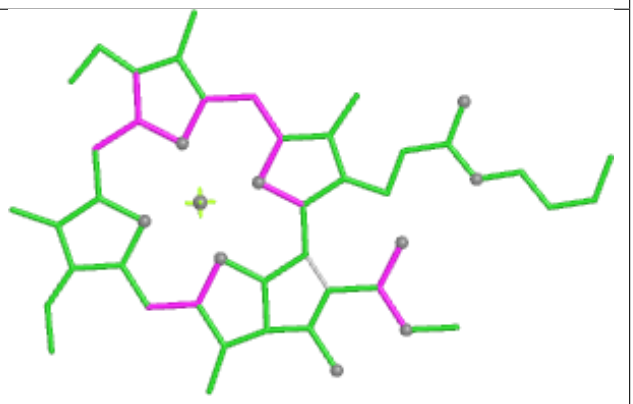


Rings

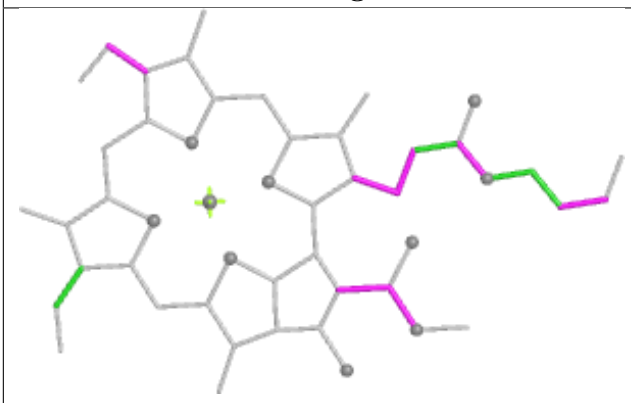
Ligand CLA 9 614



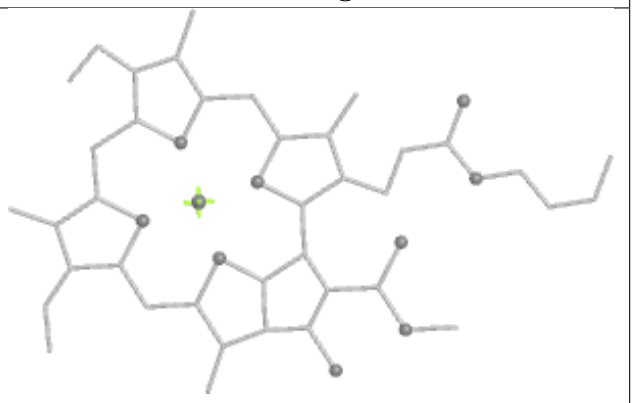
Bond lengths



Bond angles

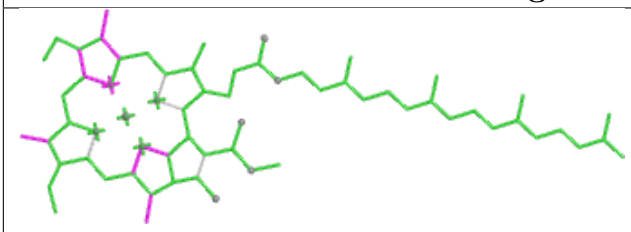


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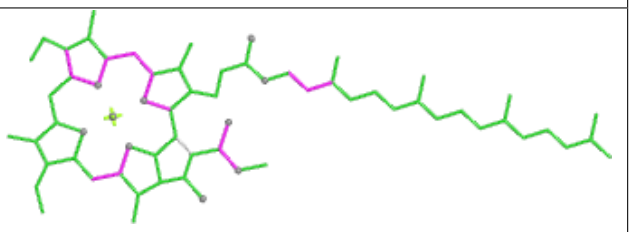


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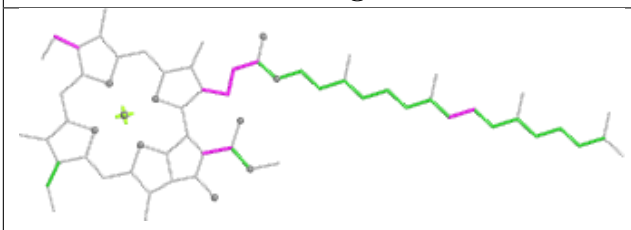
Ligand CLA 6 610



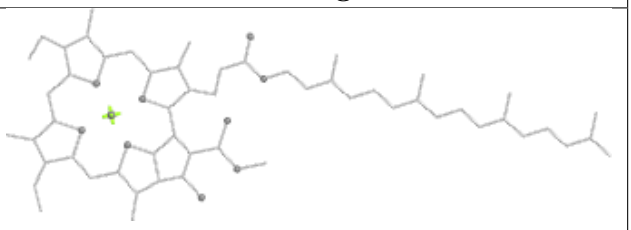
Bond lengths



Bond angles

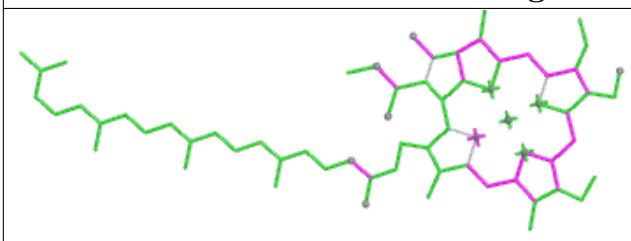


Torsions

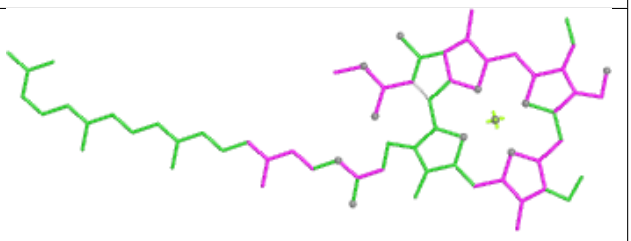


Rings

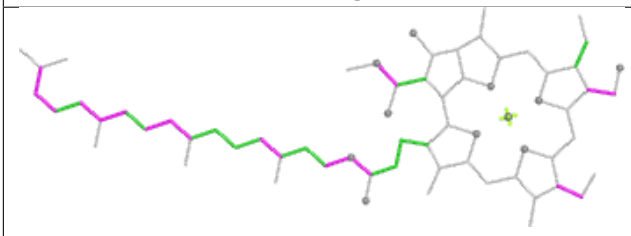
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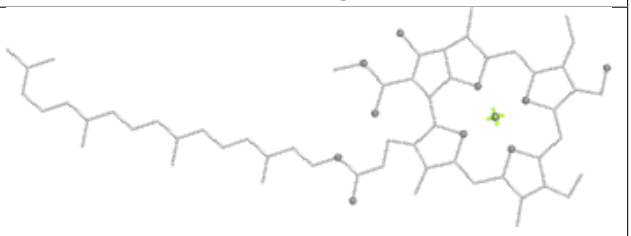
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Bond angles

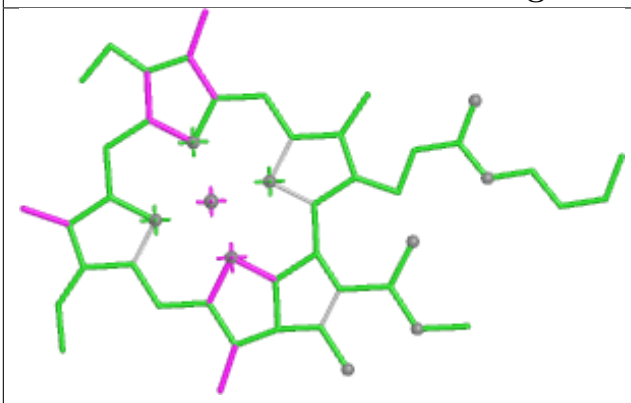


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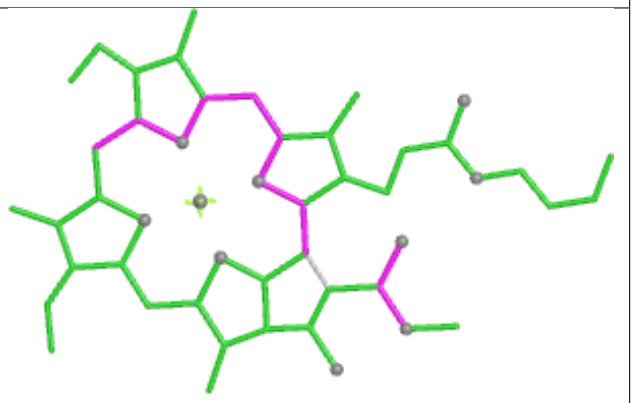


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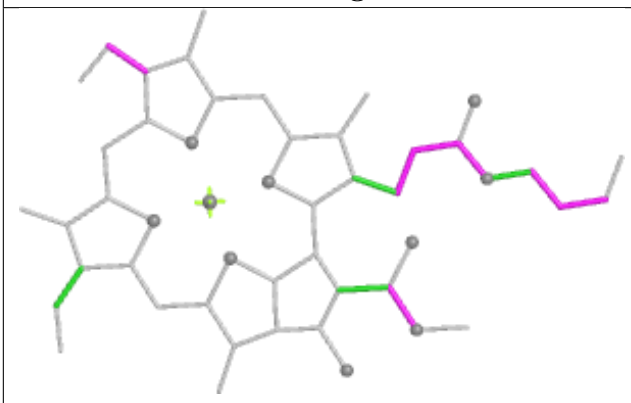
Ligand CLA S 613



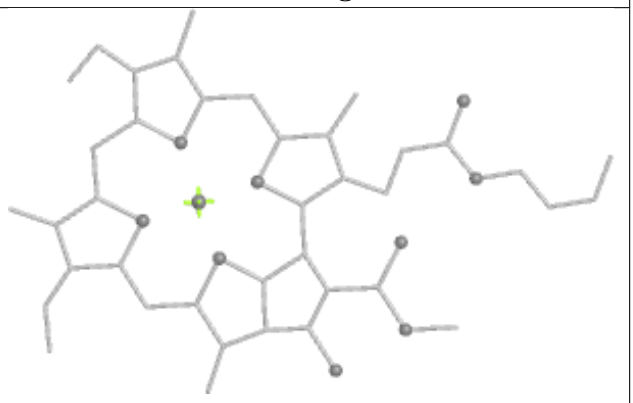
Bond lengths



Bond angles

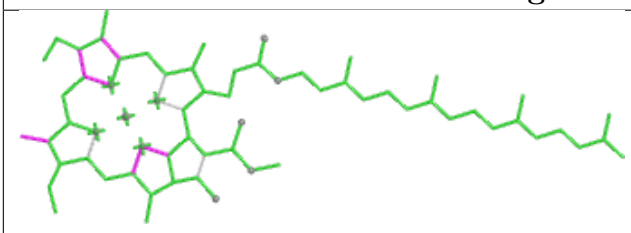


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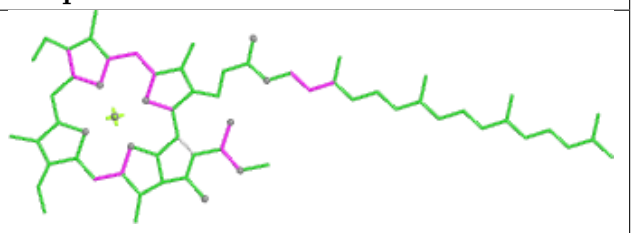


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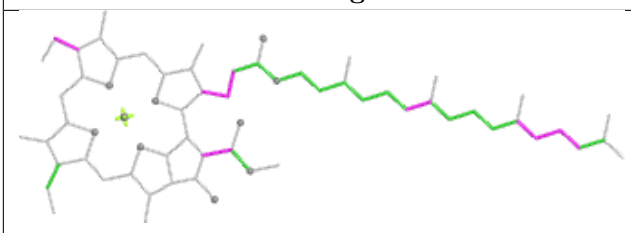
Ligand CLA q 610



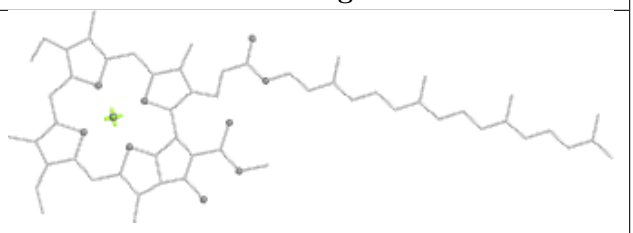
Bond lengths



Bond angles

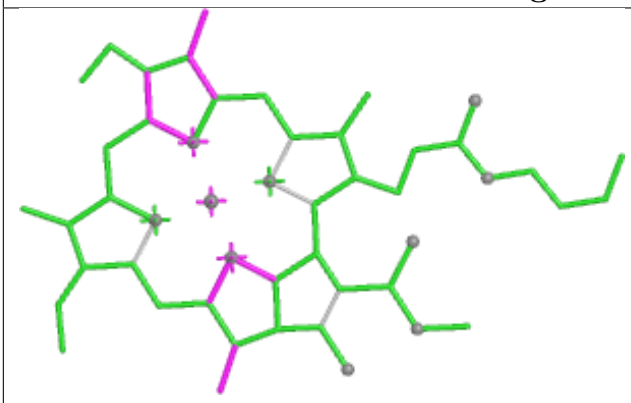


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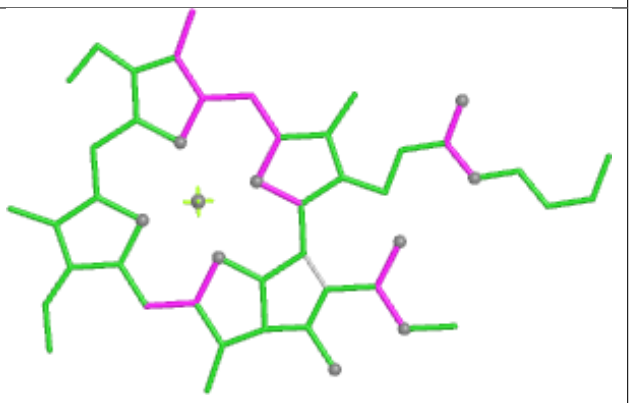


Rings

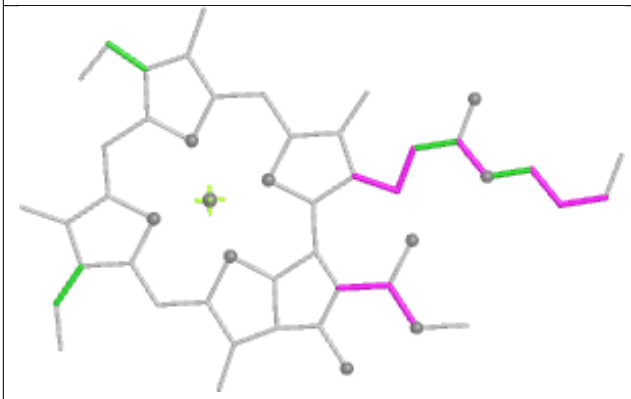
Ligand CLA s 604



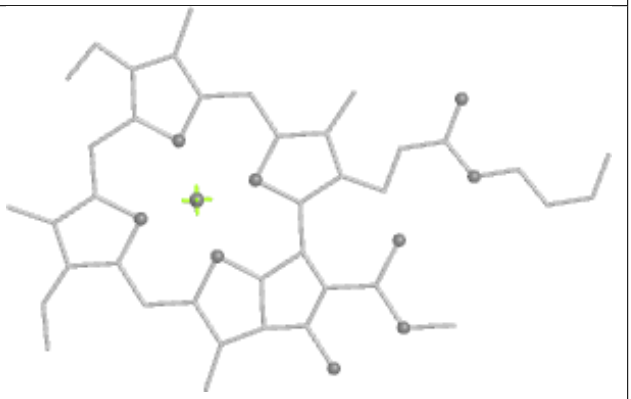
Bond lengths



Bond angles

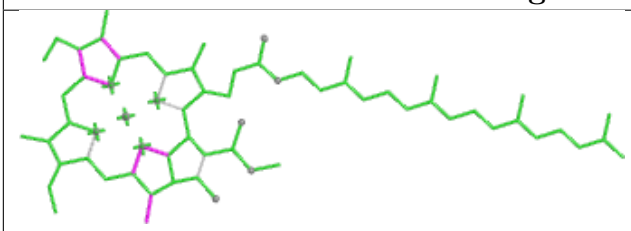


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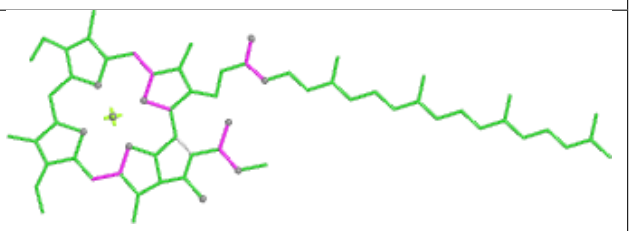


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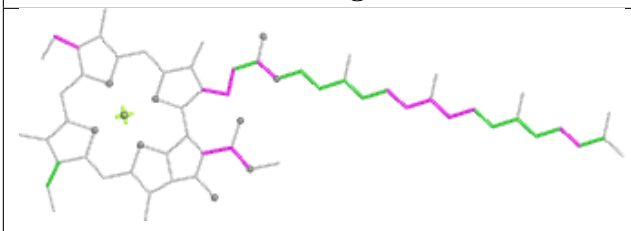
Ligand CLA 3 613



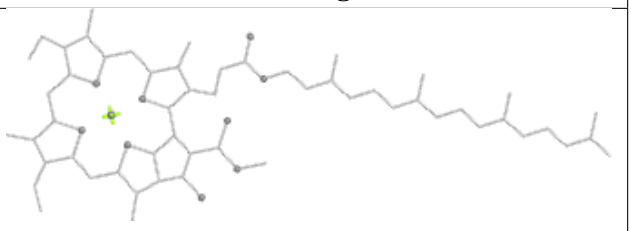
Bond lengths



Bond angles

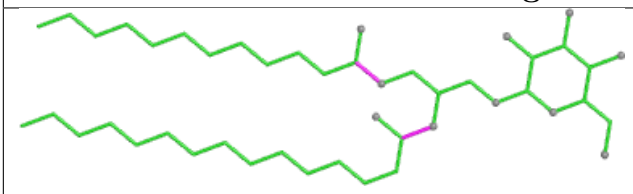


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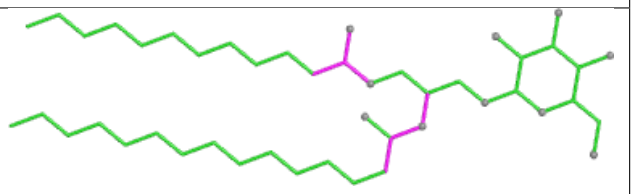


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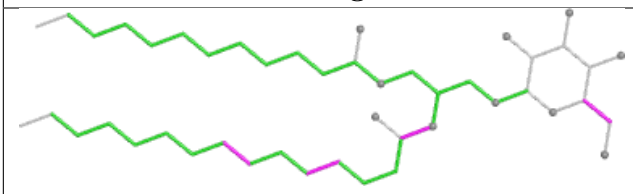
Ligand LMG d 412



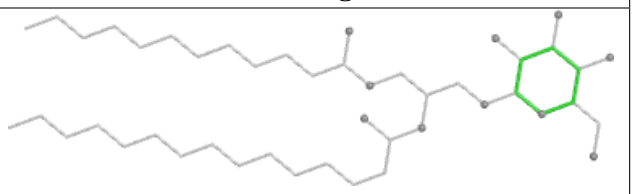
Bond lengths



Bond angles

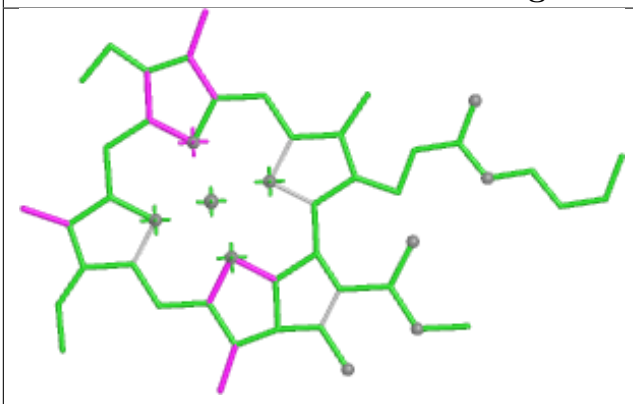


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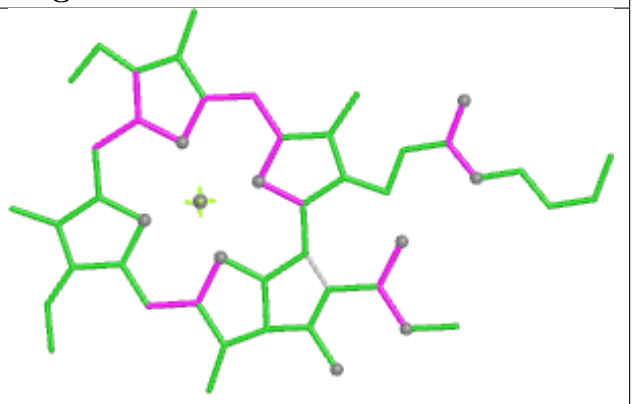


Rings

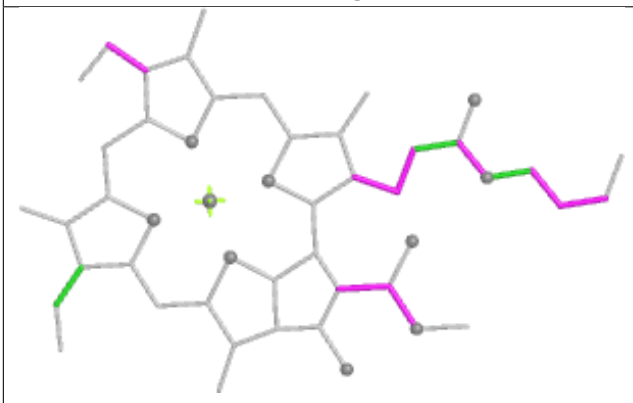
Ligand CLA g 614



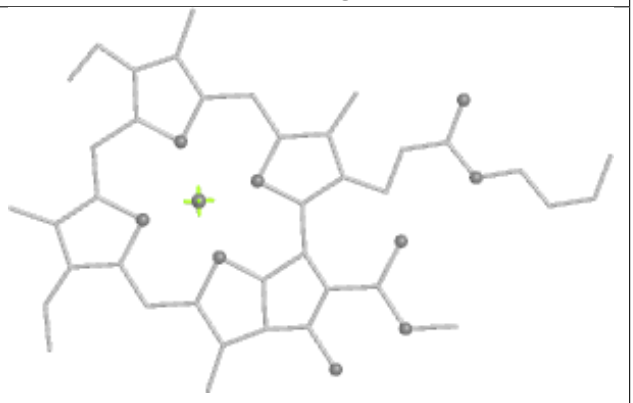
Bond lengths



Bond angles

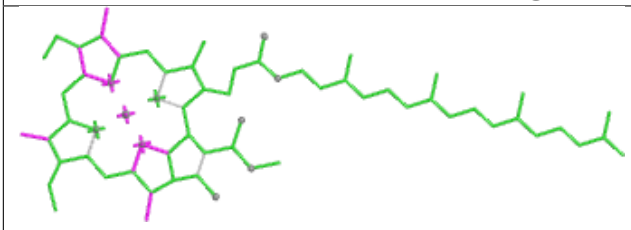


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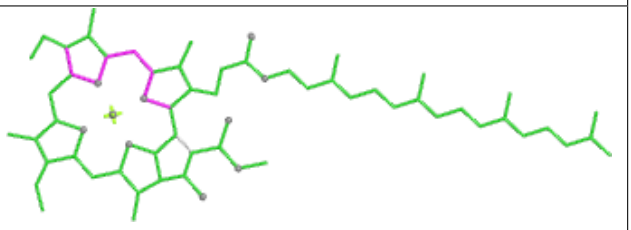


Rings

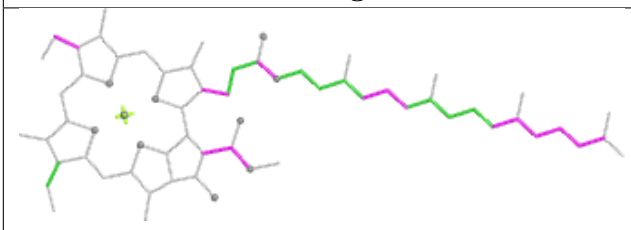
Ligand CLA b 602



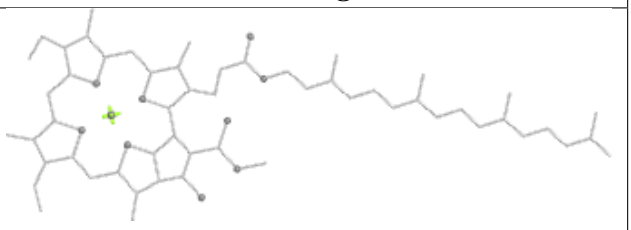
Bond lengths



Bond angles

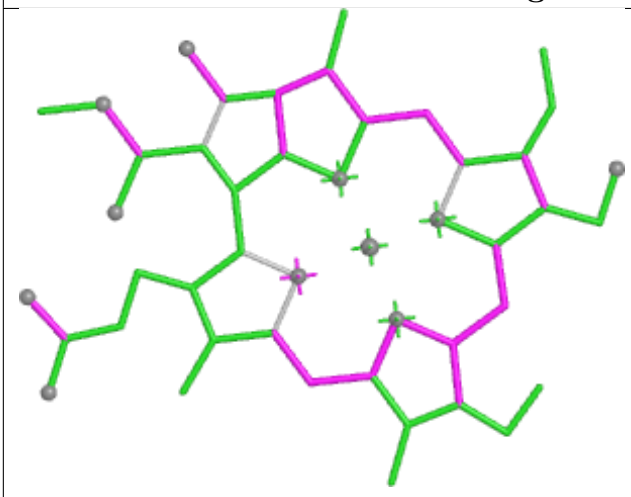


Torsions



Rings

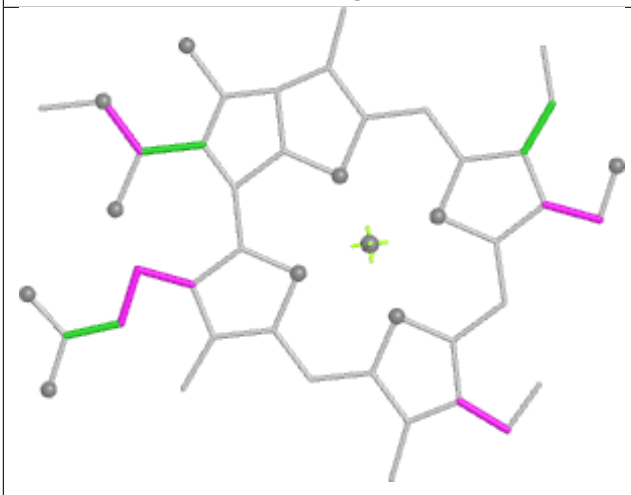
Ligand CHL y 605



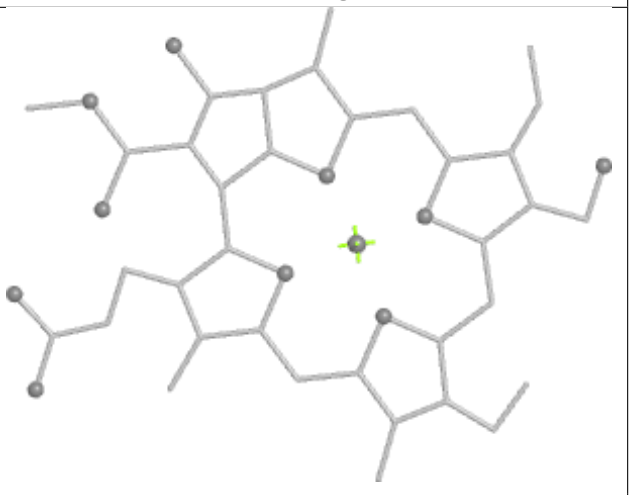
Bond lengths



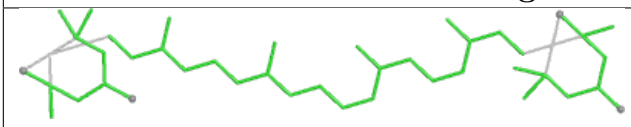
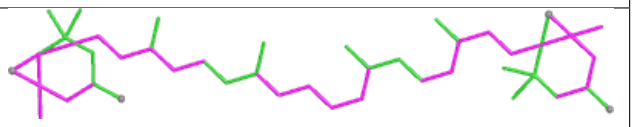
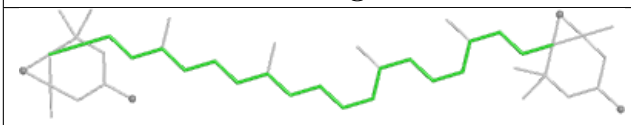
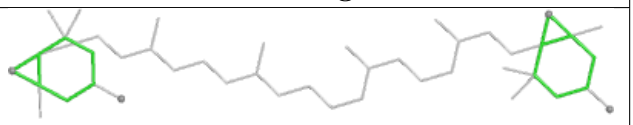
Bond angles

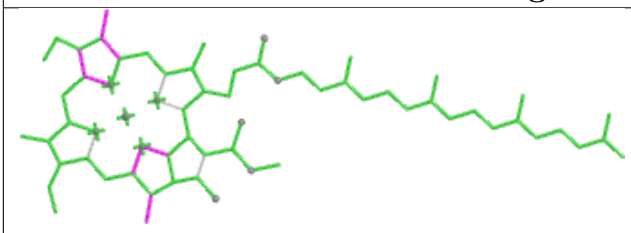
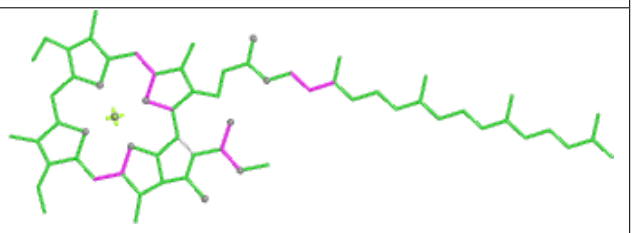
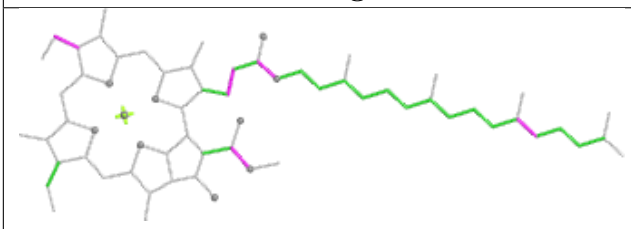
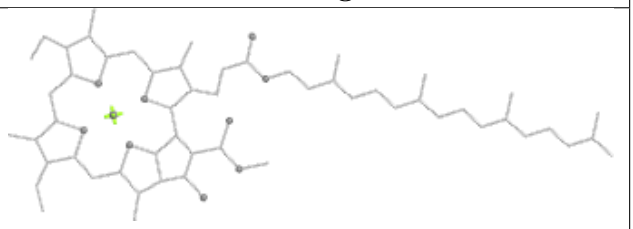


Torsions

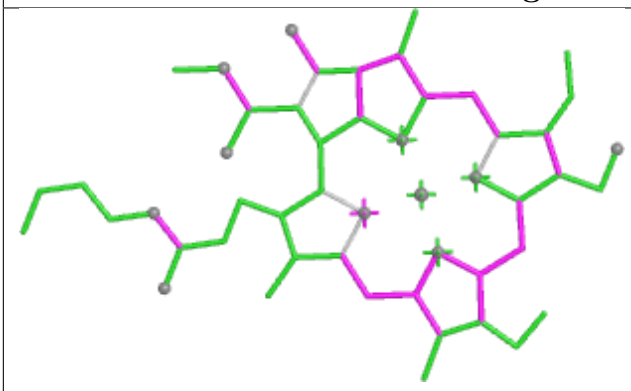


Rings

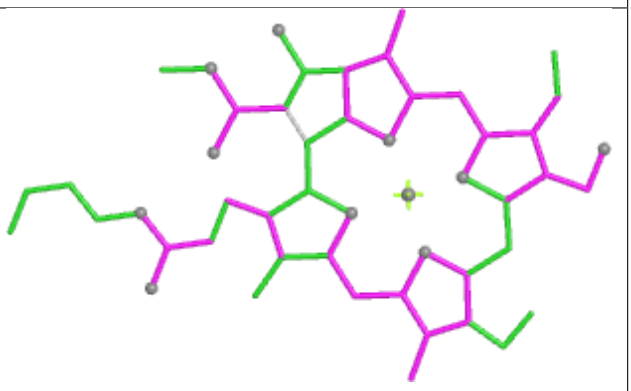
Ligand XAT 5 1622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

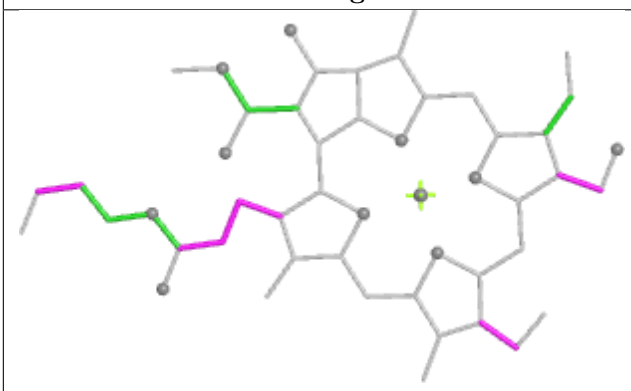
Ligand CHL G 607



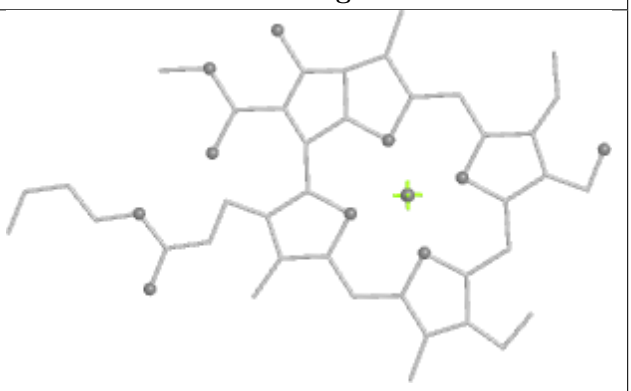
Bond lengths



Bond angles

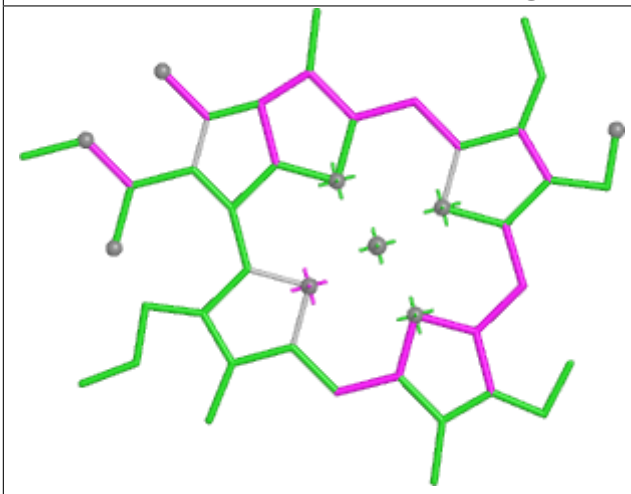


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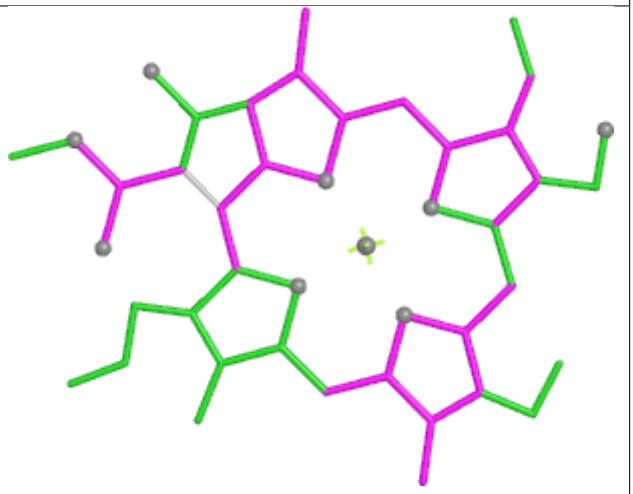


Rings

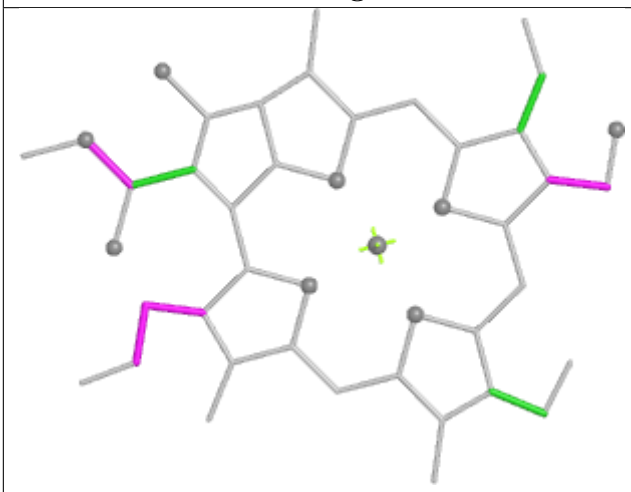
Ligand CHL G 608



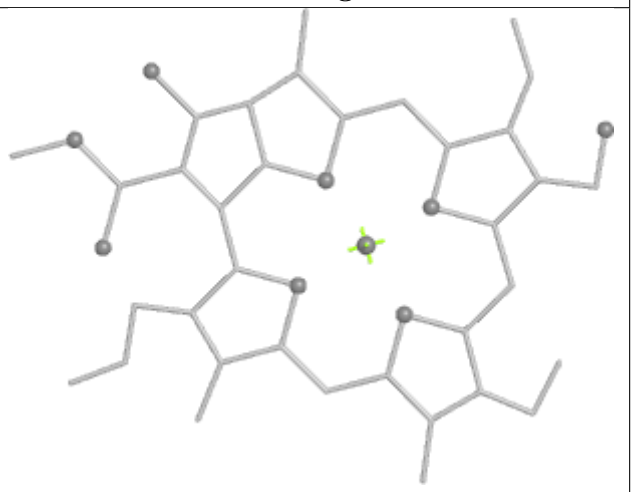
Bond lengths



Bond angles

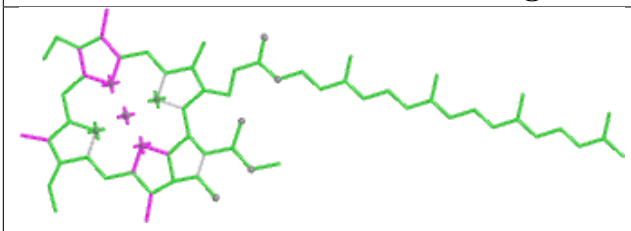


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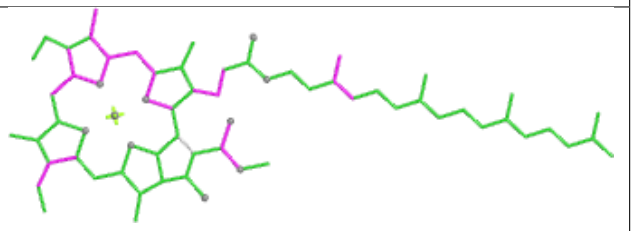


Rings

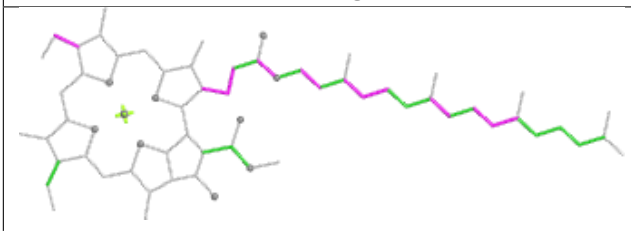
Ligand CLA D 402



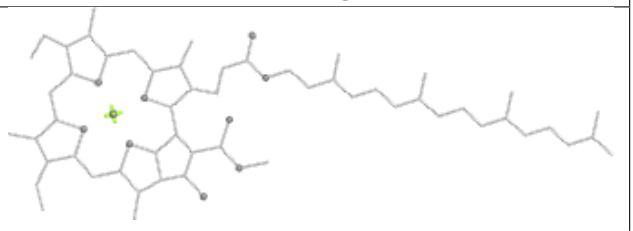
Bond lengths



Bond angles

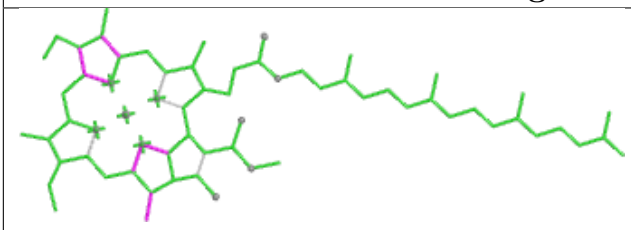


Torsions

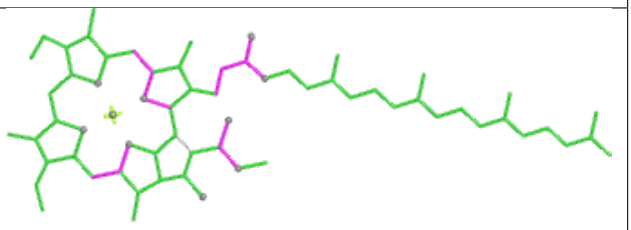


Rings

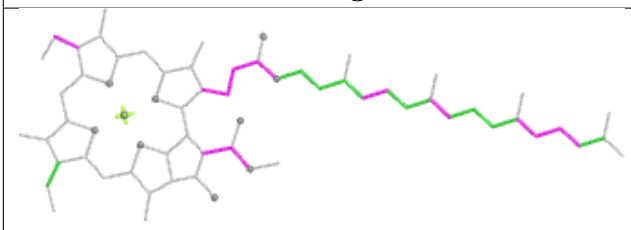
Ligand CLA 0 613



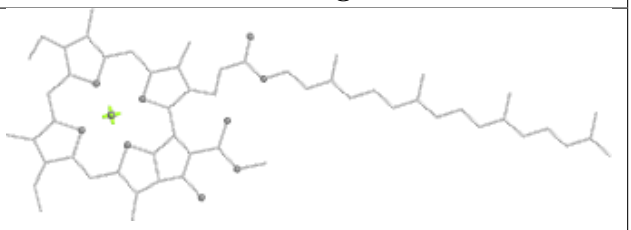
Bond lengths



Bond angles

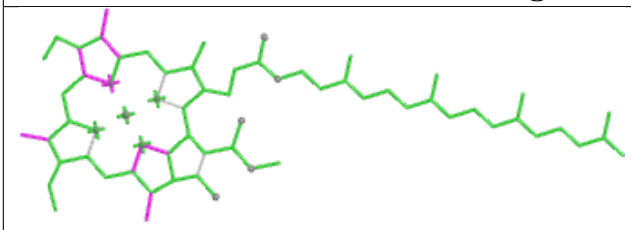


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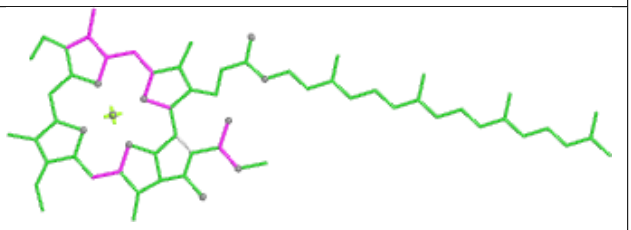


Rings

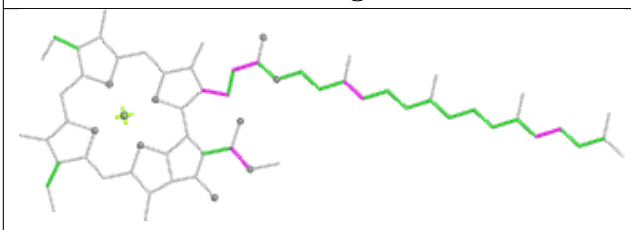
Ligand CLA 3 604



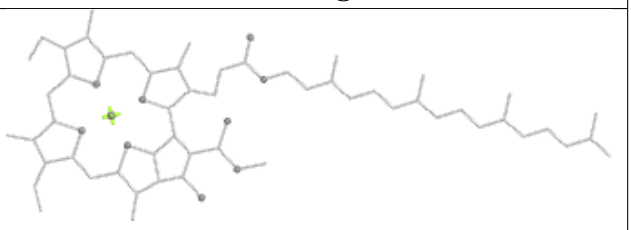
Bond lengths



Bond angles

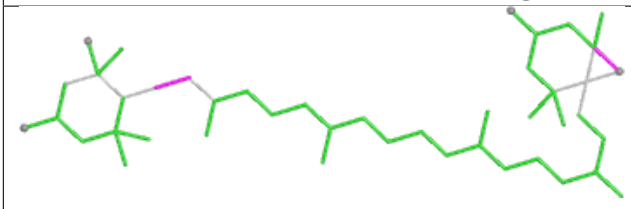


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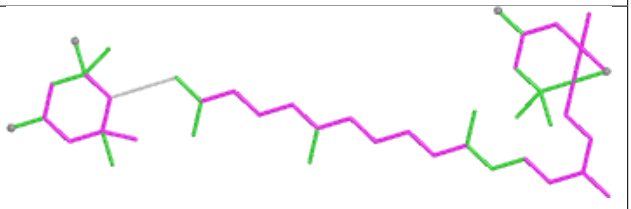


Rings

Ligand NEX 4 1623



Bond lengths



Bond angles

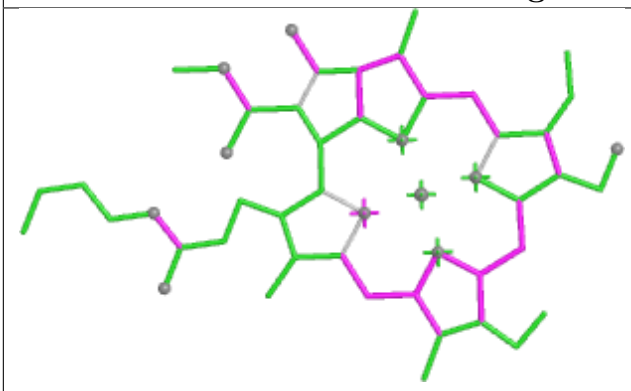


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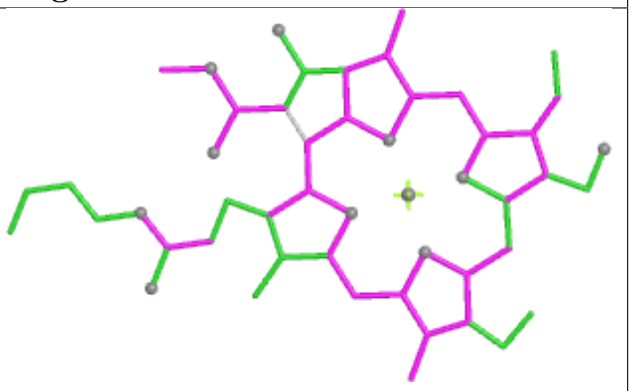


Rings

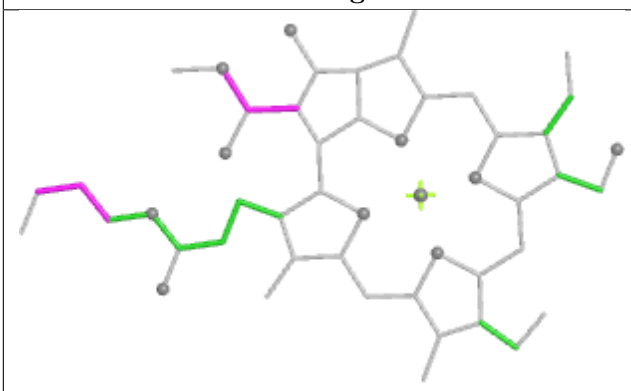
Ligand CHL g 606



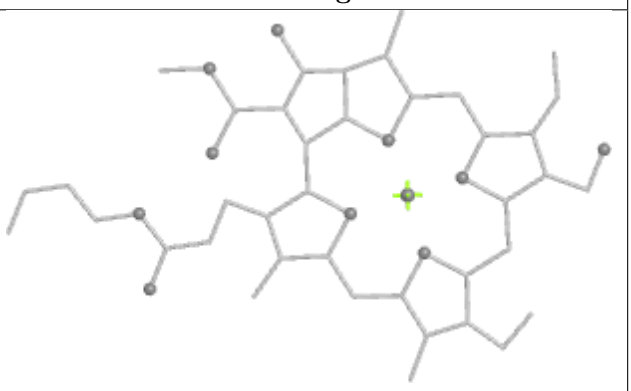
Bond lengths



Bond angles

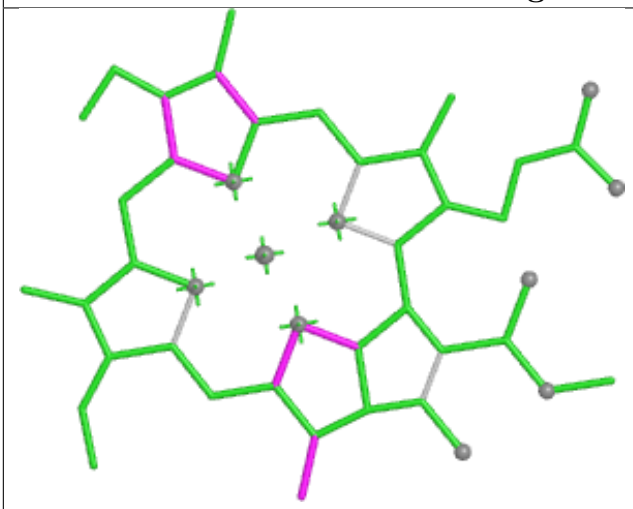


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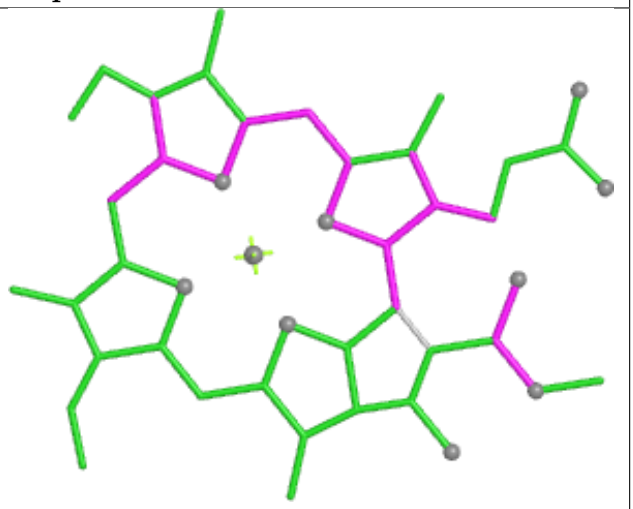


Rings

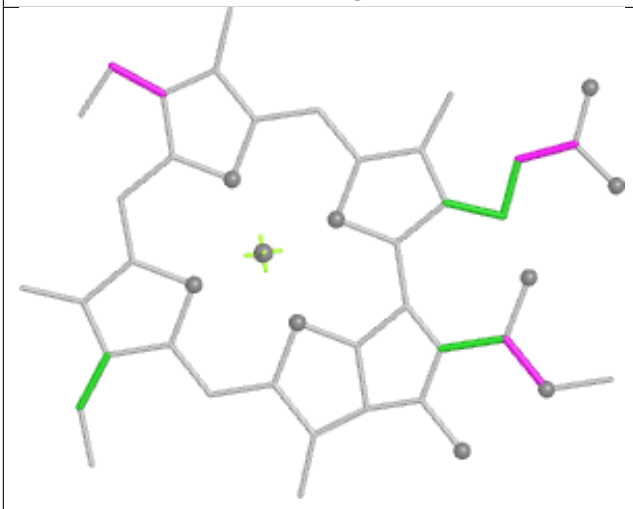
Ligand CLA p 612



Bond lengths



Bond angles

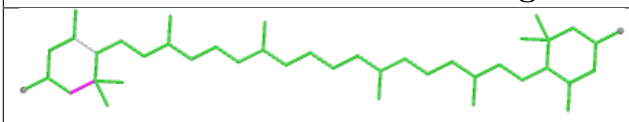


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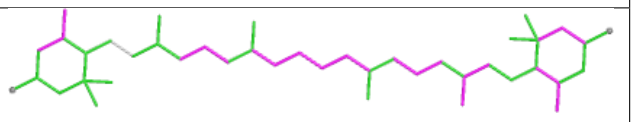


Rings

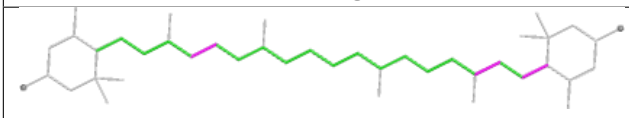
Ligand LUT n 1621



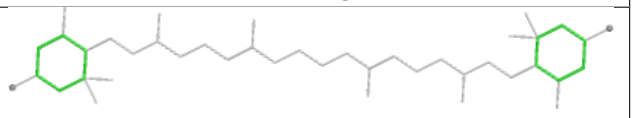
Bond lengths



Bond angles

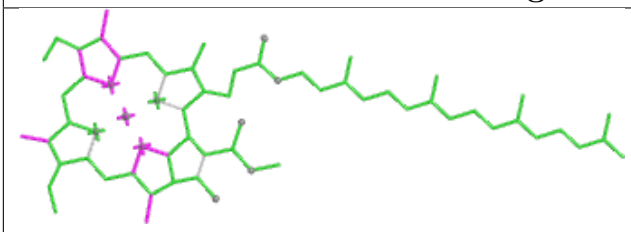


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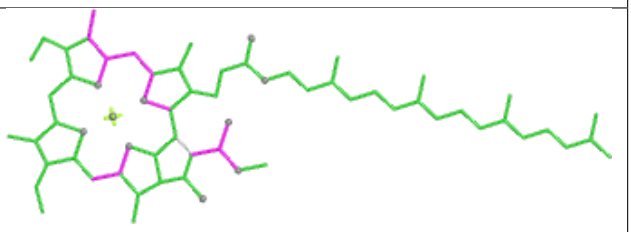


Rings

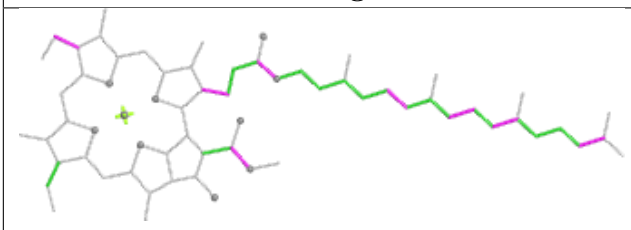
Ligand CLA d 403



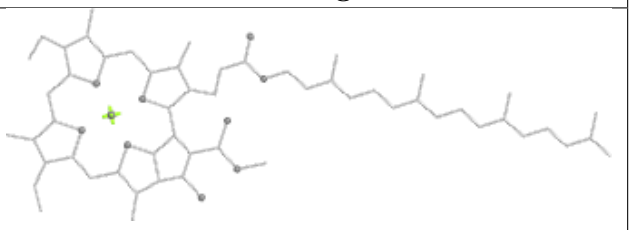
Bond lengths



Bond angles

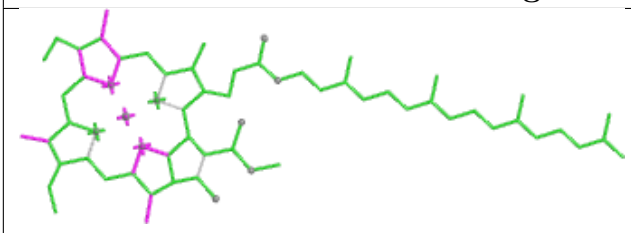


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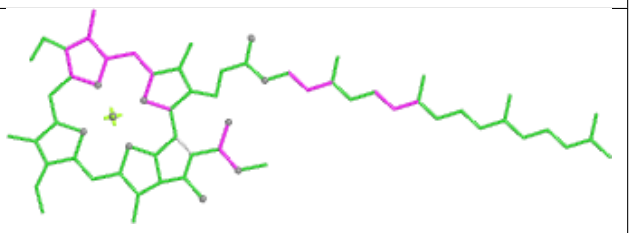


Rings

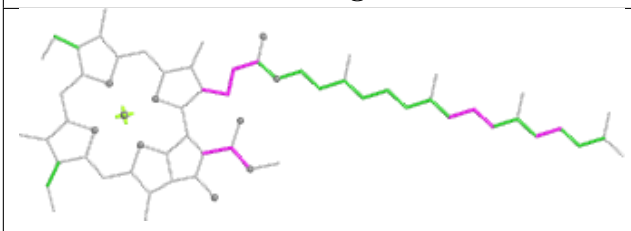
Ligand CLA G 602



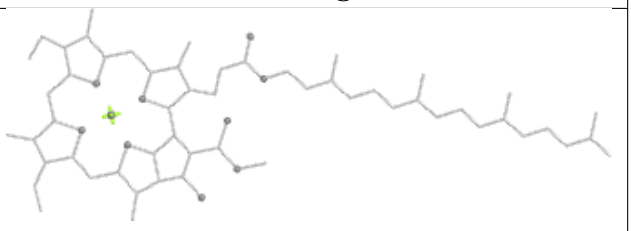
Bond lengths



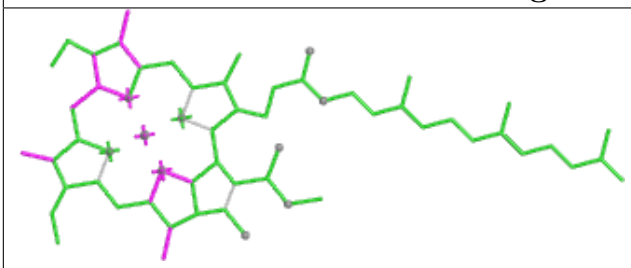
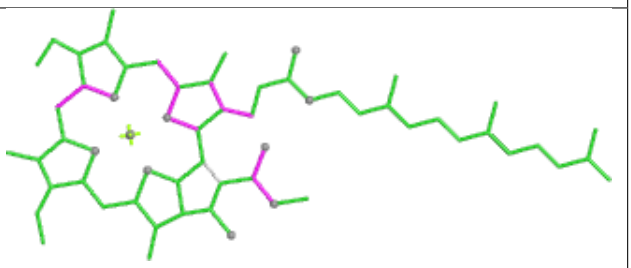
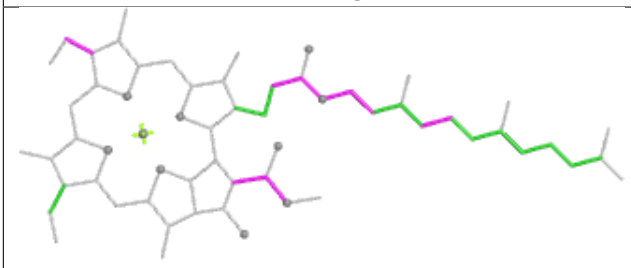
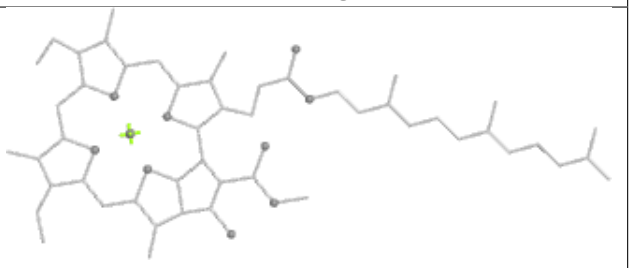
Bond angles

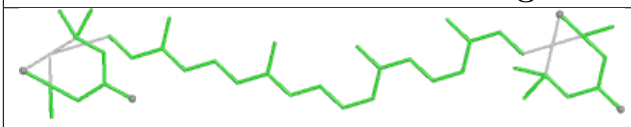
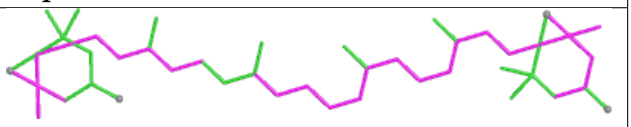
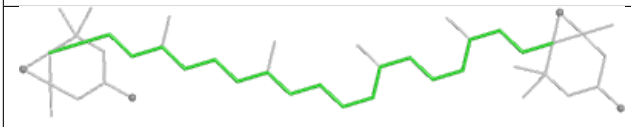
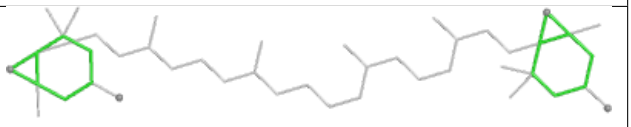


Torsions

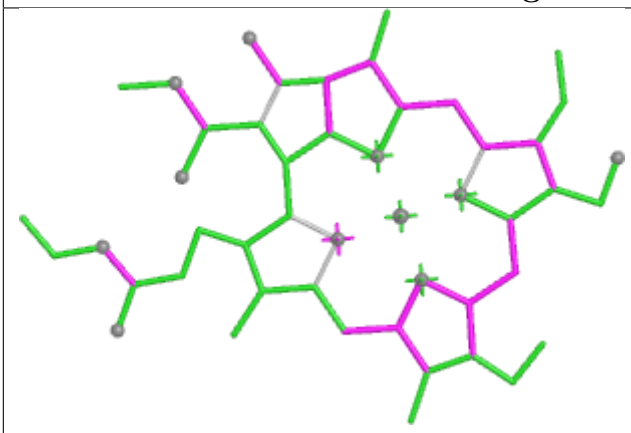


Rings

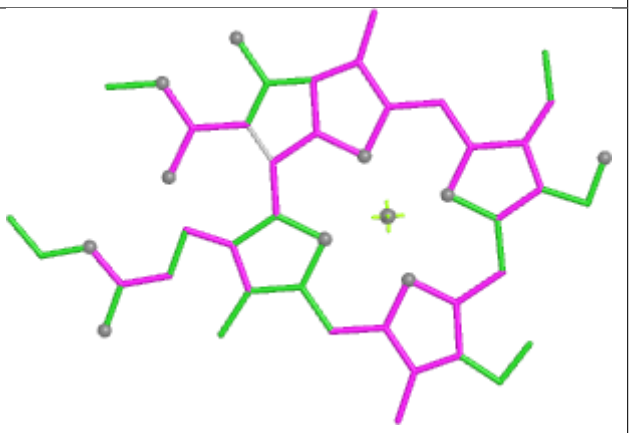
Ligand CLA r 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT p 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

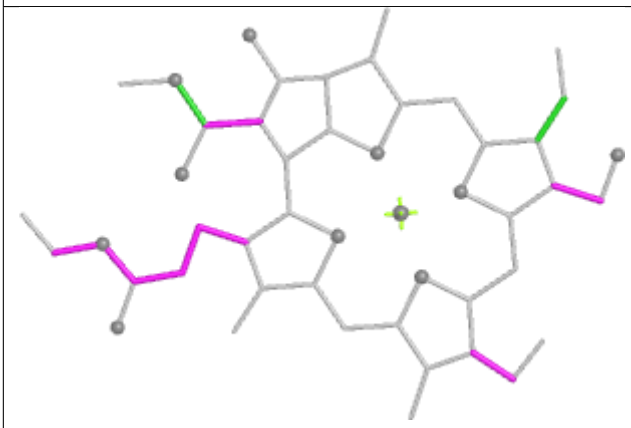
Ligand CHL G 605



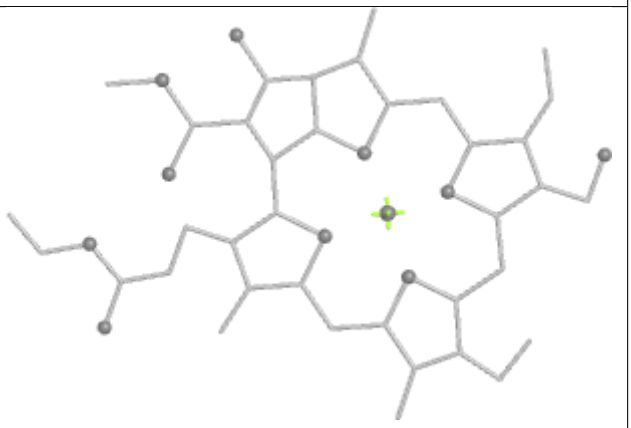
Bond lengths



Bond angles

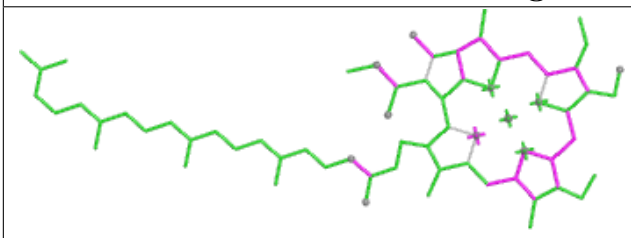


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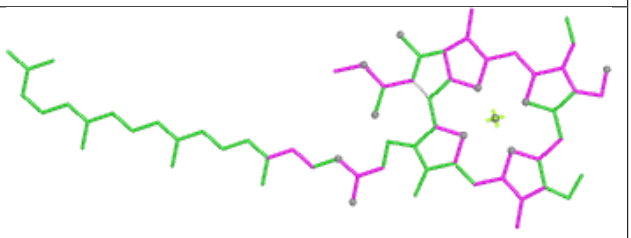


Rings

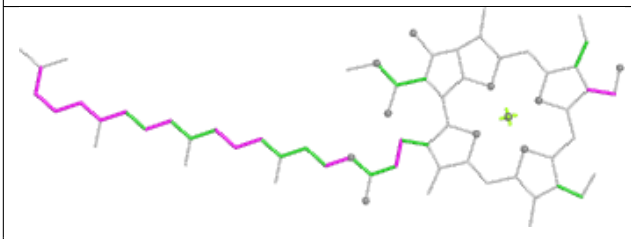
Ligand CHL 8 605



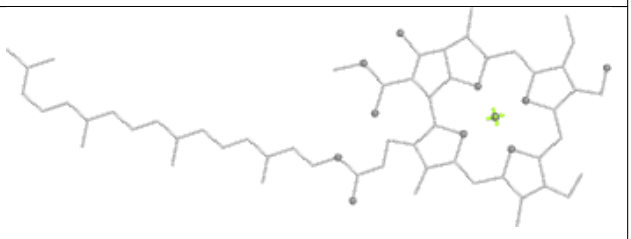
Bond lengths



Bond angles

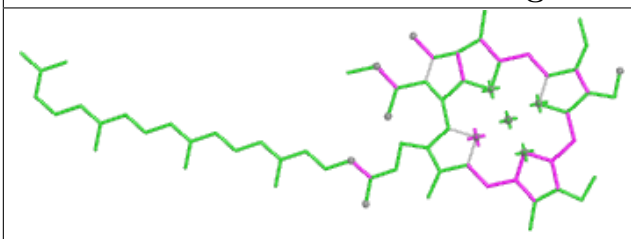


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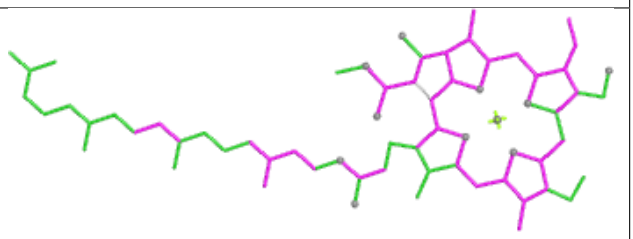


Rings

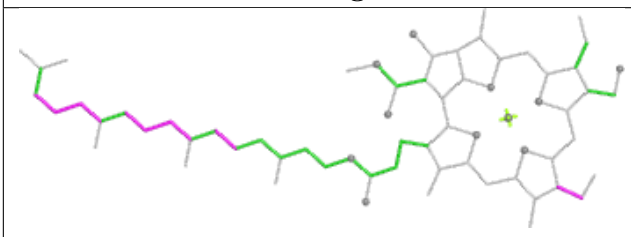
Ligand CHL n 601



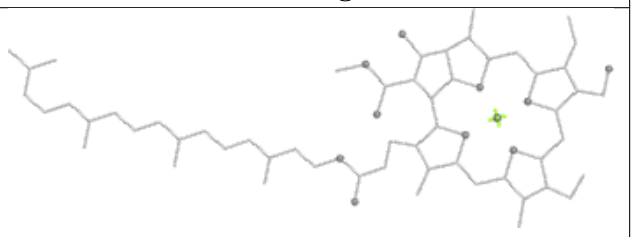
Bond lengths



Bond angles

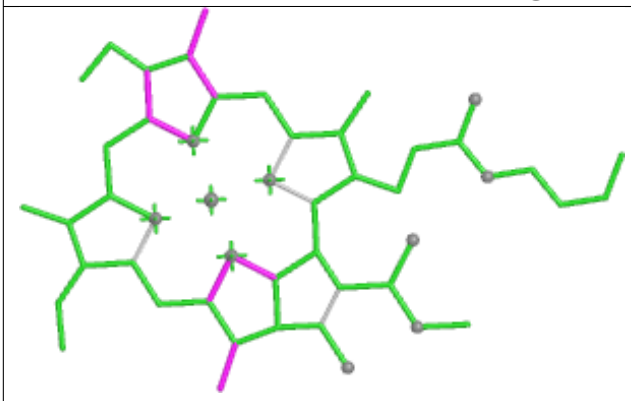


Torsions

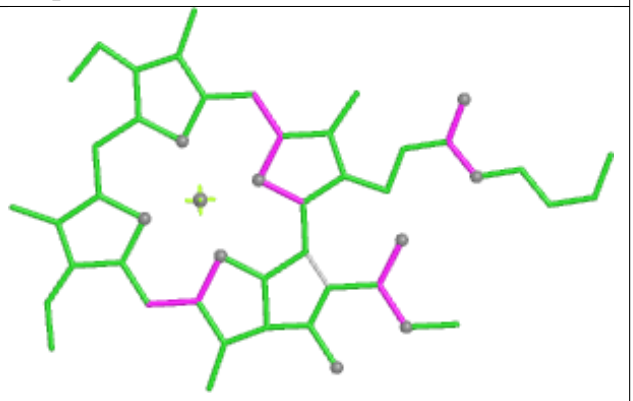


Rings

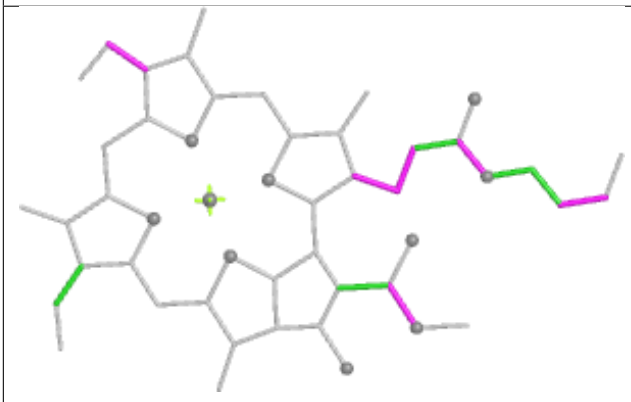
Ligand CLA p 614



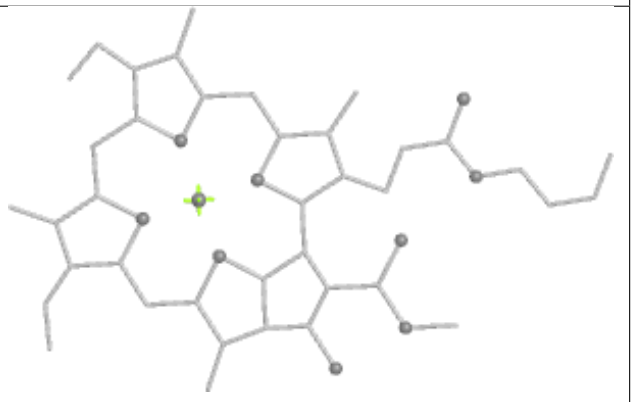
Bond lengths



Bond angles

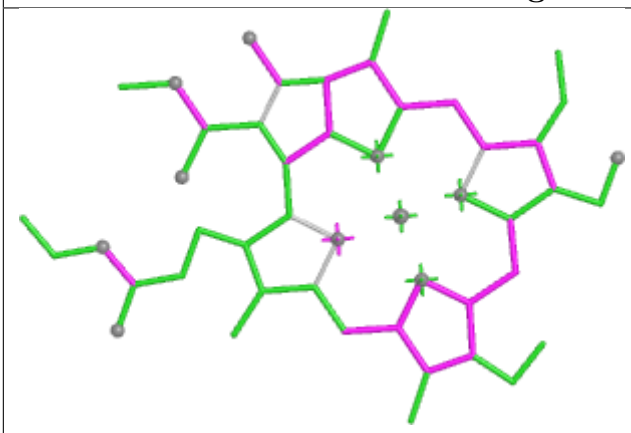


Torsions

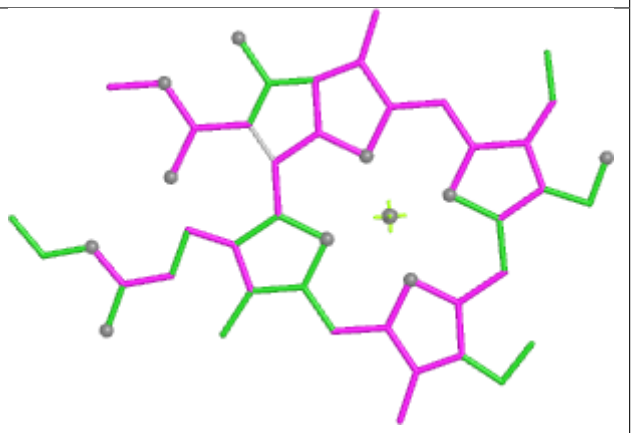


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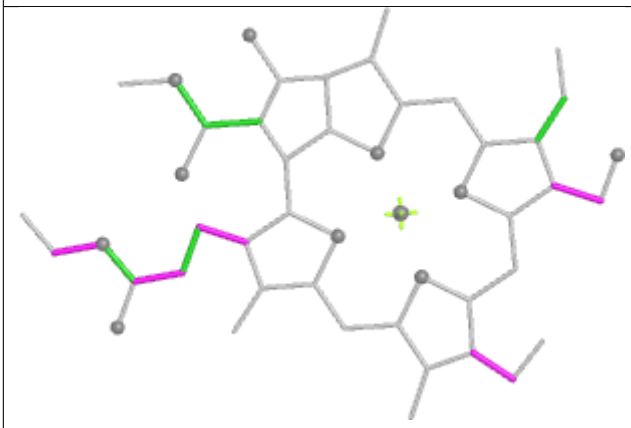
Ligand CHL 2 605



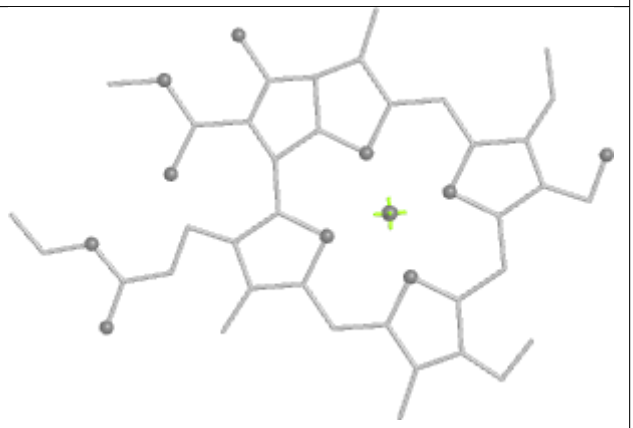
Bond lengths



Bond angles

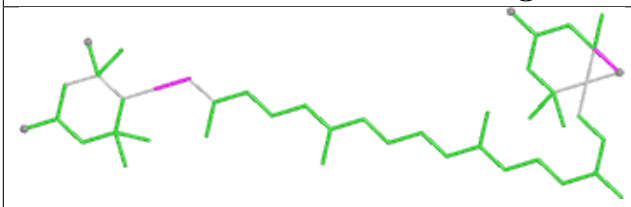


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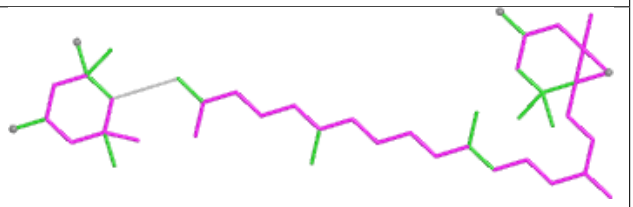


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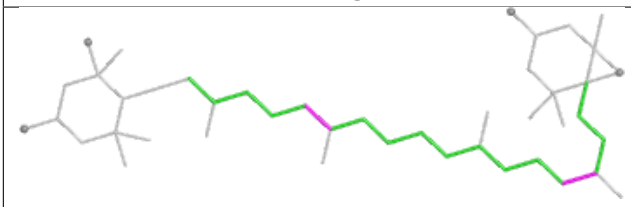
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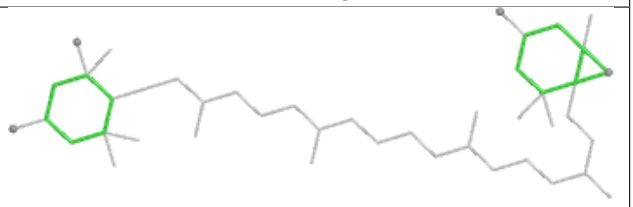
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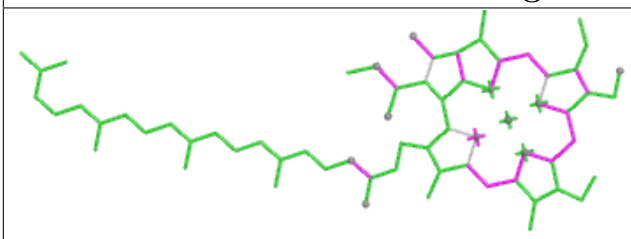


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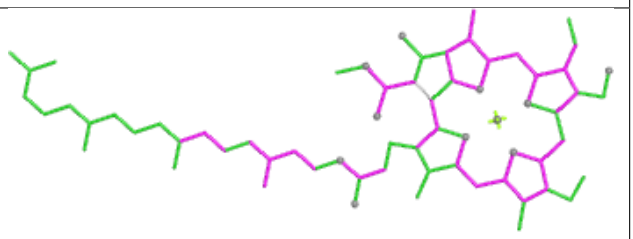


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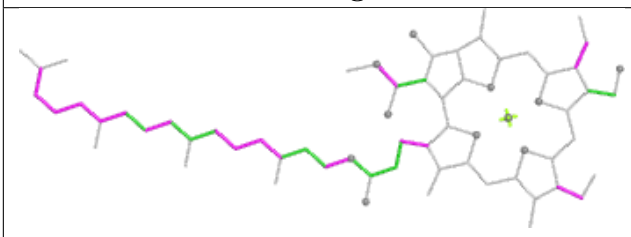
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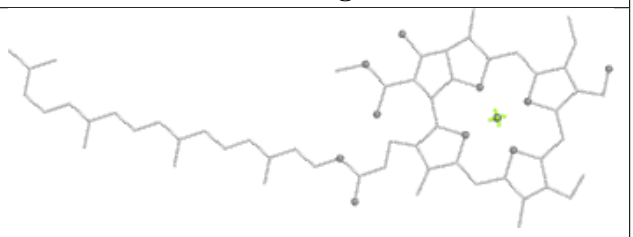
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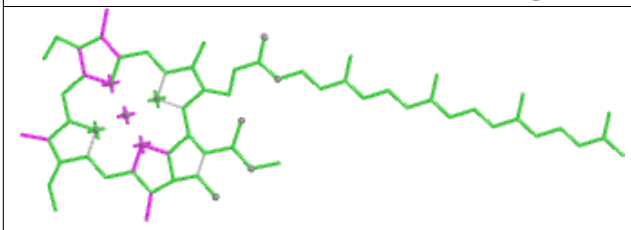


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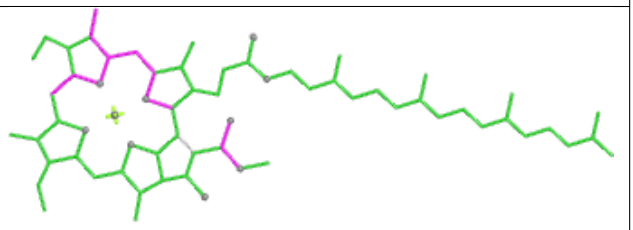


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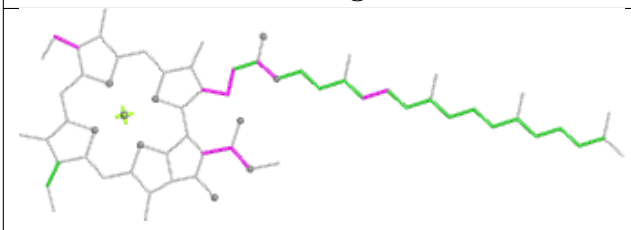
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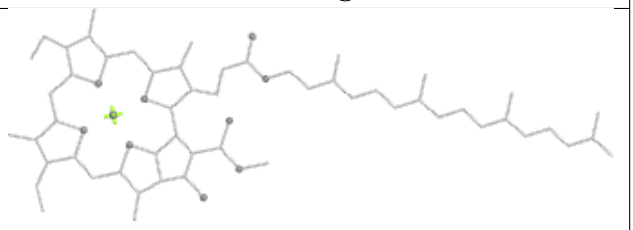
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Bond angles

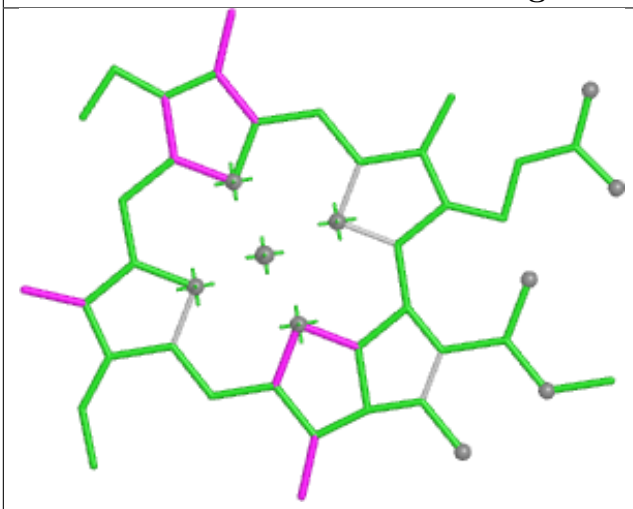


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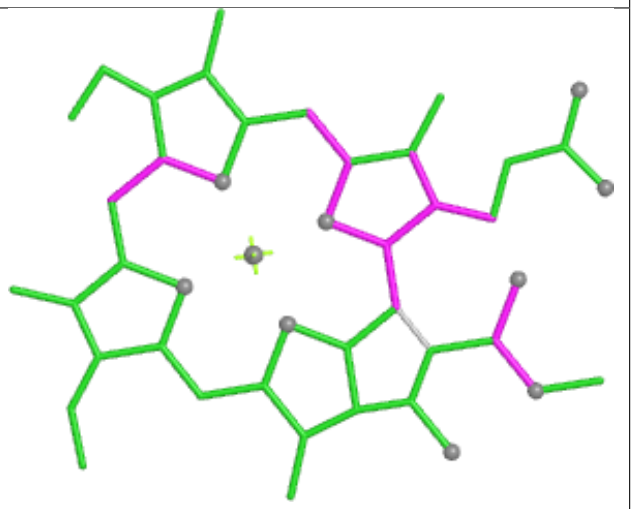


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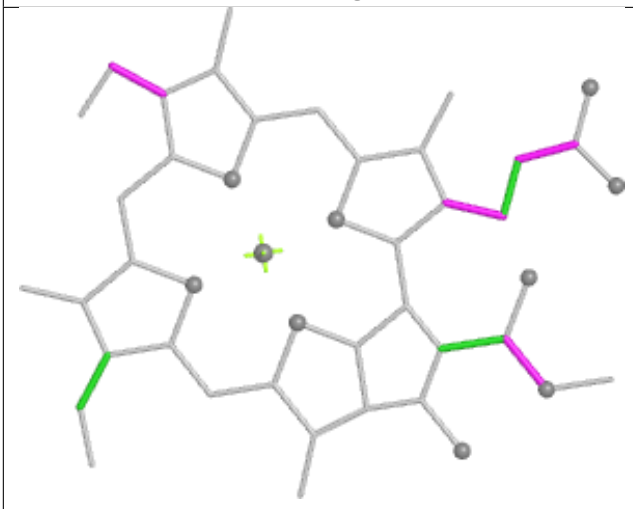
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Bond lengths



Bond angles

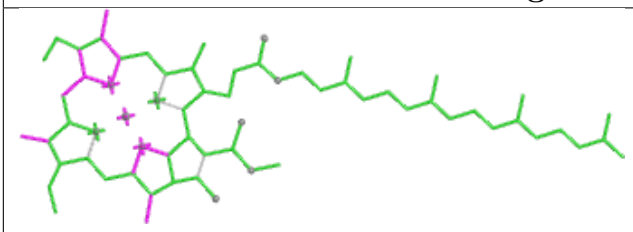


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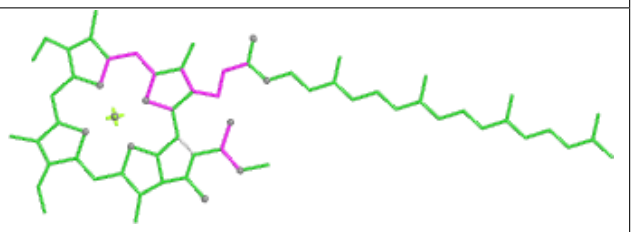


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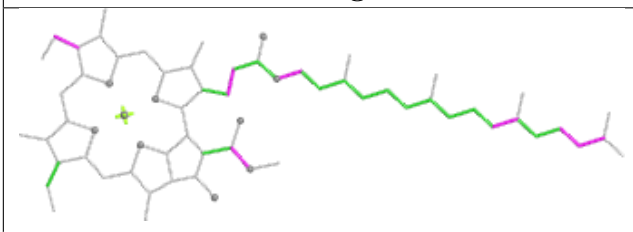
Ligand CLA b 611



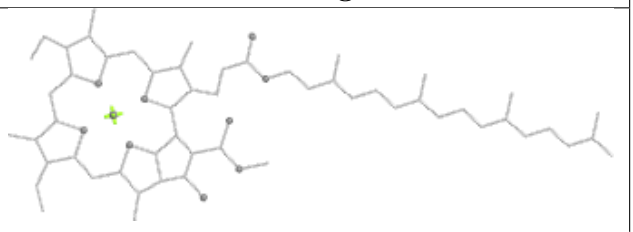
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Bond angles

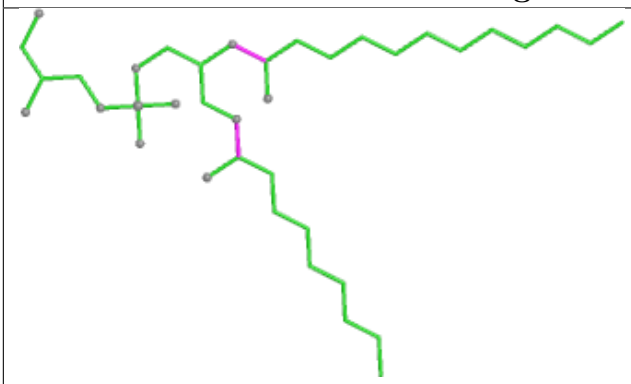


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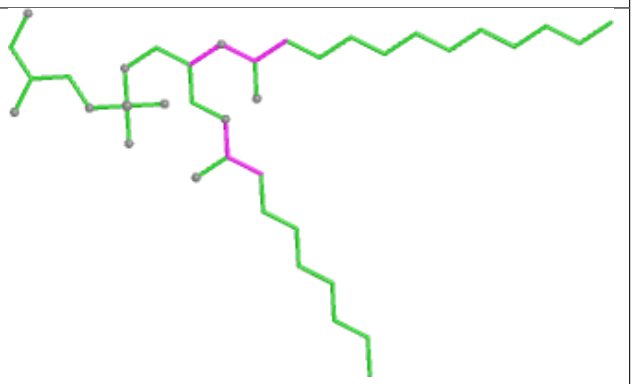


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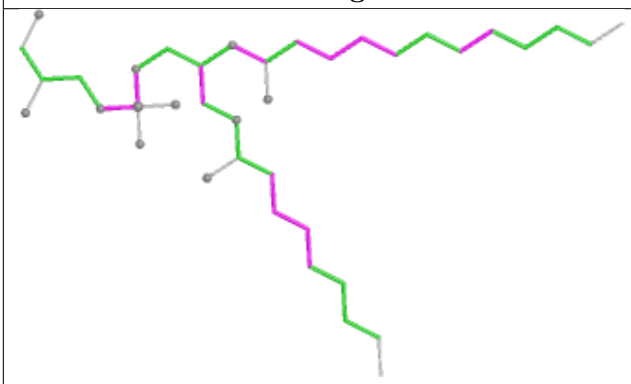
Ligand LHG R 2630



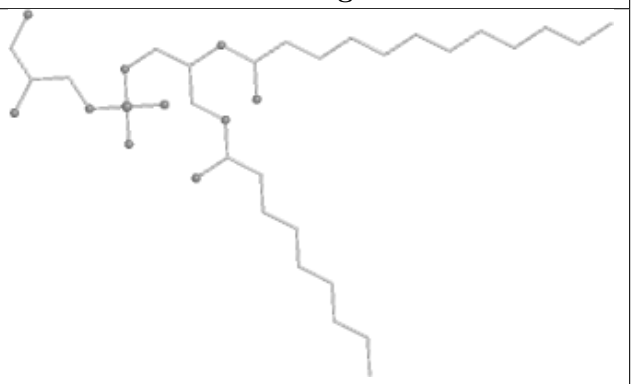
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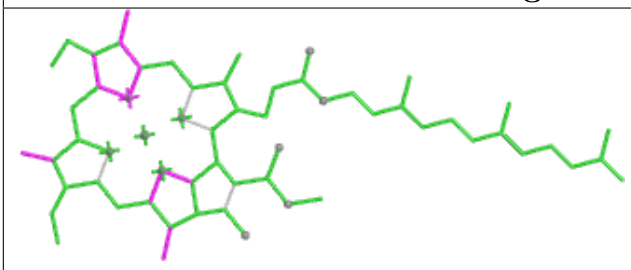


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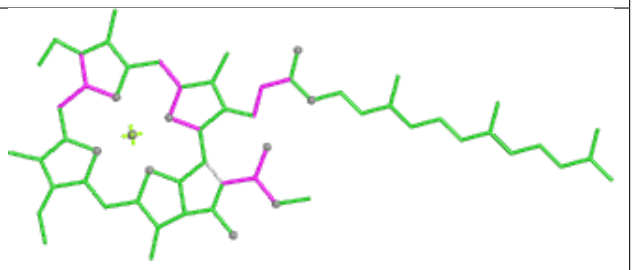


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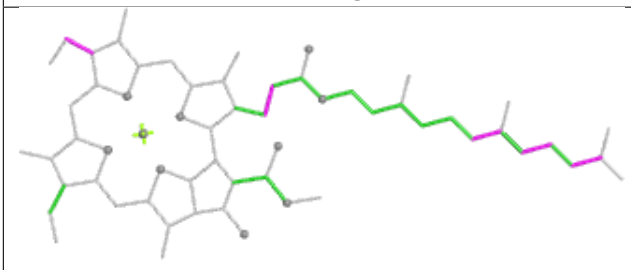
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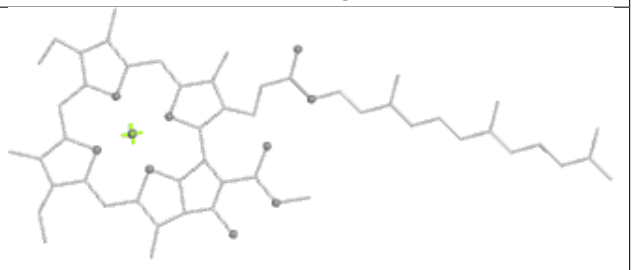
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Bond angles

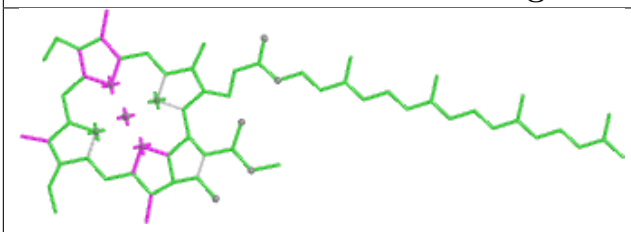


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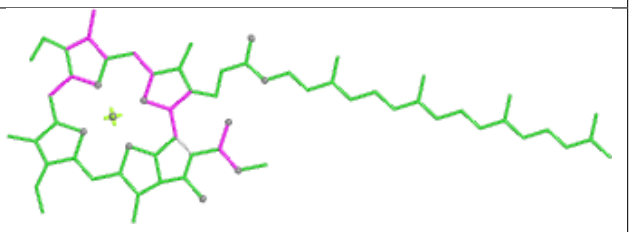


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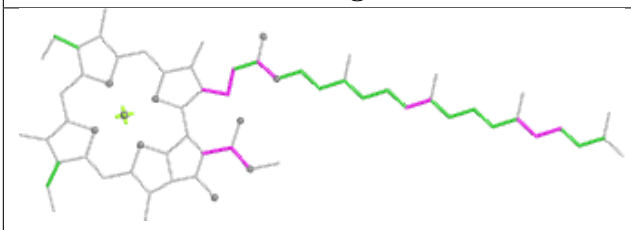
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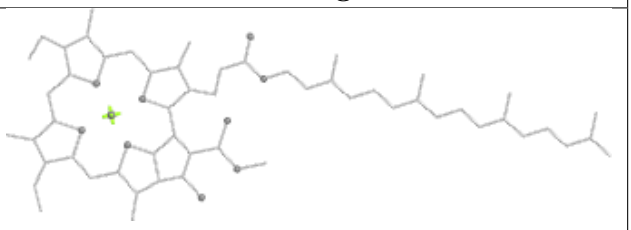
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Bond angles

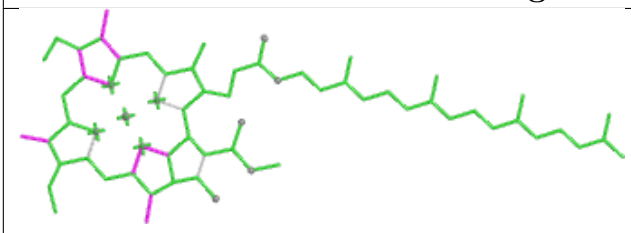


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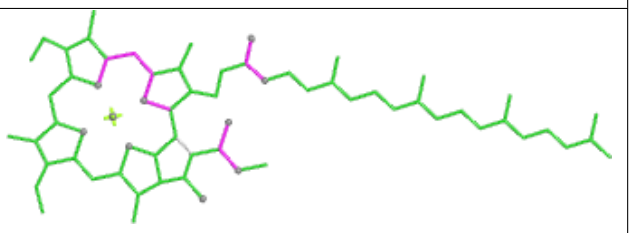


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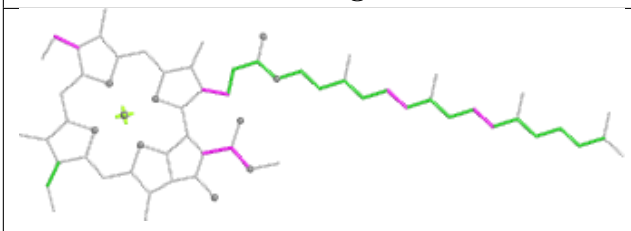
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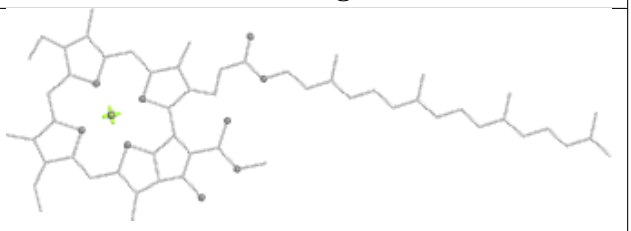
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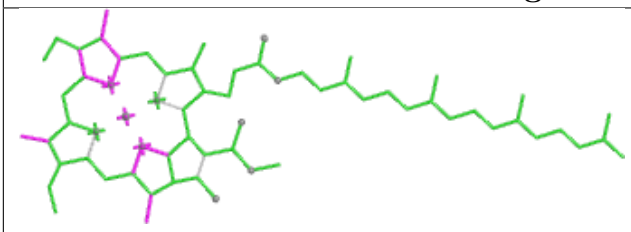


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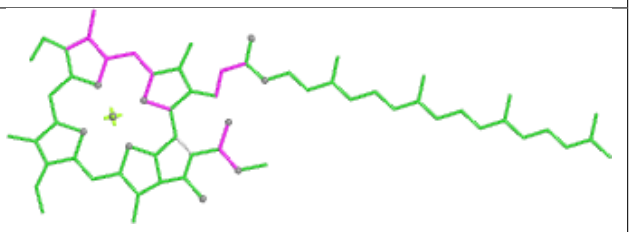


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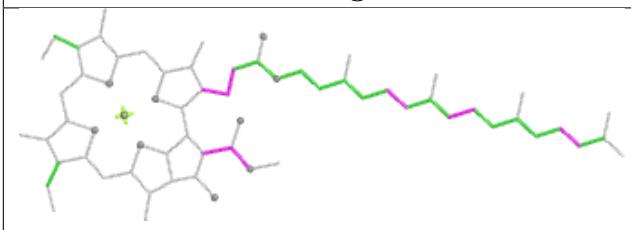
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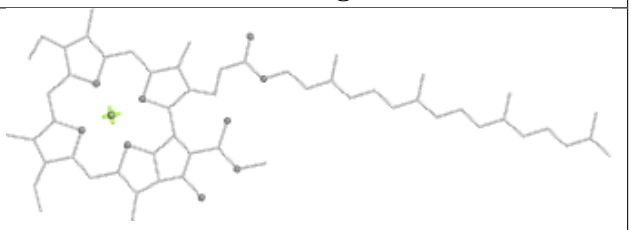
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Bond angles

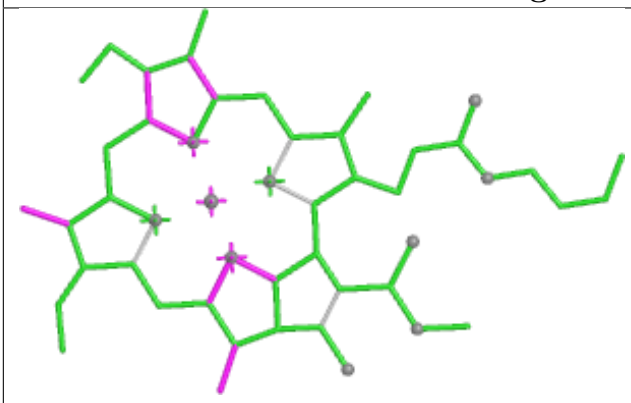


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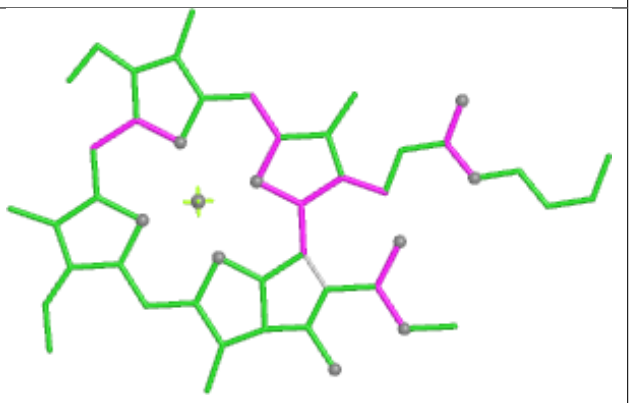


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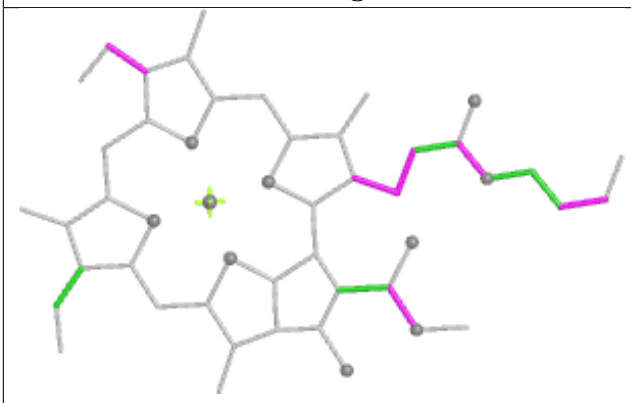
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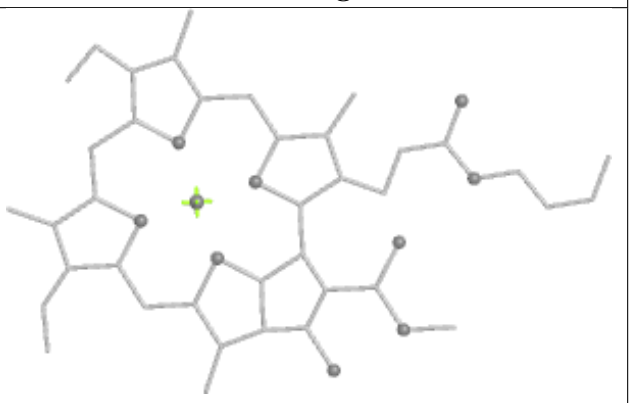
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Bond angles

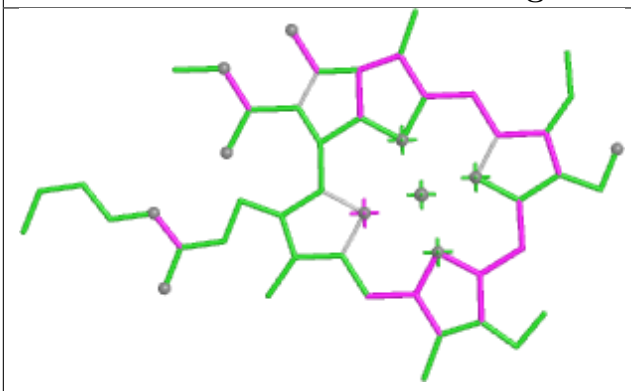


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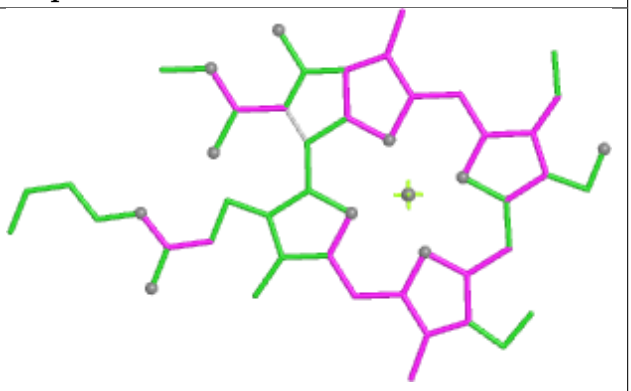


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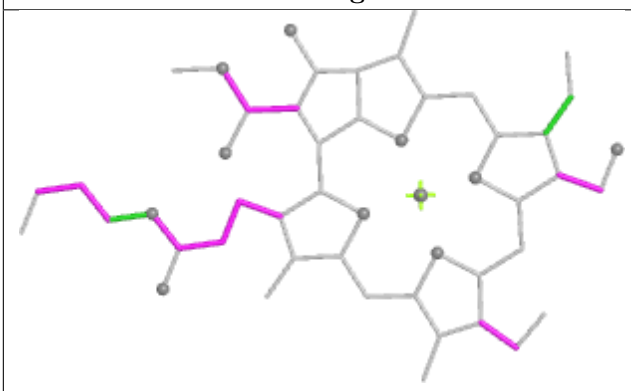
Ligand CHL p 608



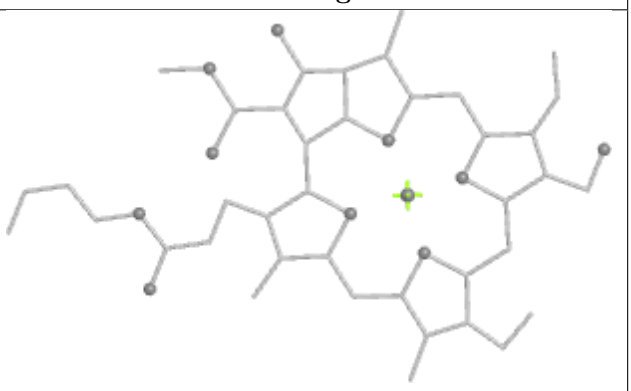
Bond lengths



Bond angles

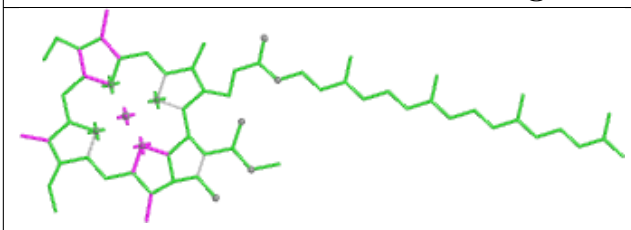


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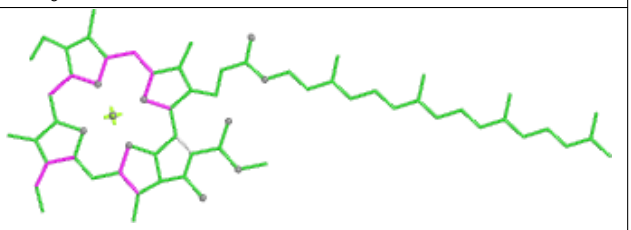


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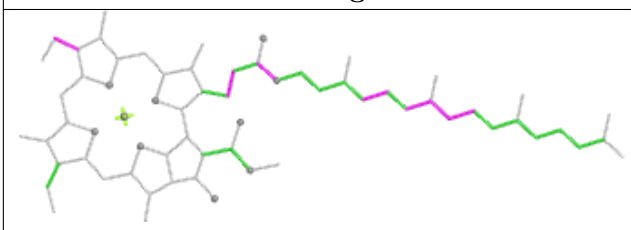
Ligand CLA y 613



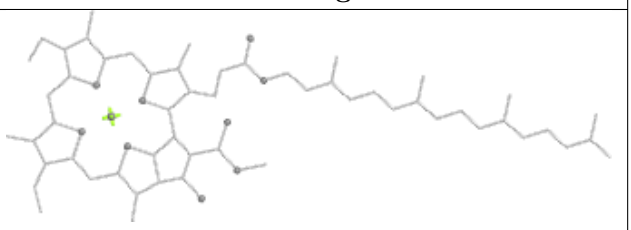
Bond lengths



Bond angles

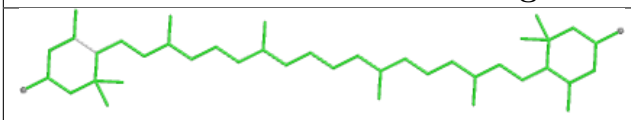


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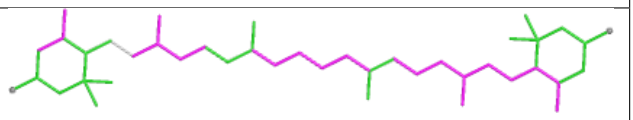


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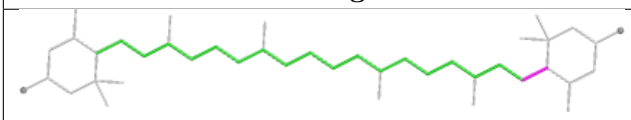
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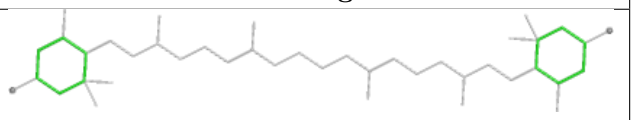
Bond lengths



Bond angles

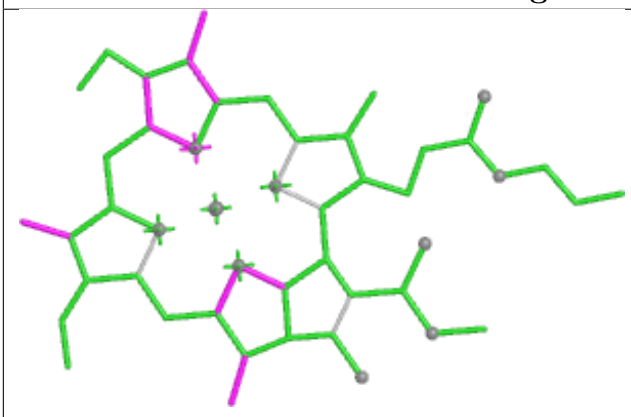


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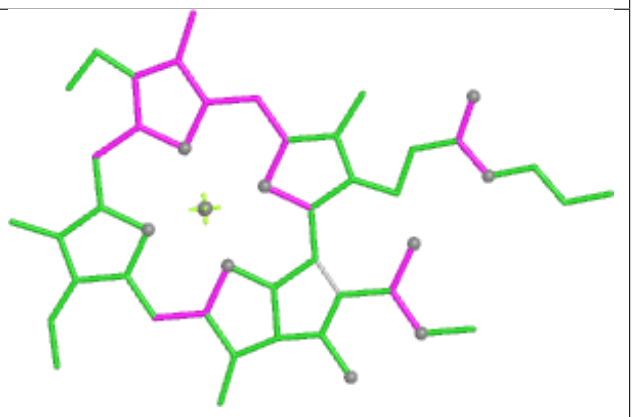


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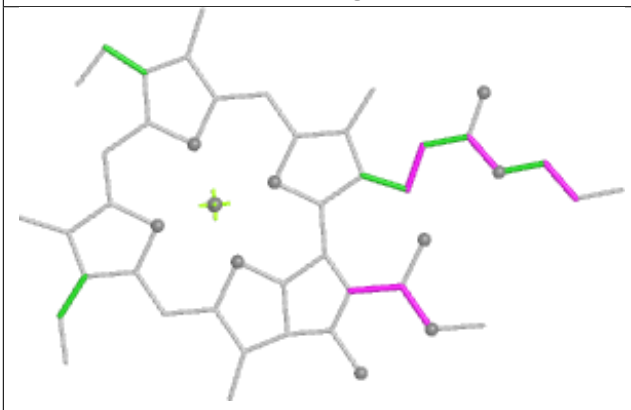
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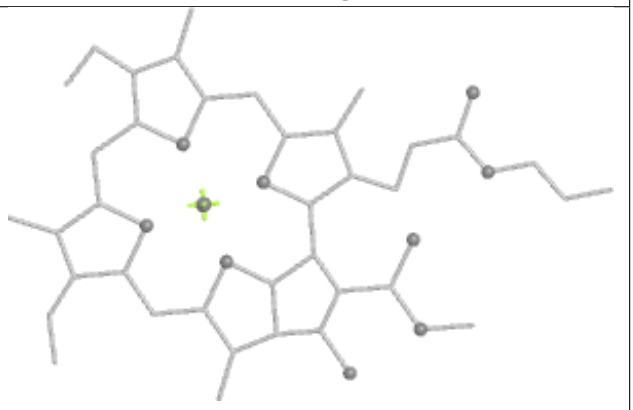
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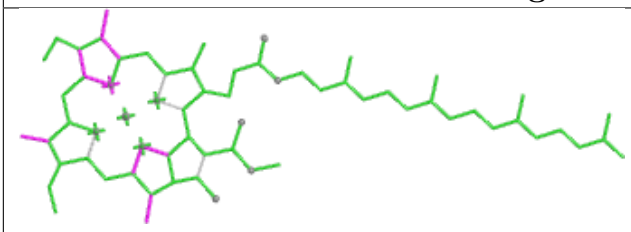


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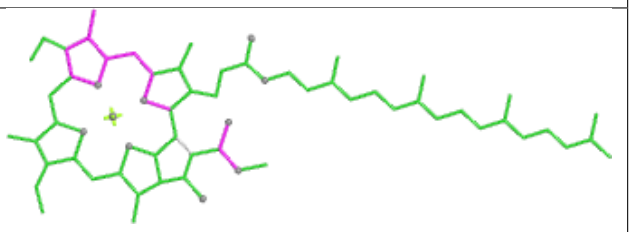


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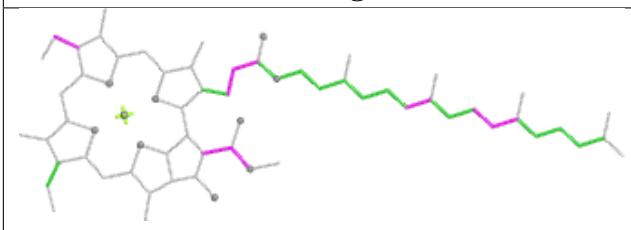
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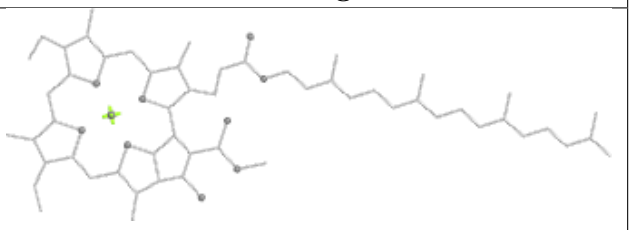
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Bond angles



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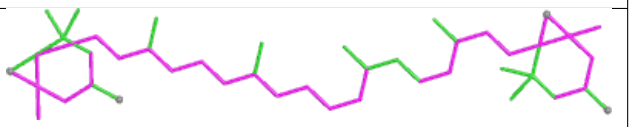


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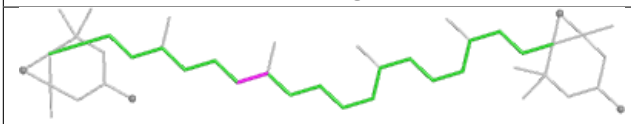
Ligand XAT 2 1622



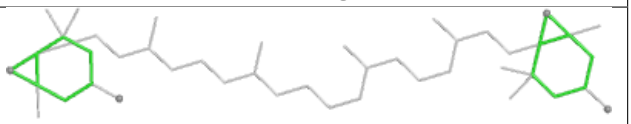
Bond lengths



Bond angles

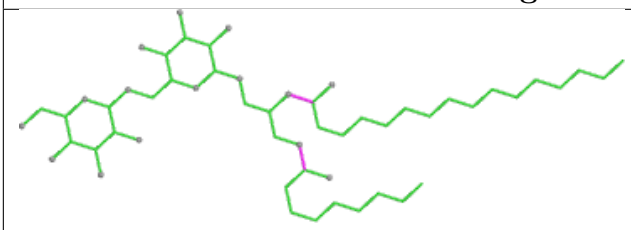


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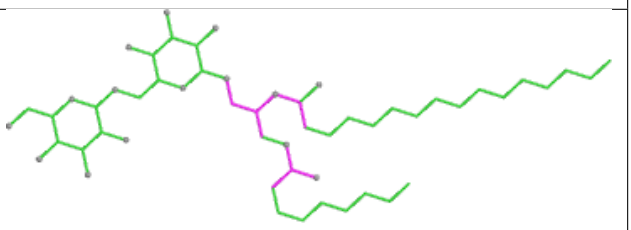


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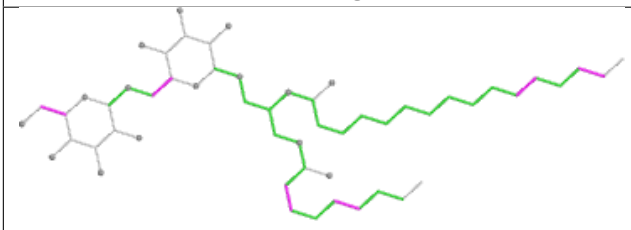
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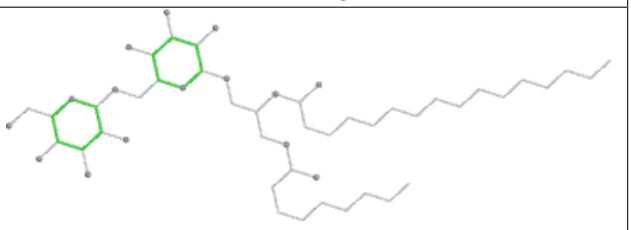
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Bond angles

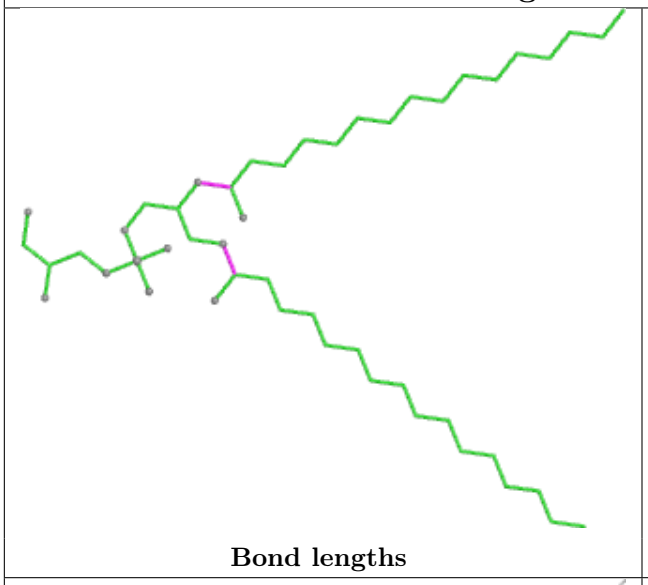


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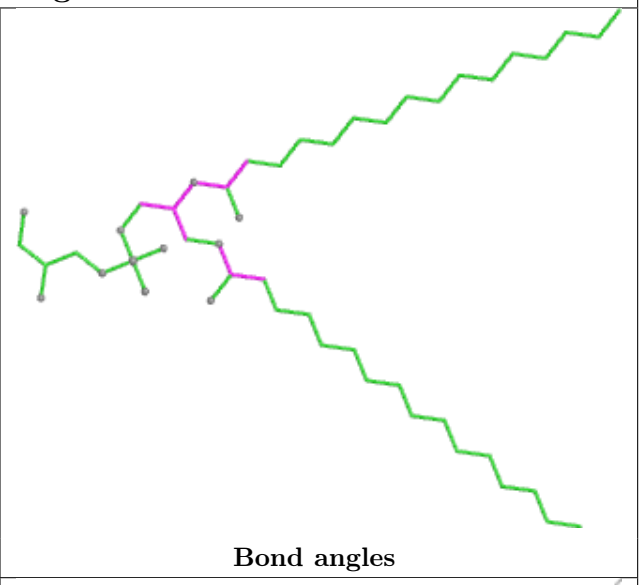


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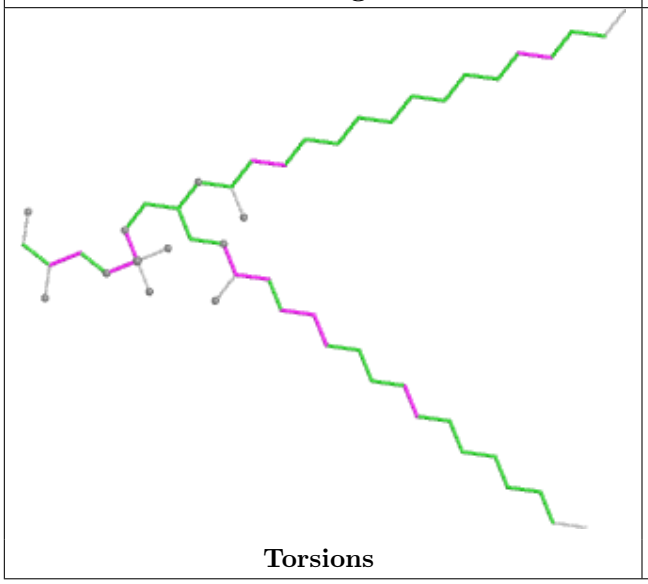
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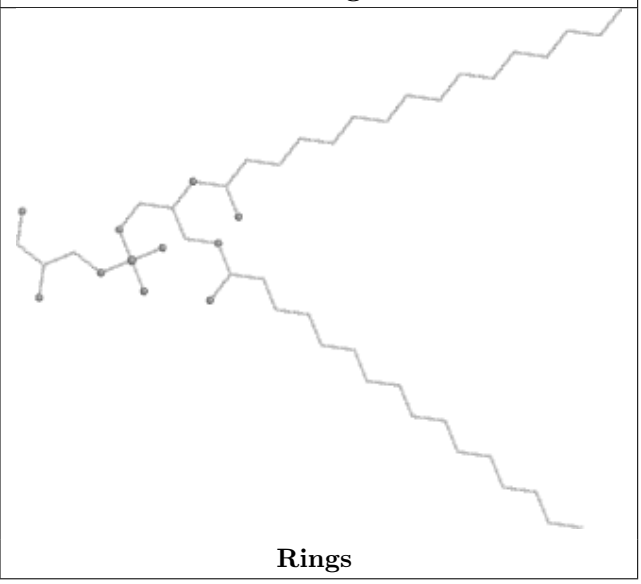
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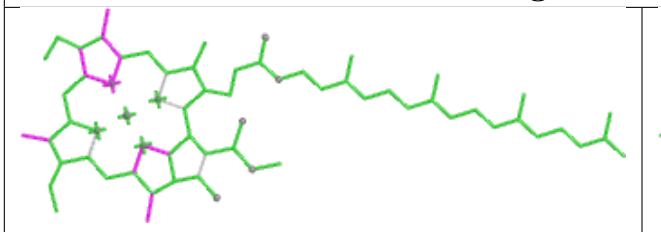


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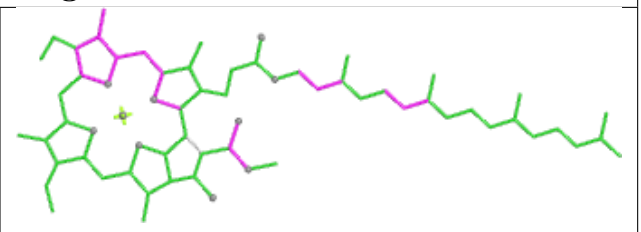


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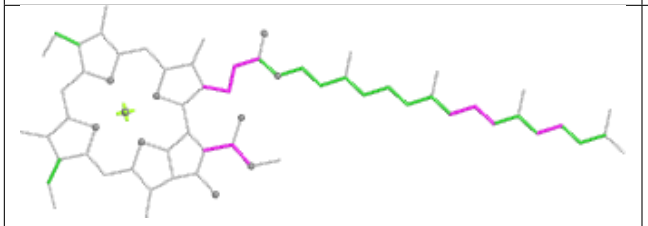
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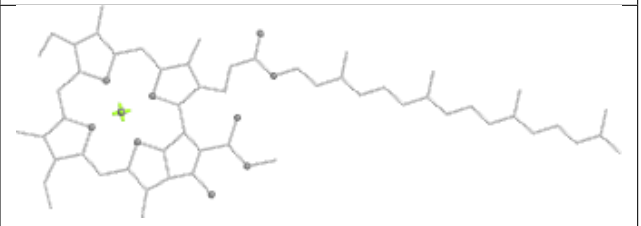
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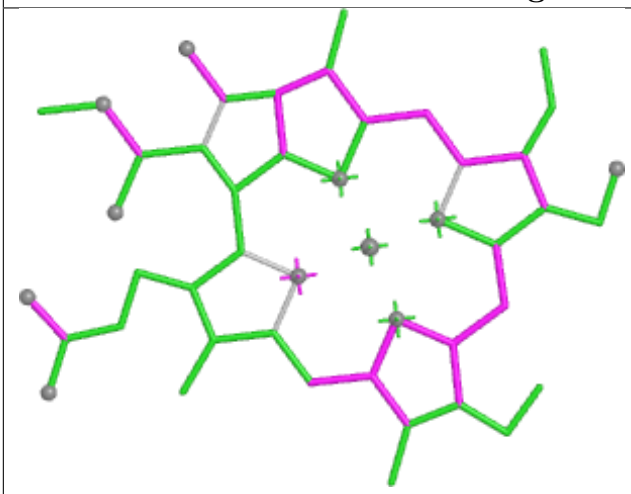


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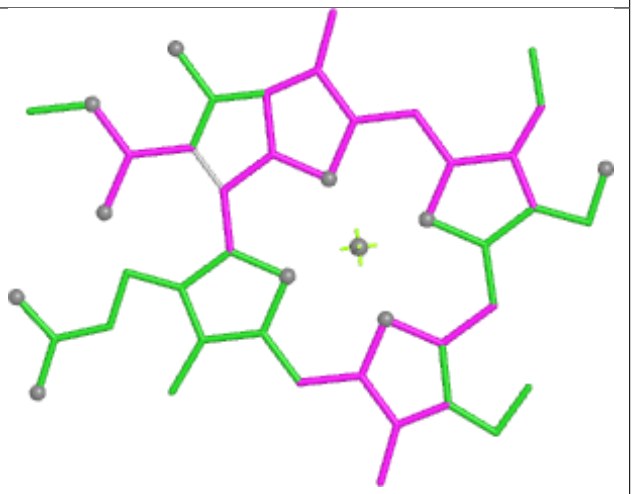


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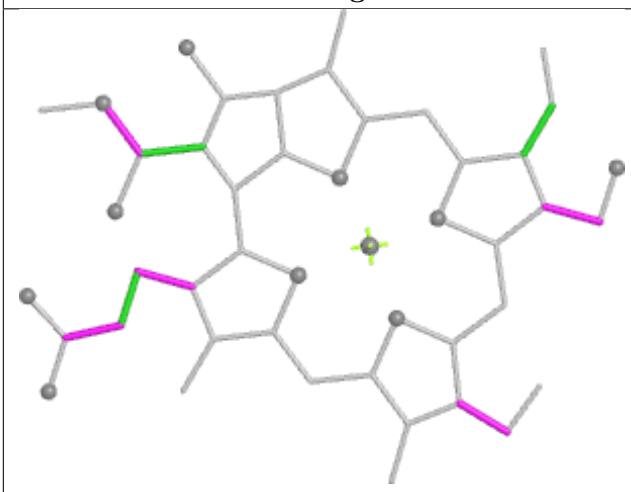
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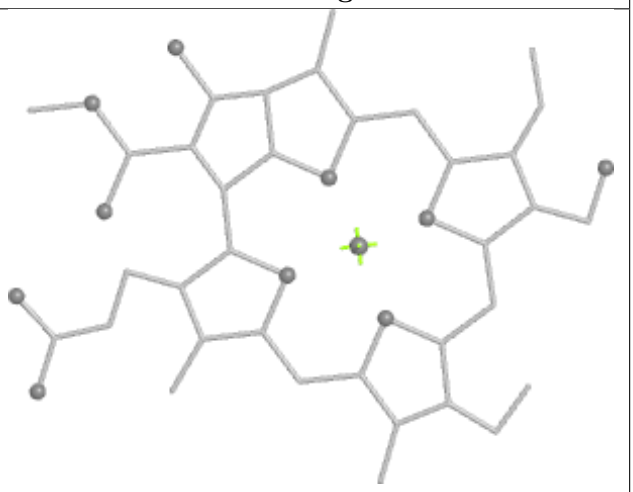
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Bond angles

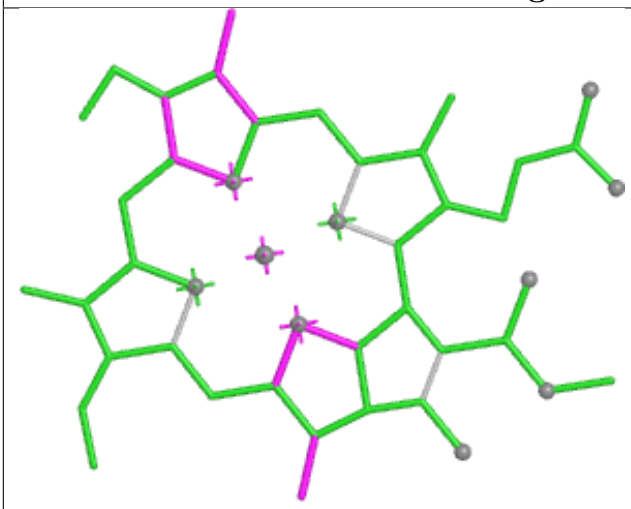


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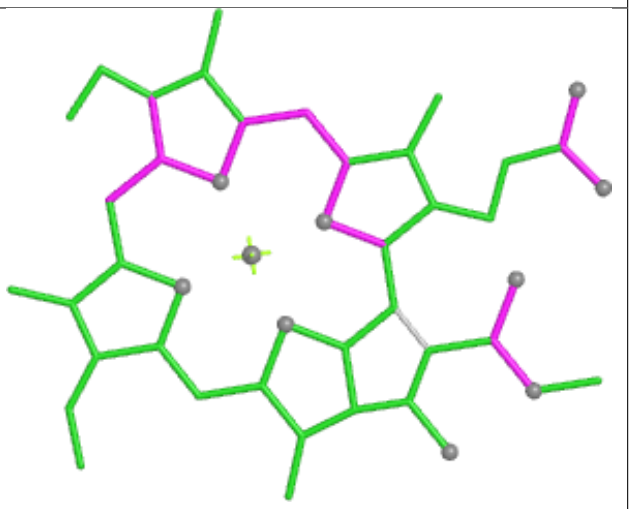


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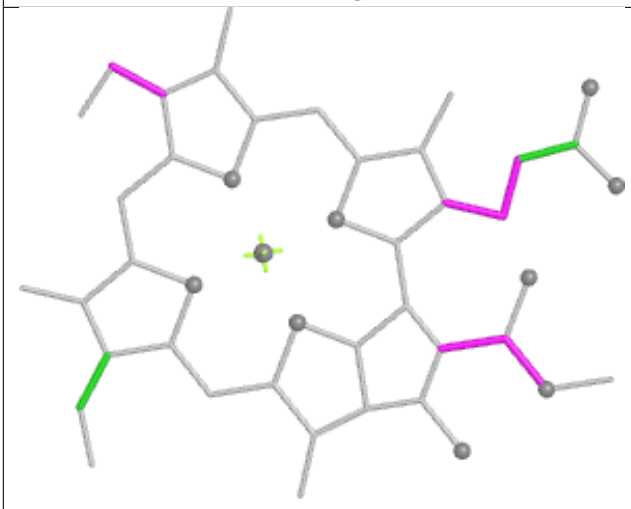
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Bond lengths



Bond angles

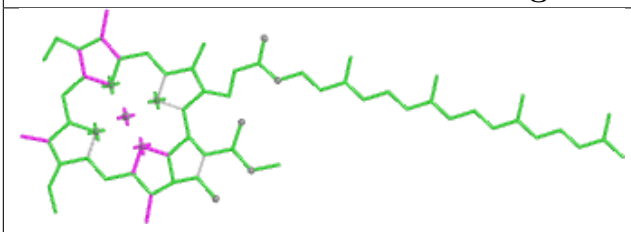


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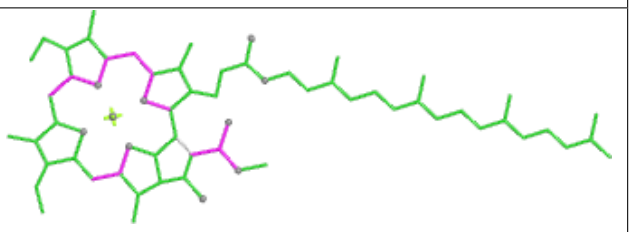


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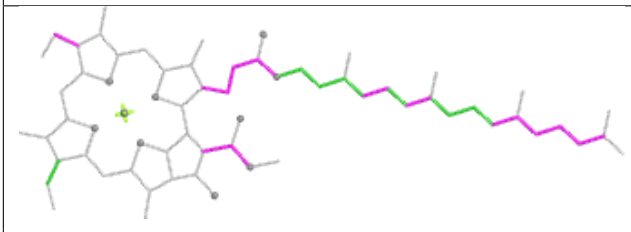
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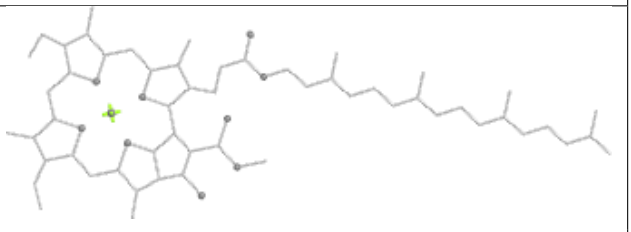
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Bond angles

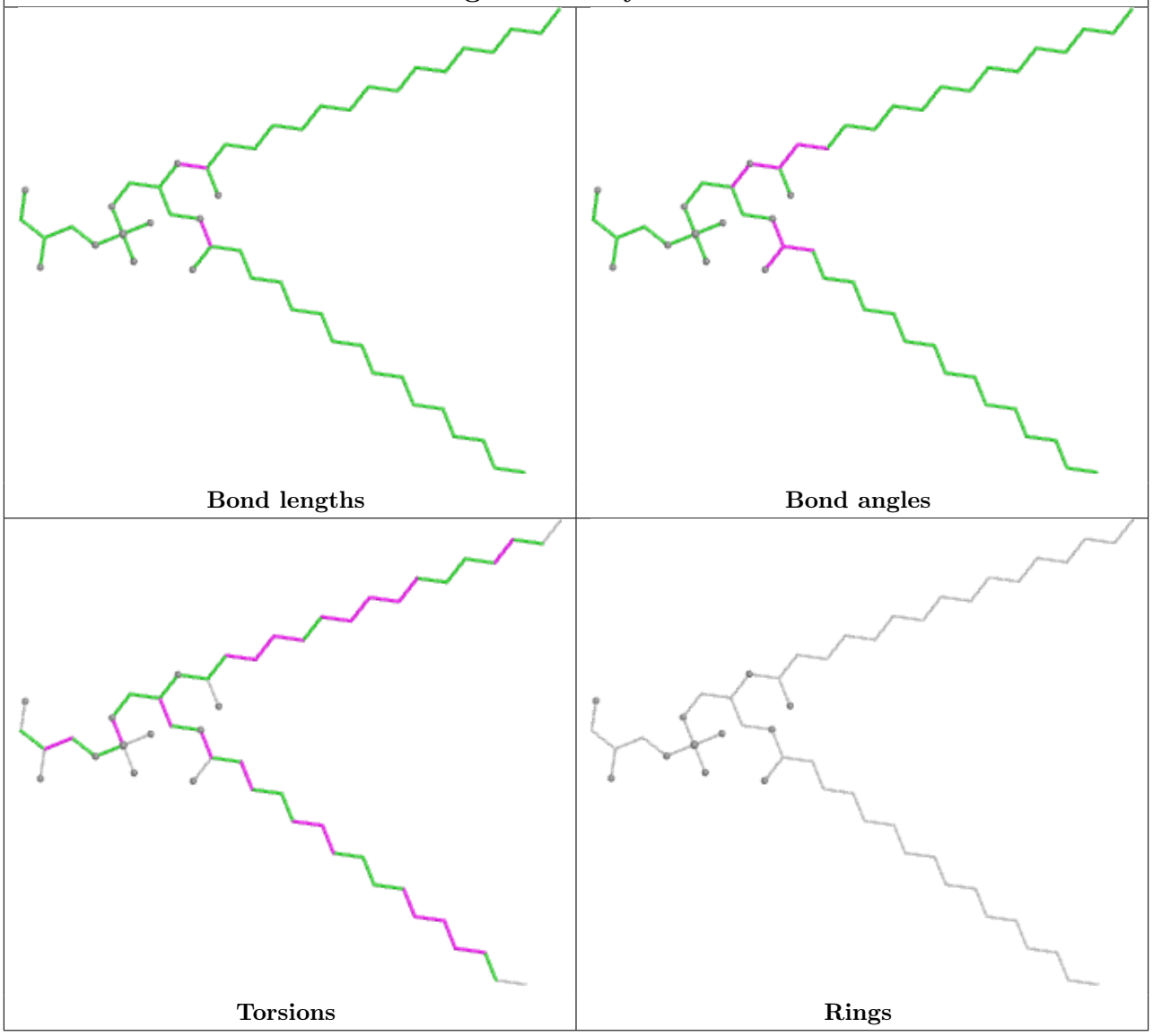


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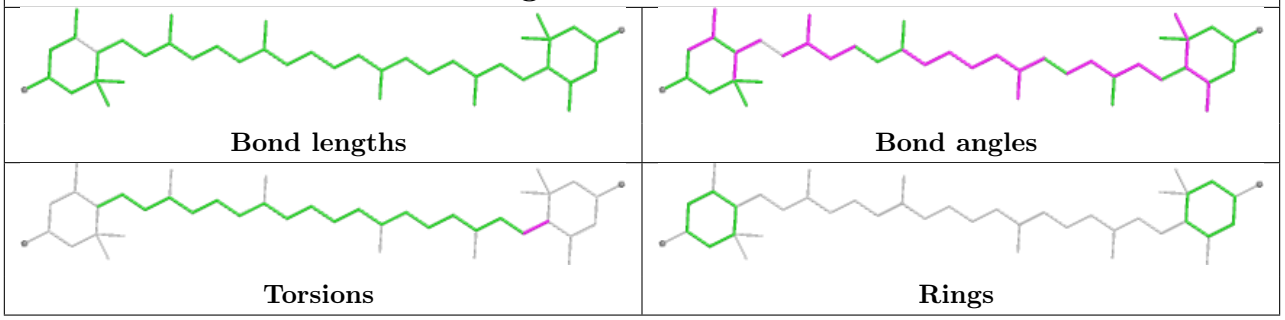


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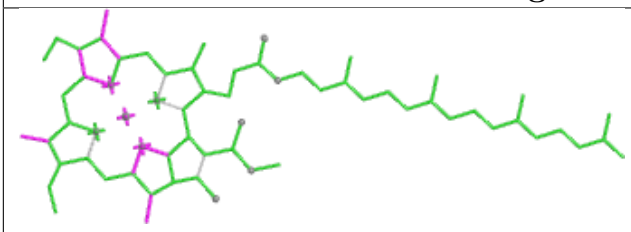
Ligand LHG y 2630



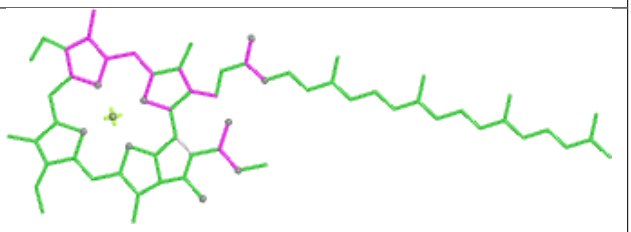
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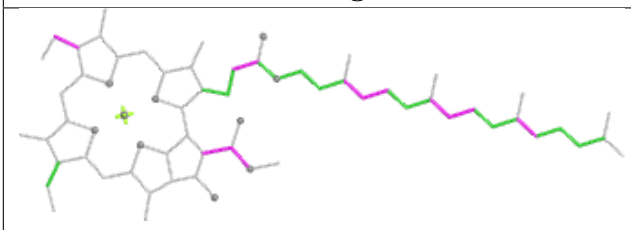
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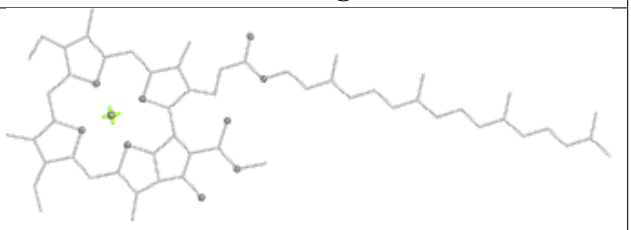
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Bond angles



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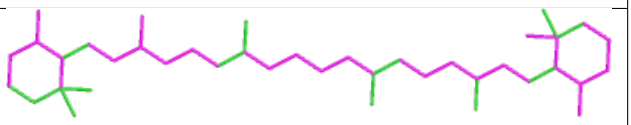


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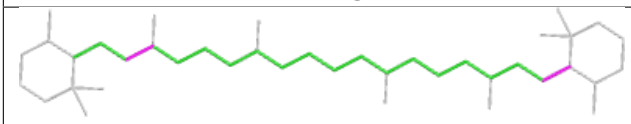
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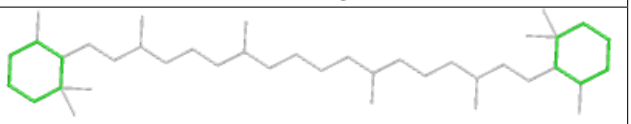
Bond lengths



Bond angles

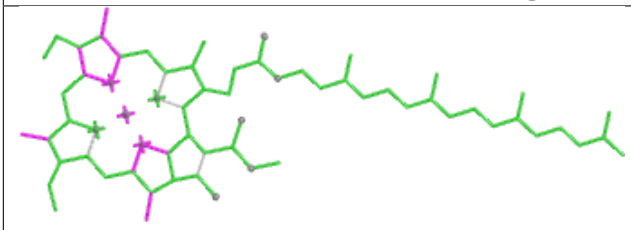


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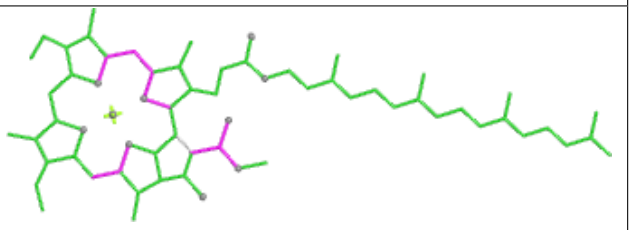


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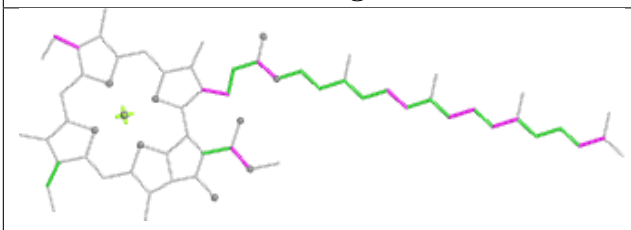
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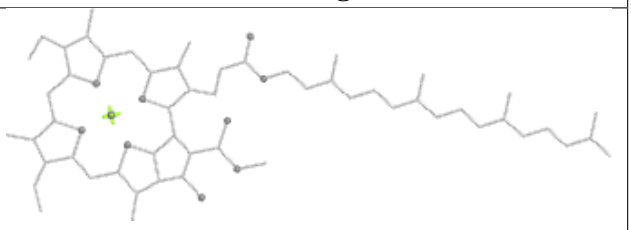
Bond lengths



Bond angles

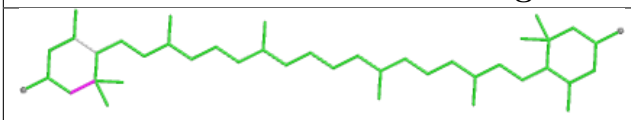


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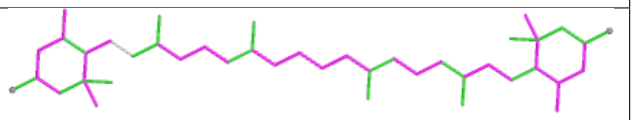


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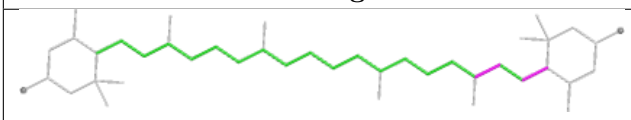
Ligand LUT Y 1621



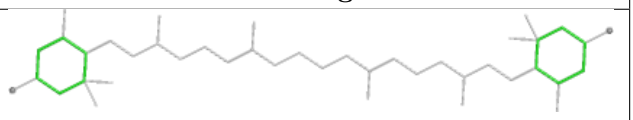
Bond lengths



Bond angles

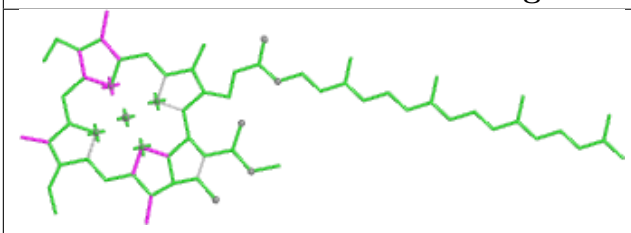


Torsions

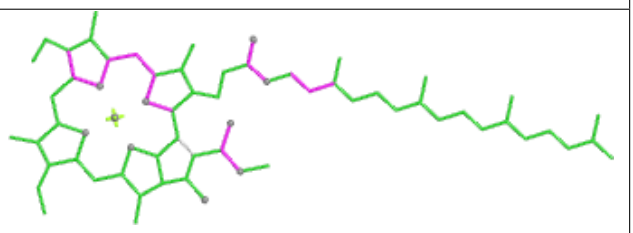


Rings

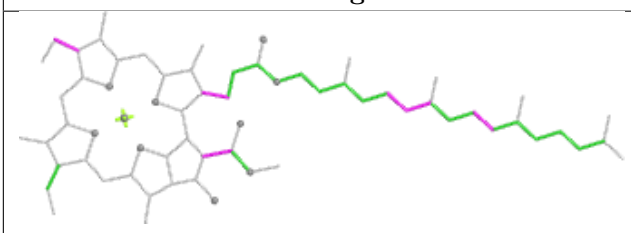
Ligand CLA N 610



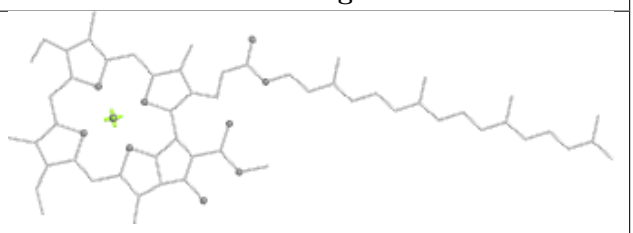
Bond lengths



Bond angles

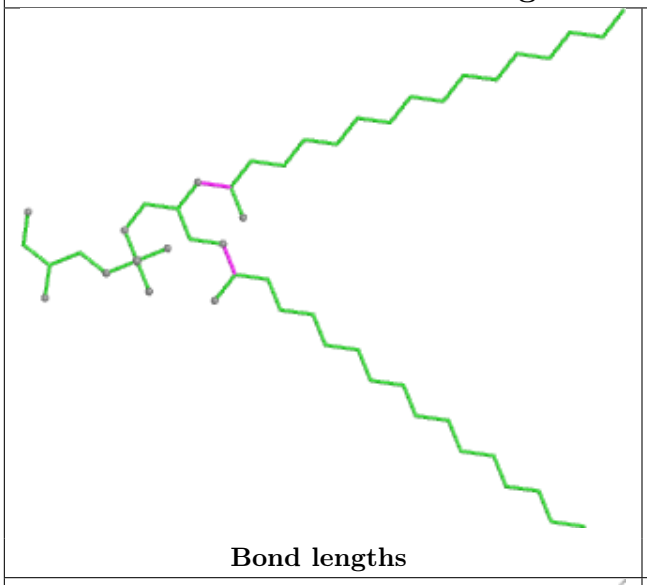


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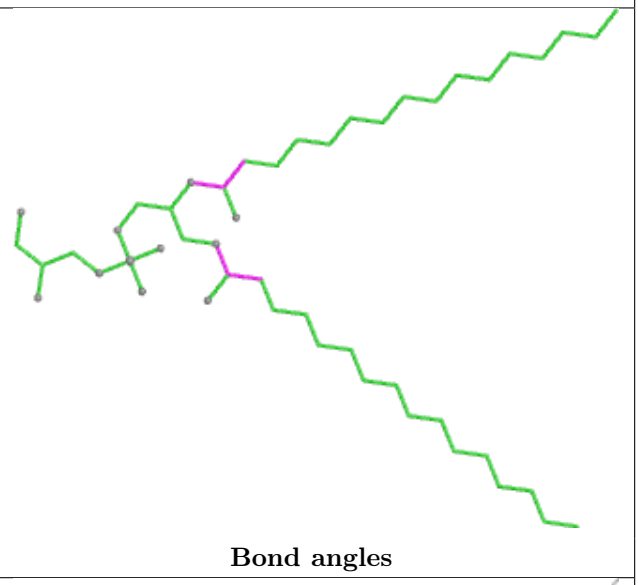


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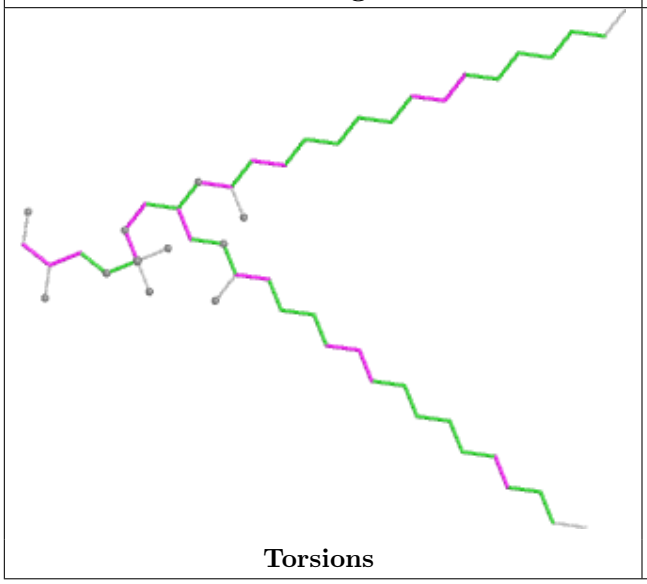
Ligand LHG 6 2630



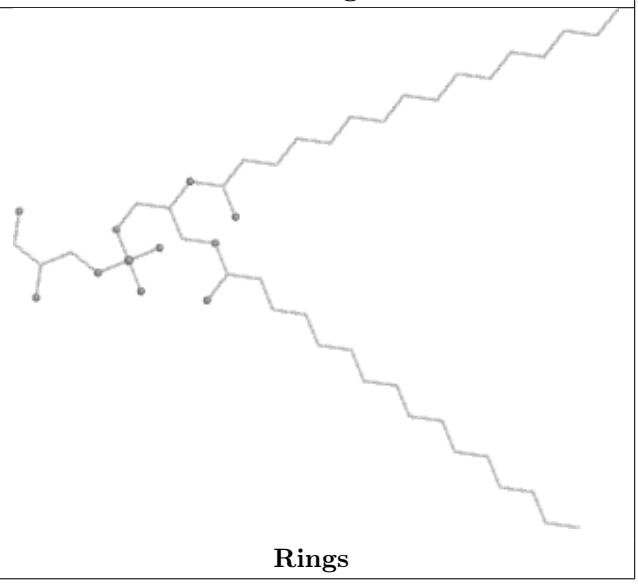
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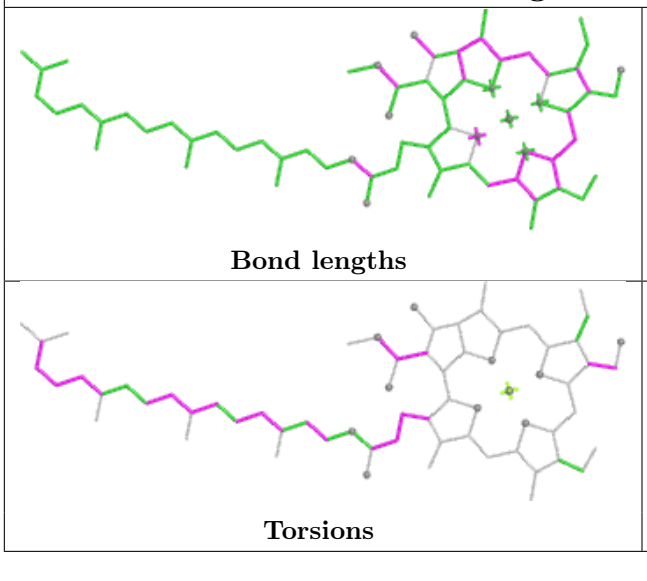


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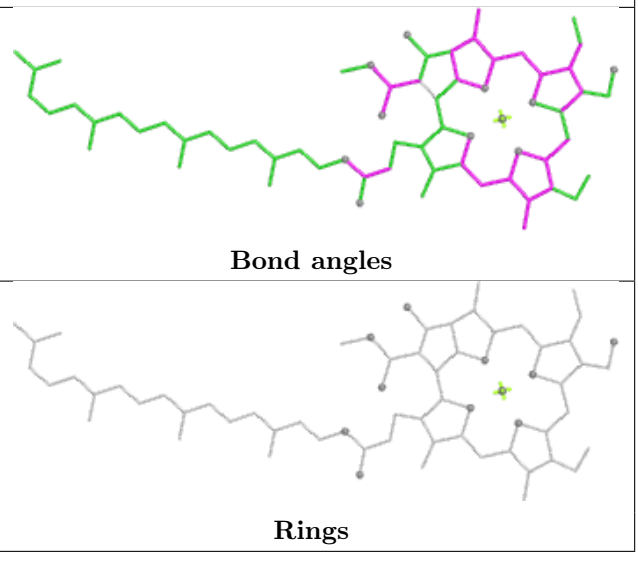


Rings

Ligand CHL 0 607



Bond lengths

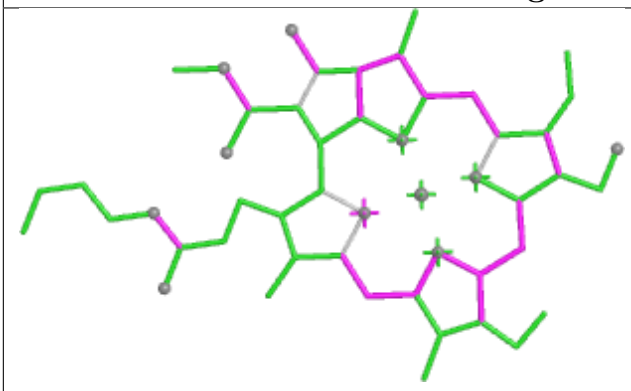


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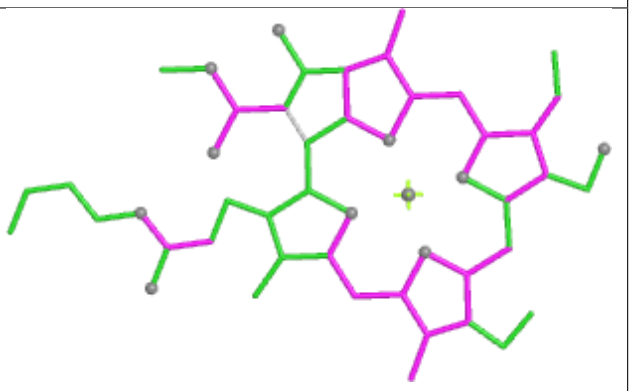
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Rings

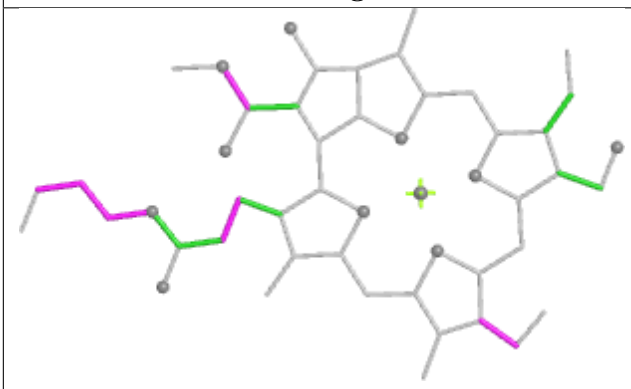
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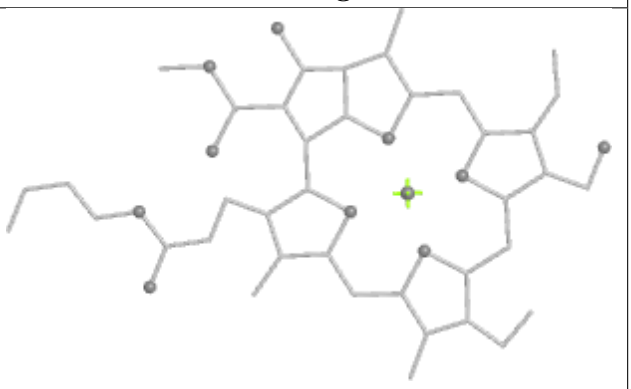
Bond lengths



Bond angles

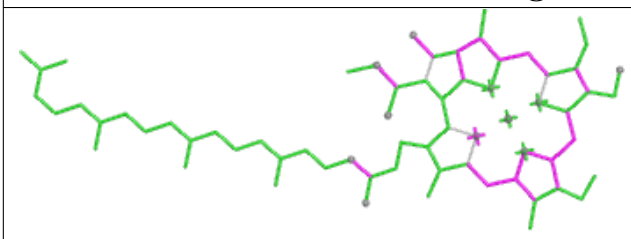


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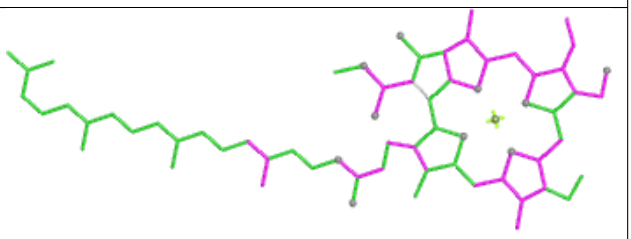


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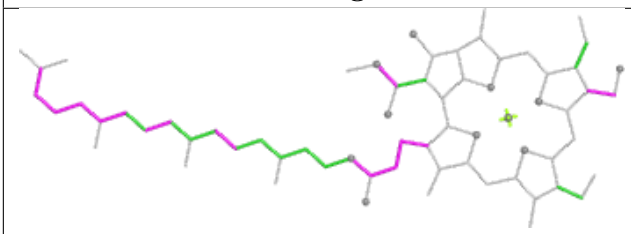
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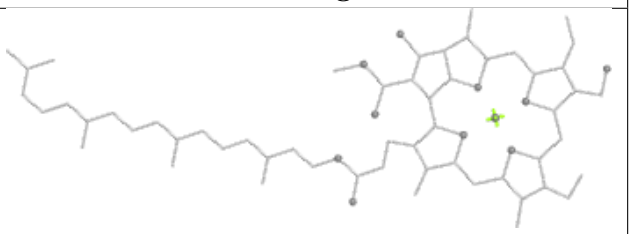
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Bond angles

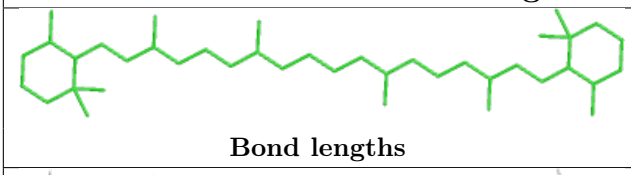


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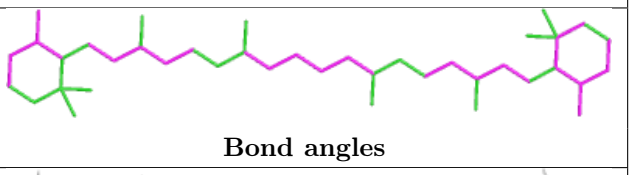


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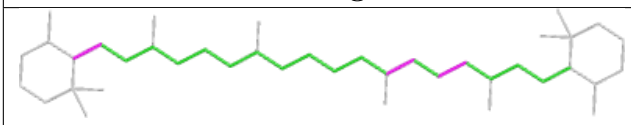
Ligand BCR B 618



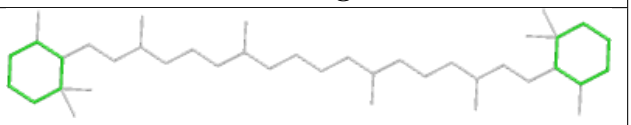
Bond lengths



Bond angles

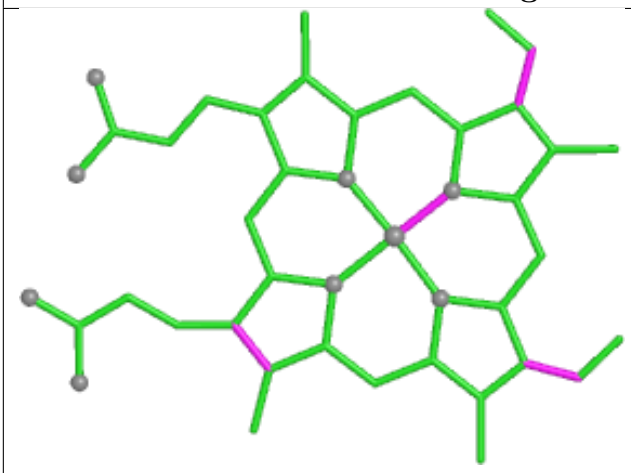


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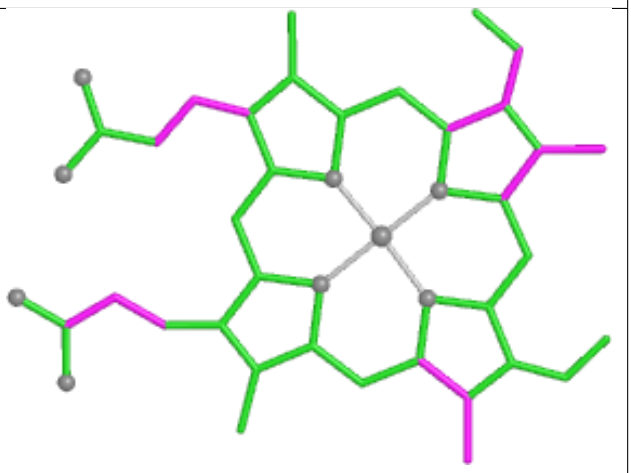


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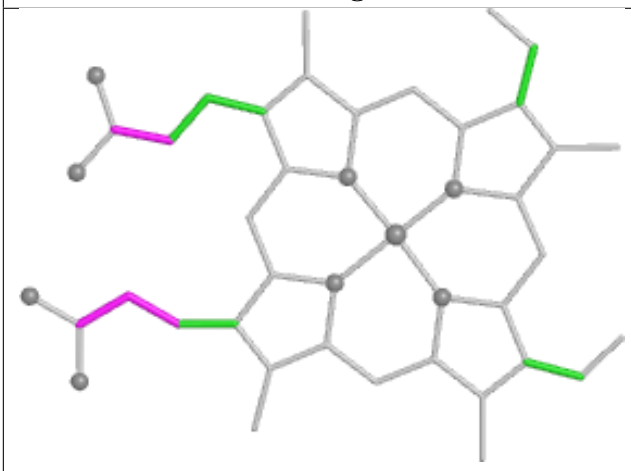
Ligand HEM F 101



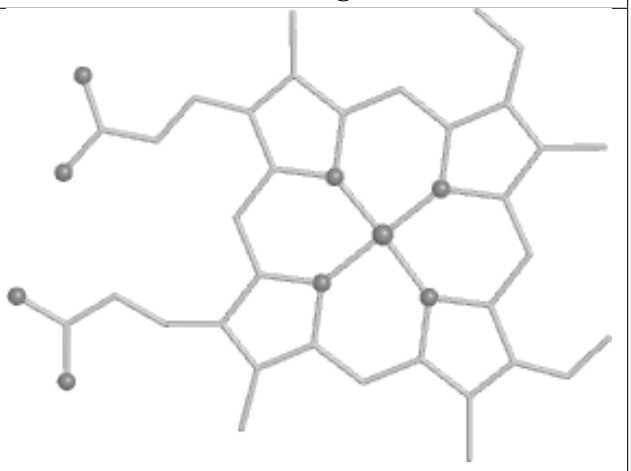
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Bond angles

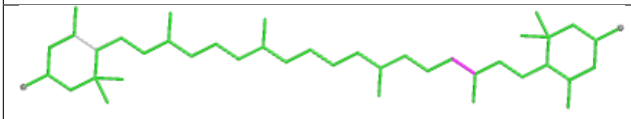


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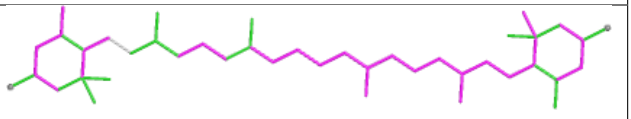


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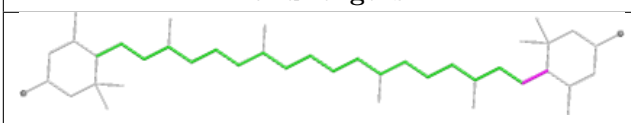
Ligand LUT y 1620



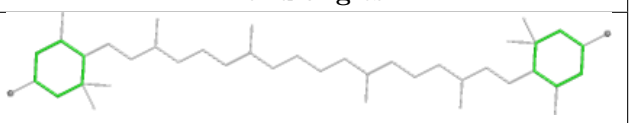
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Bond angles

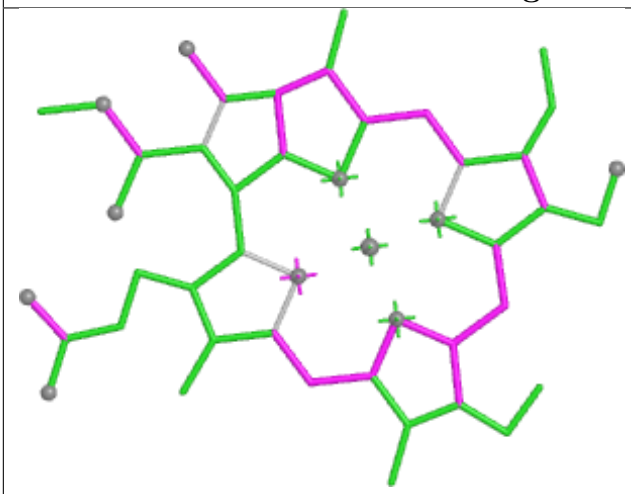


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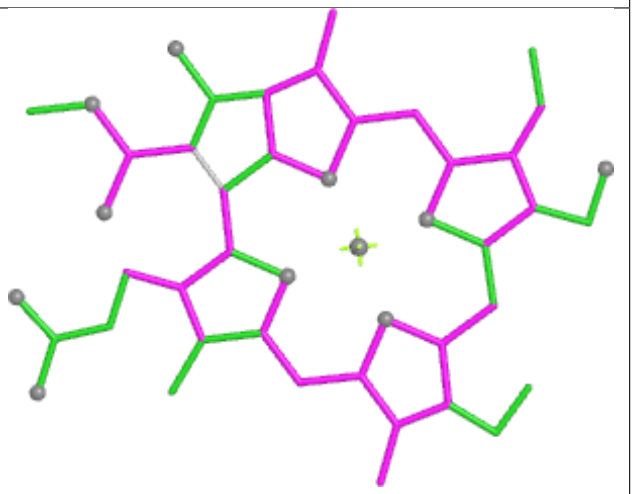


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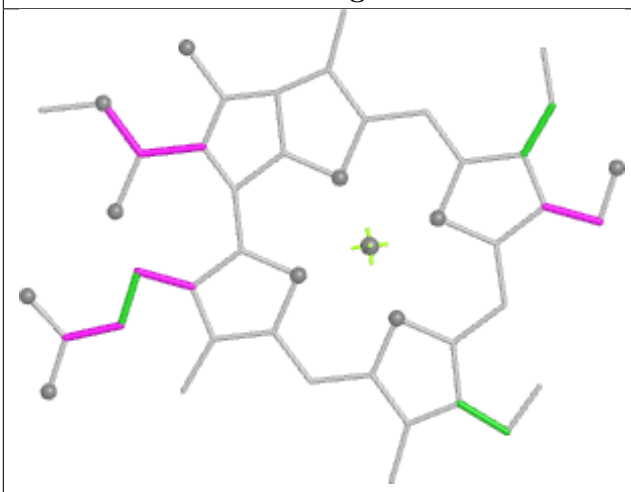
Ligand CHL N 606



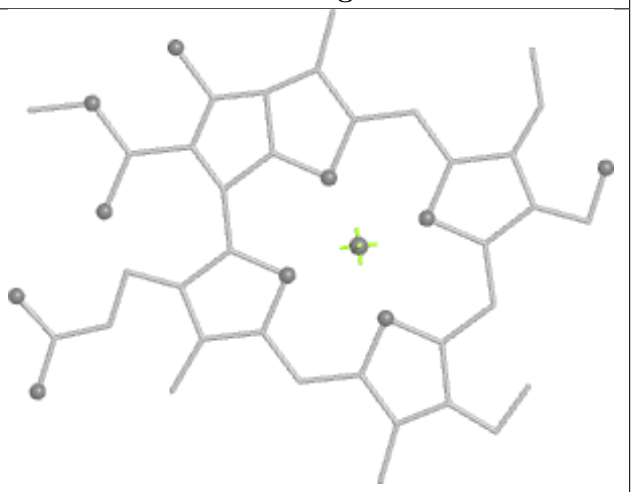
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Bond angles

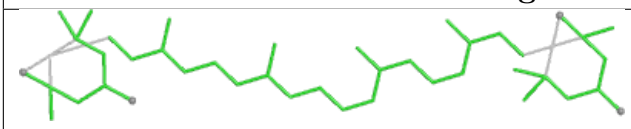


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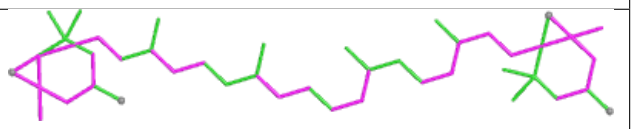


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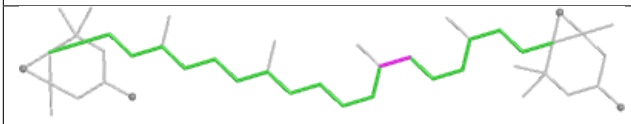
Ligand XAT 4 1622



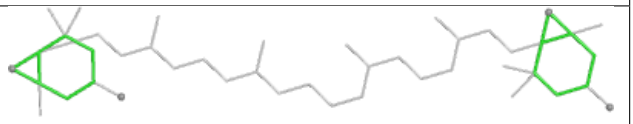
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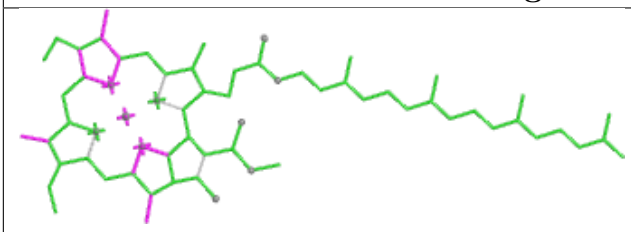


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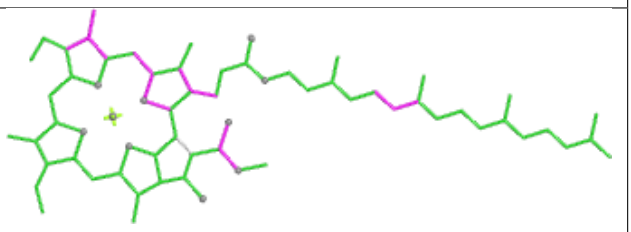


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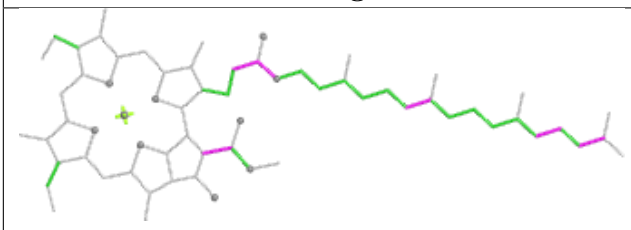
Ligand CLA C 510



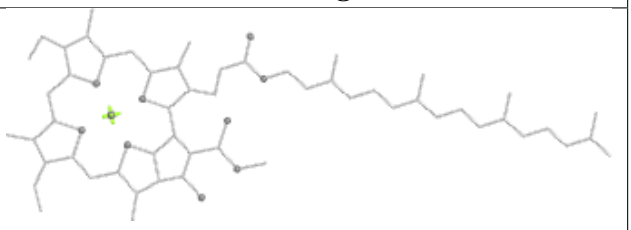
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Bond angles

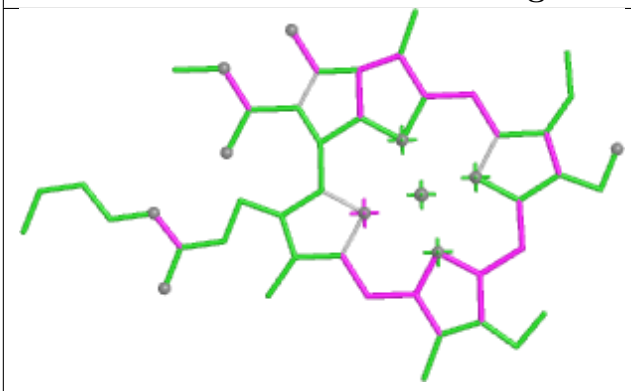


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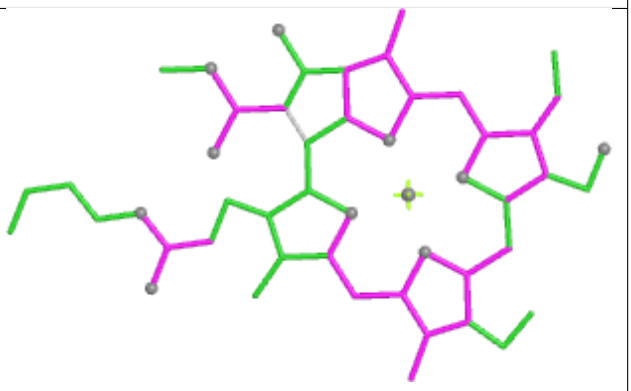


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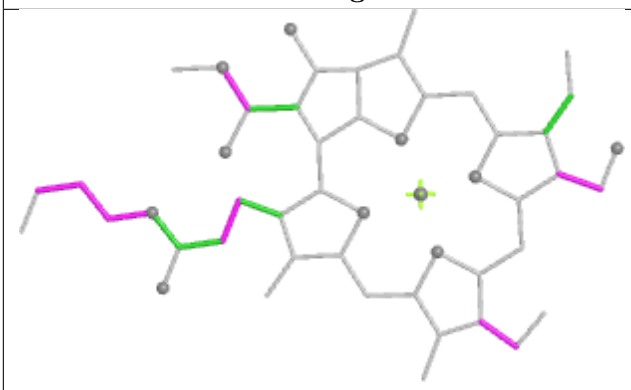
Ligand CHL 6 608



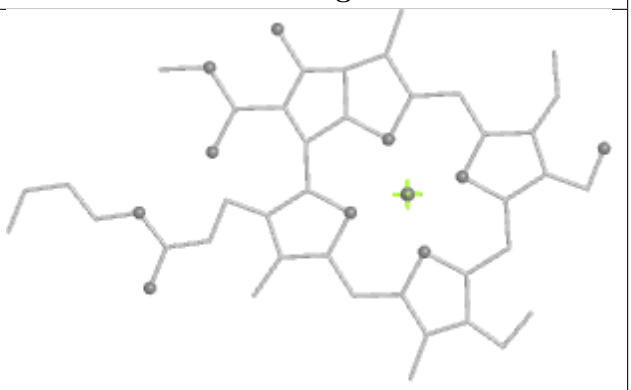
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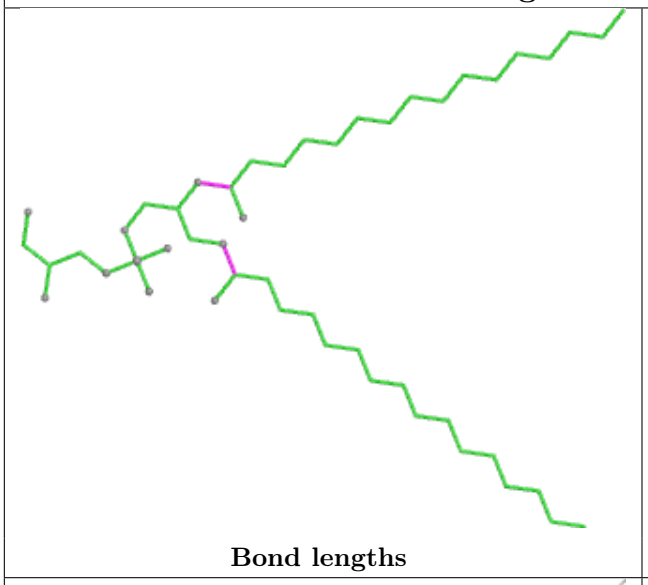


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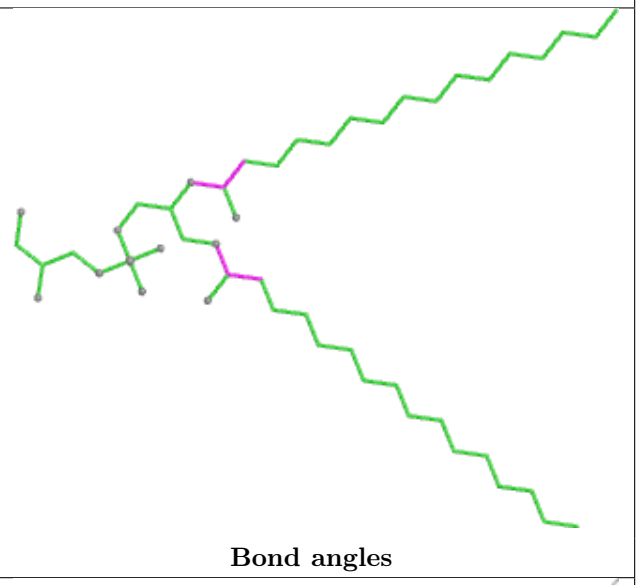


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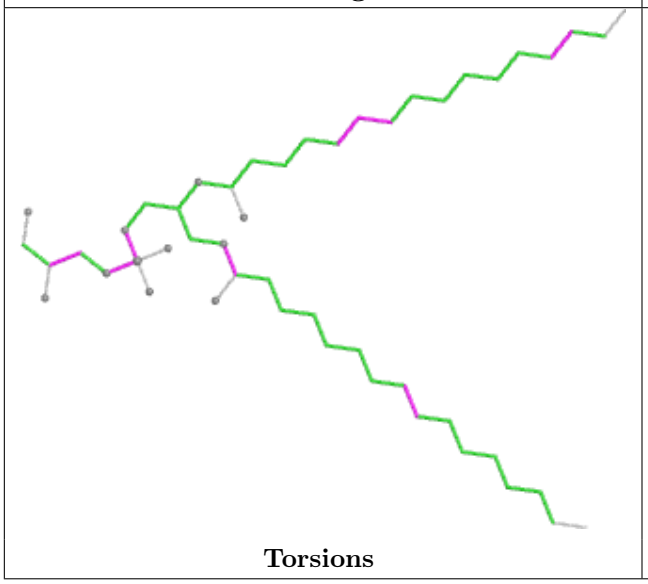
Ligand LHG 3 2630



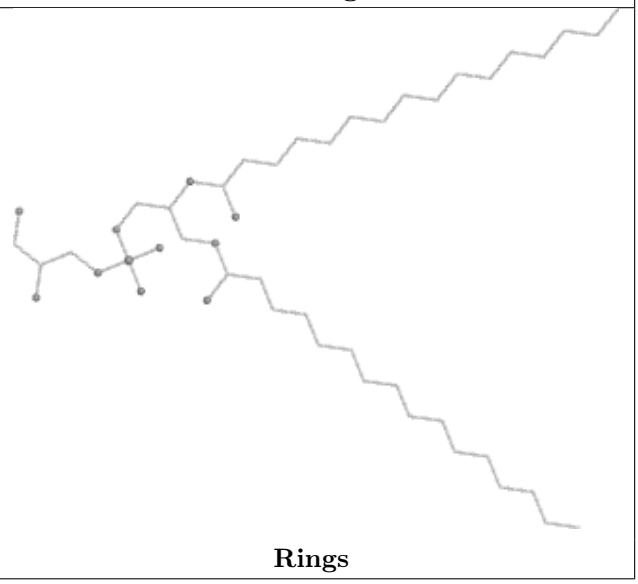
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Bond angles

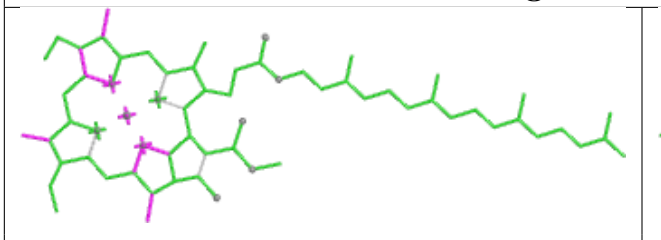


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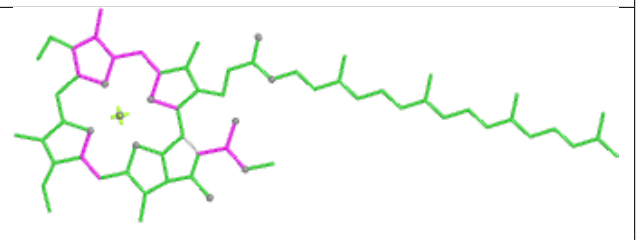


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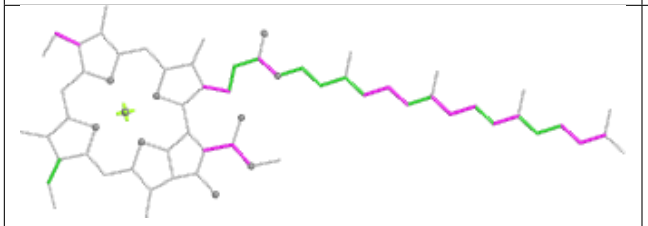
Ligand CLA C 508



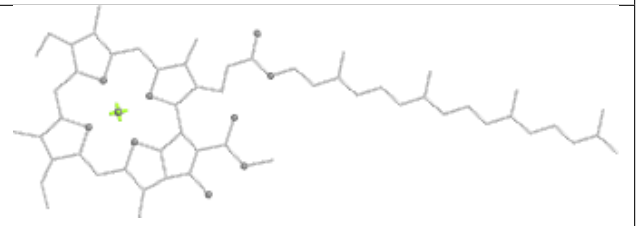
Bond lengths



Bond angles

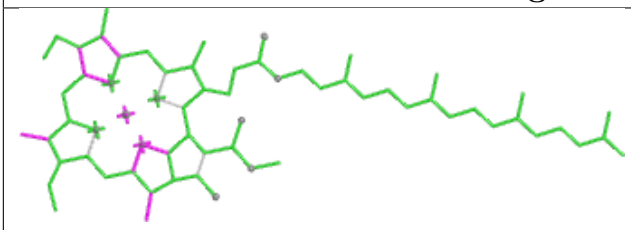


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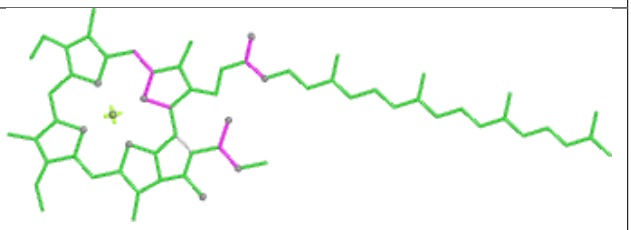


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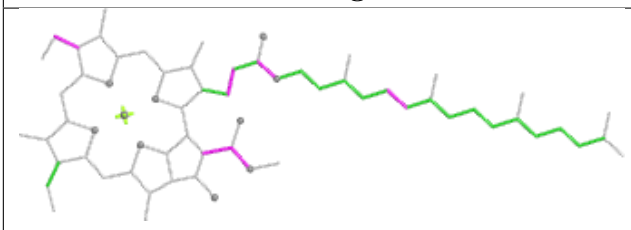
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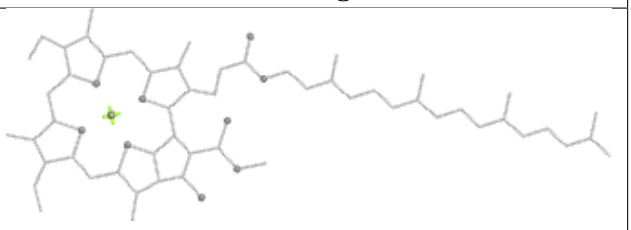
Bond lengths



Bond angles

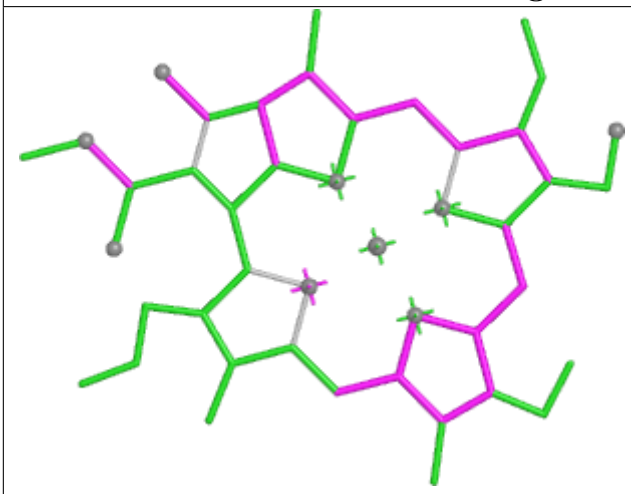


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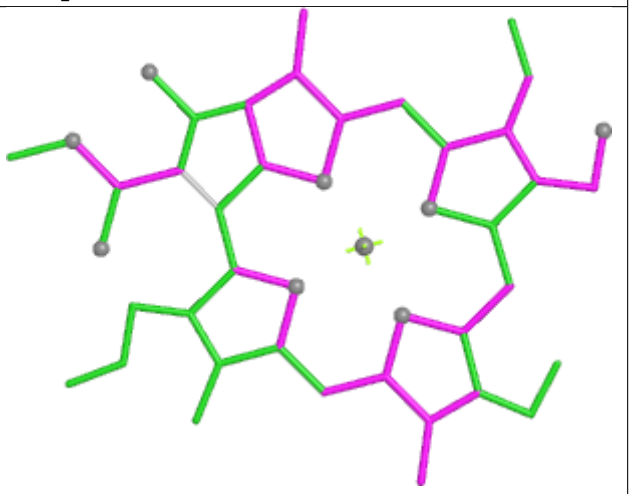


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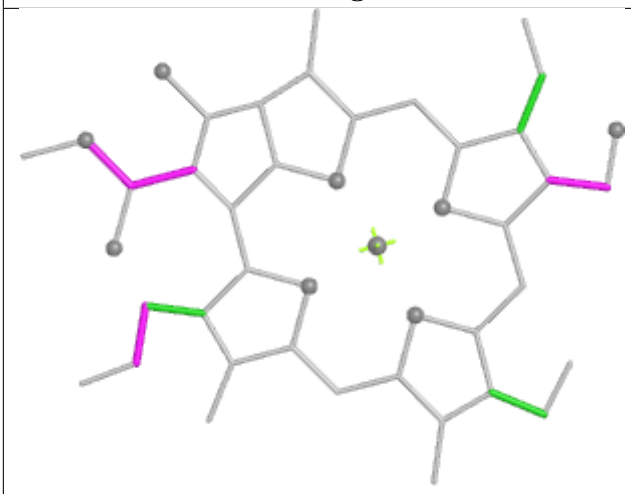
Ligand CHL q 608



Bond lengths



Bond angles

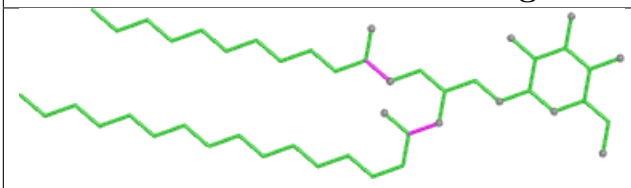


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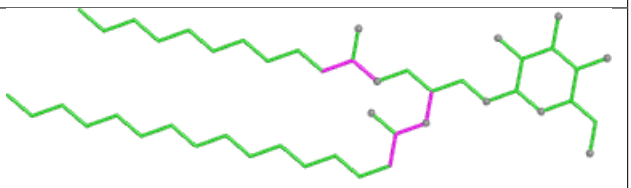


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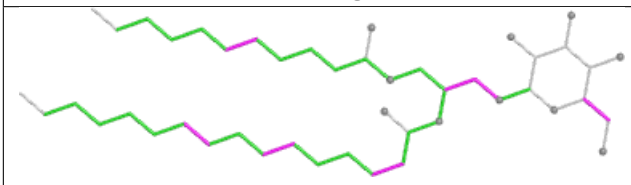
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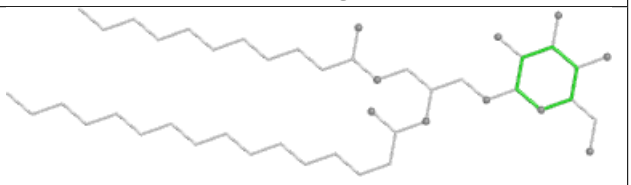
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Bond angles

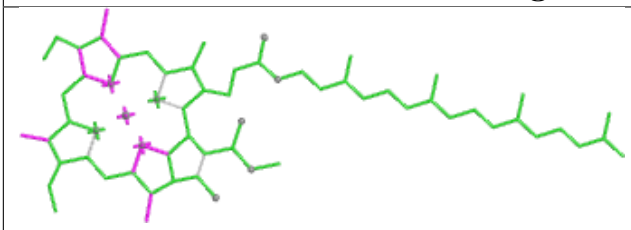


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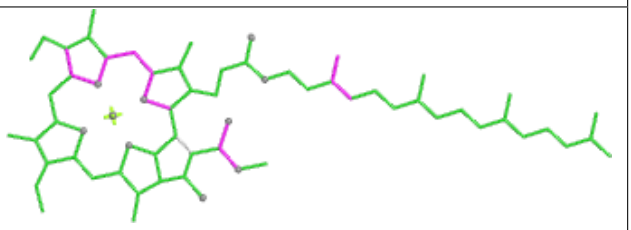


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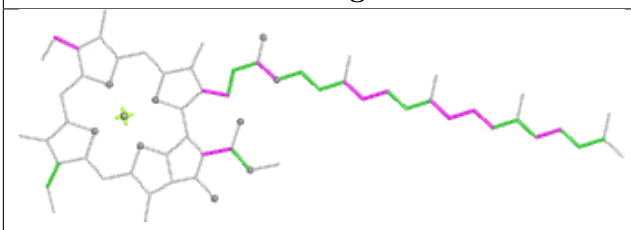
Ligand CLA c 504



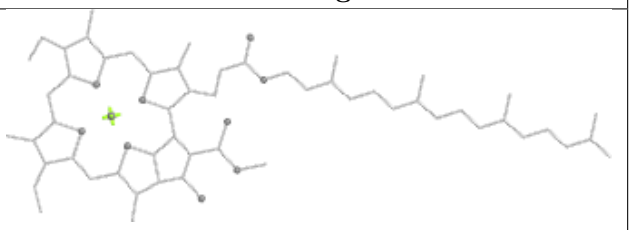
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Bond angles

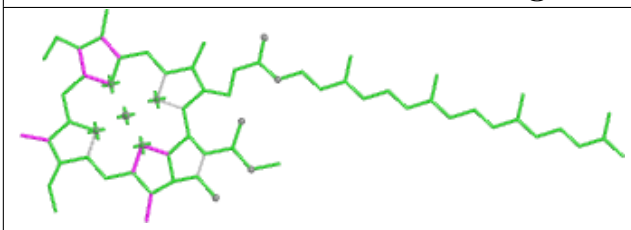


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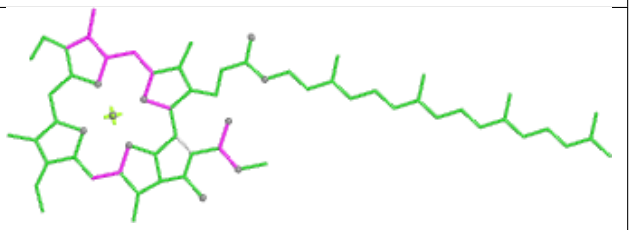


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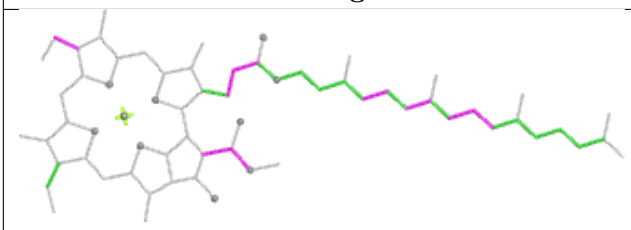
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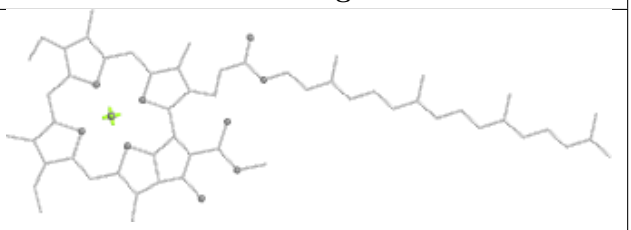
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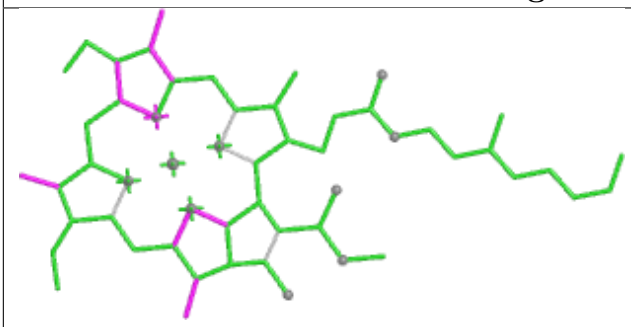


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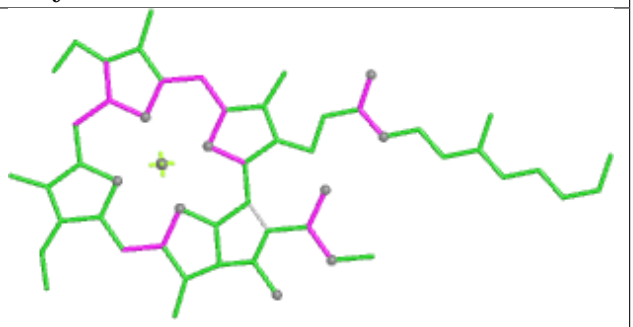


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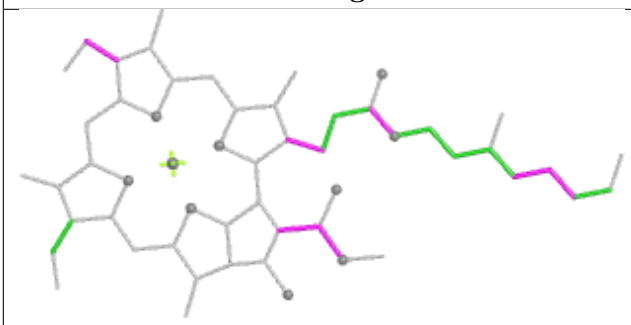
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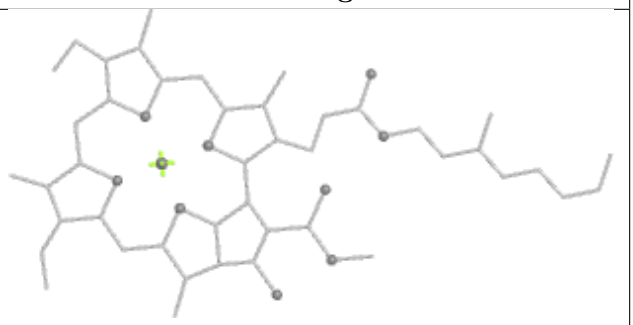
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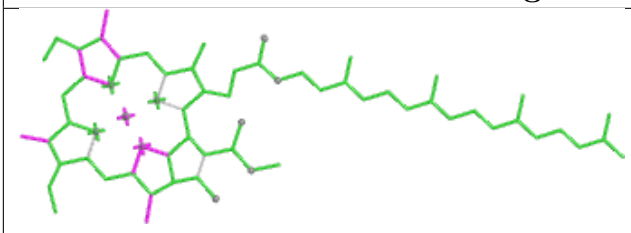


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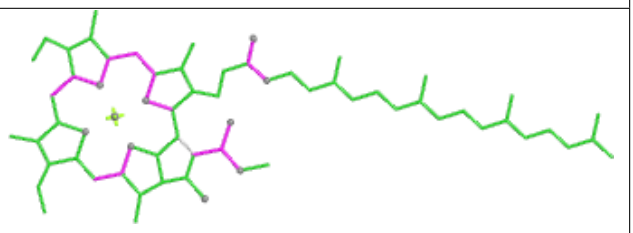


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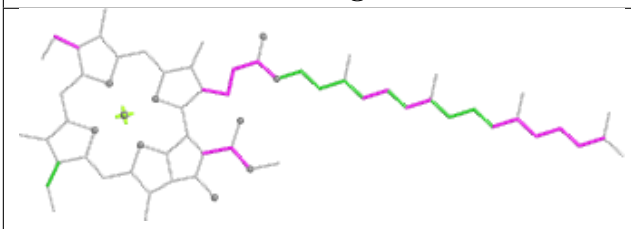
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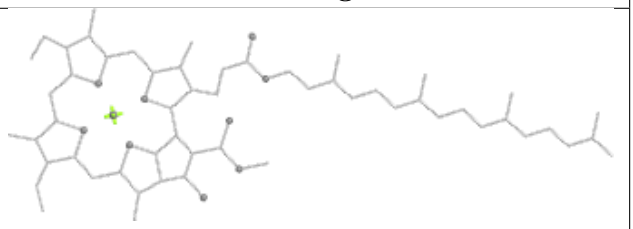
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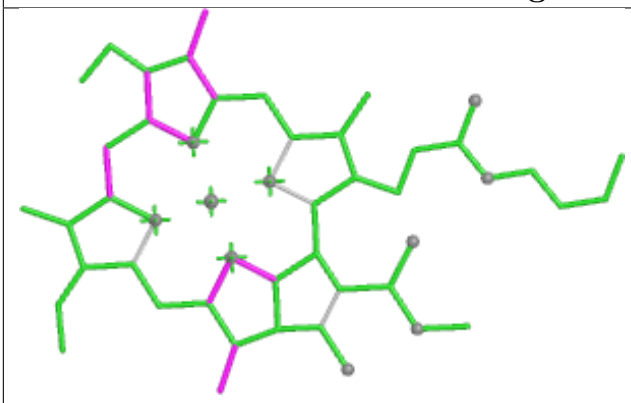


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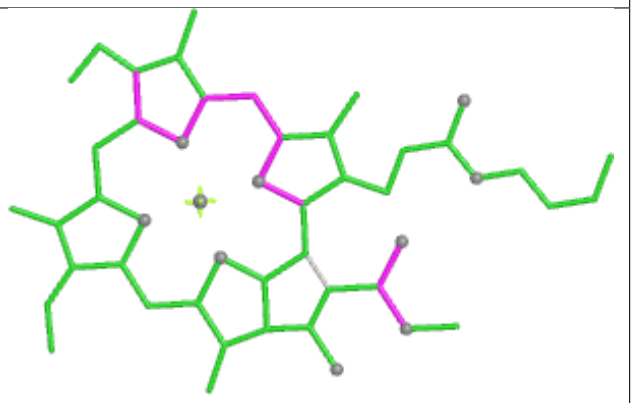


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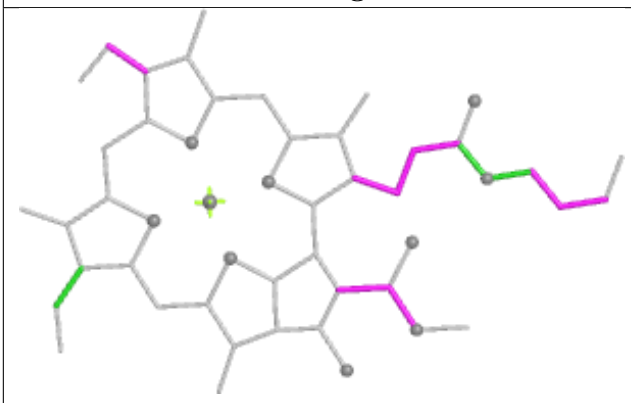
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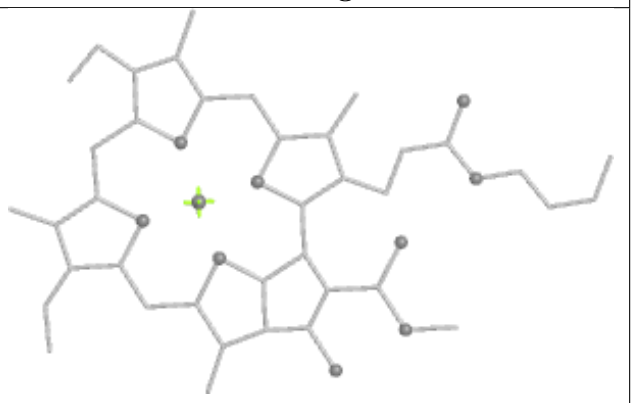
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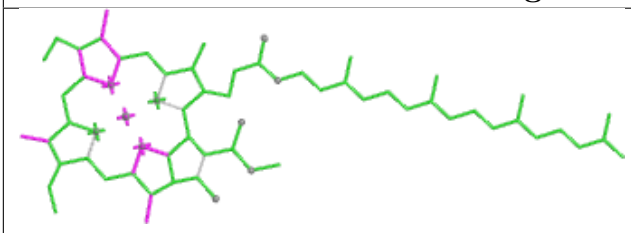


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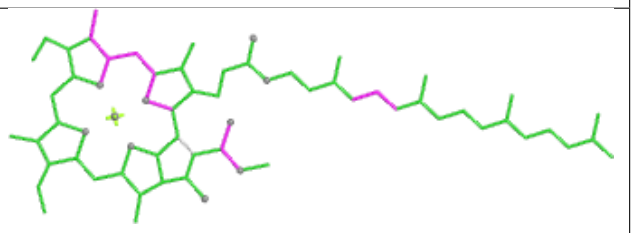


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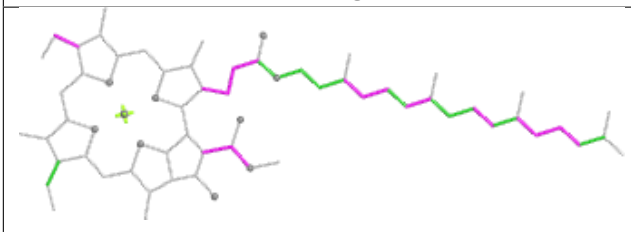
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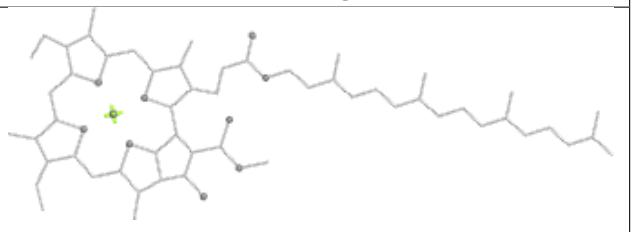
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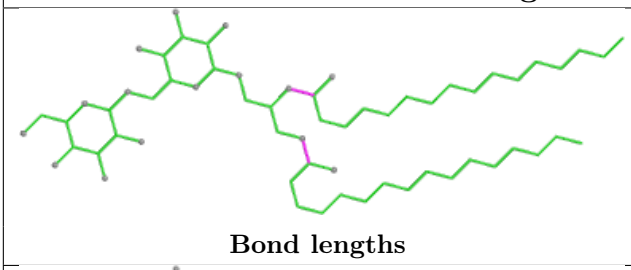


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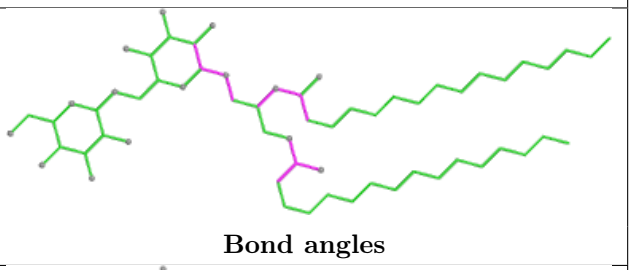


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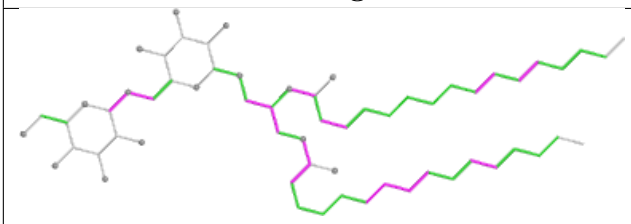
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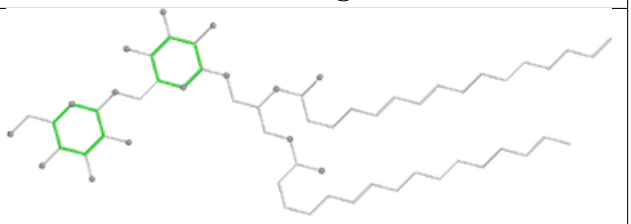
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Bond angles

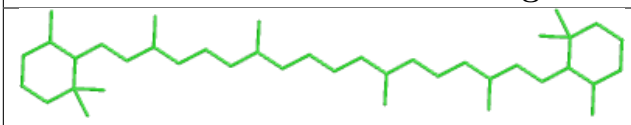


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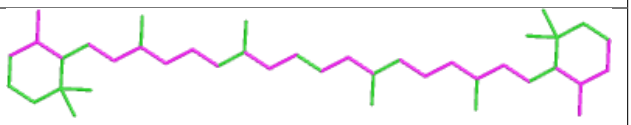


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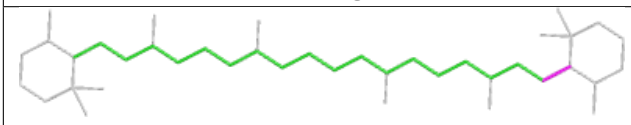
Ligand BCR A 411



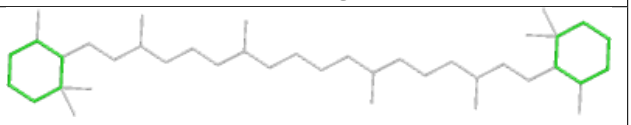
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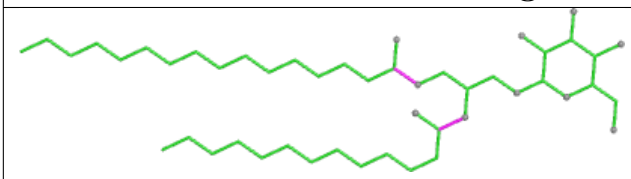


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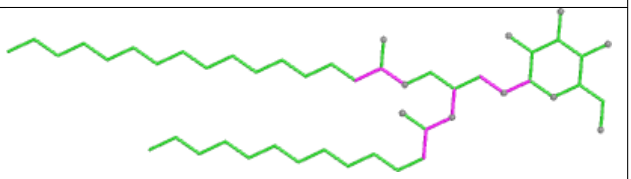


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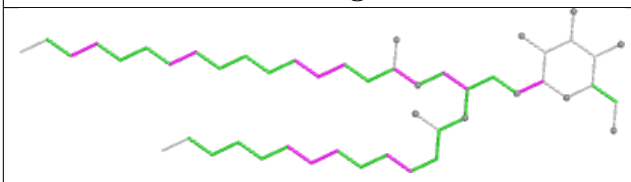
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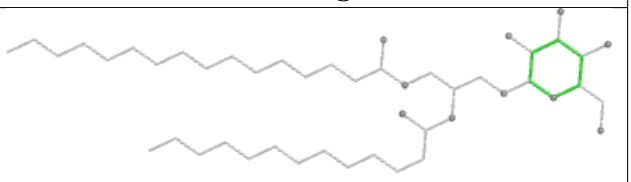
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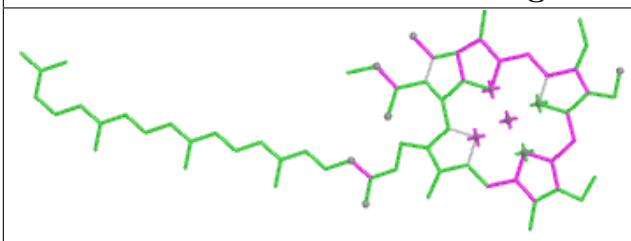


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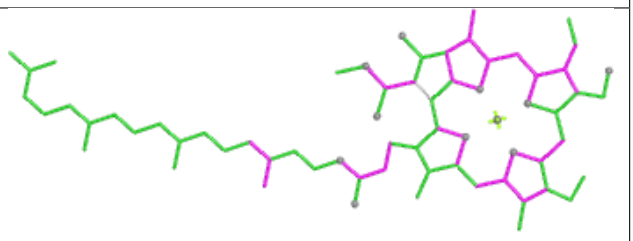


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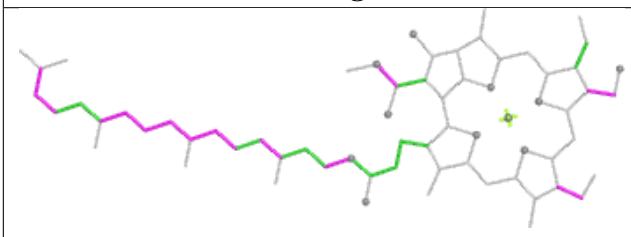
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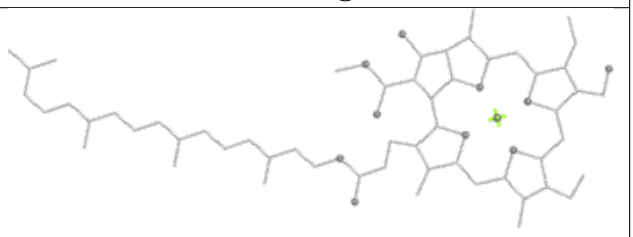
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Bond angles

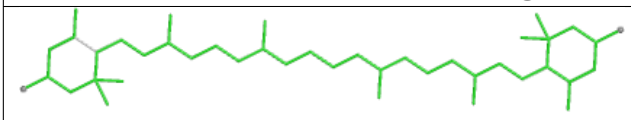


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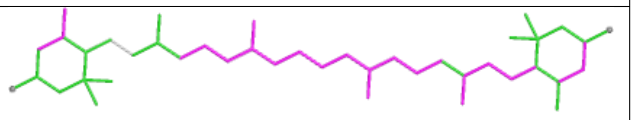


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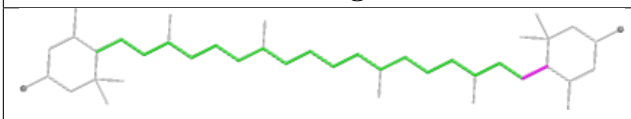
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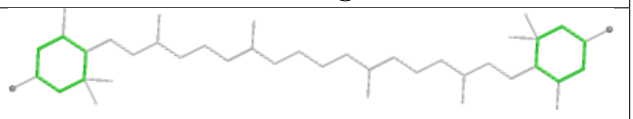
Bond lengths



Bond angles

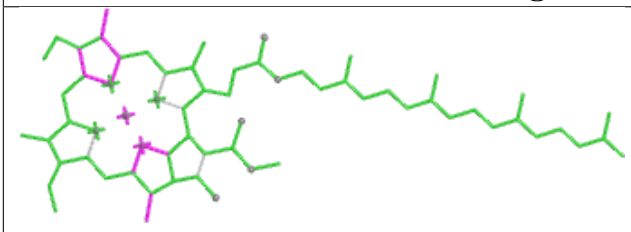


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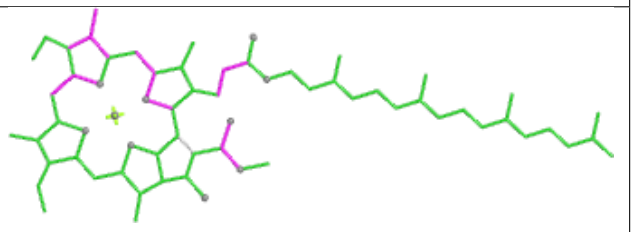


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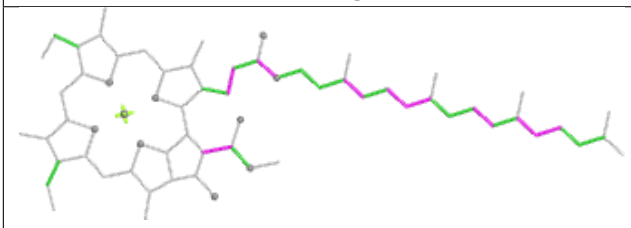
Ligand CLA 1 613



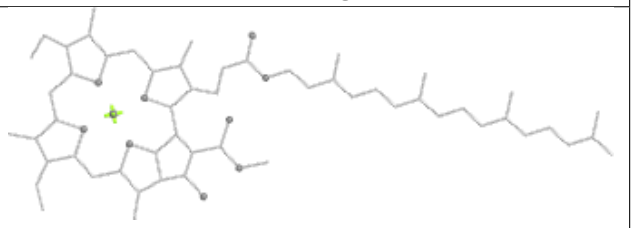
Bond lengths



Bond angles

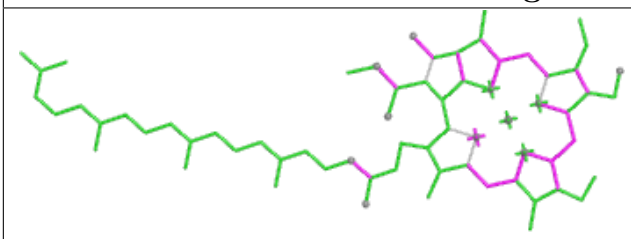


Torsions

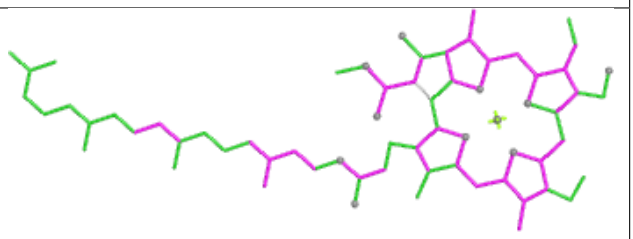


Rings

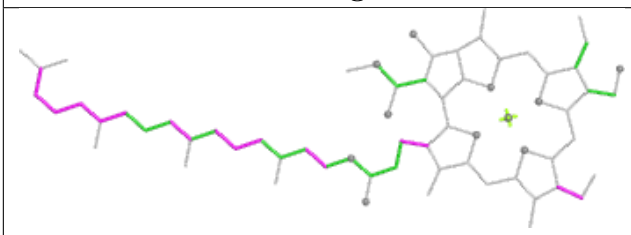
Ligand CHL Y 601



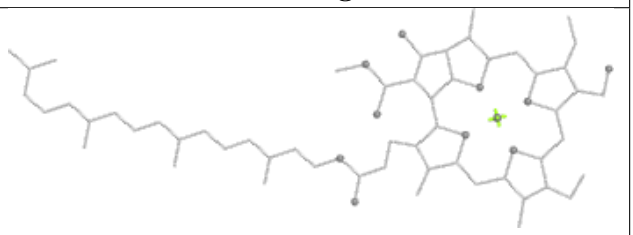
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Bond angles

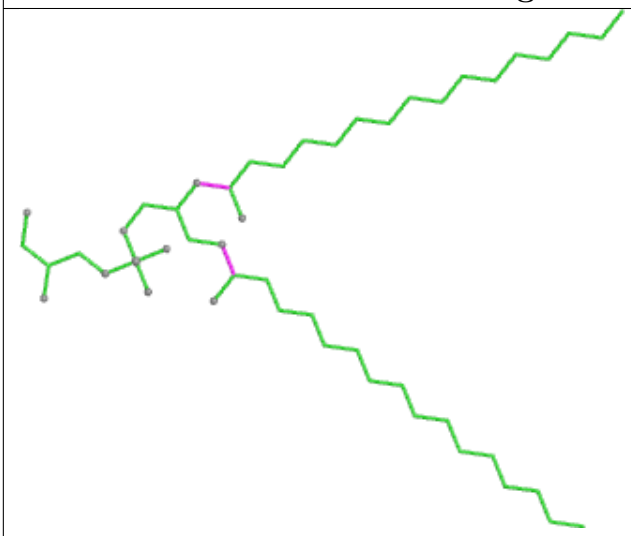


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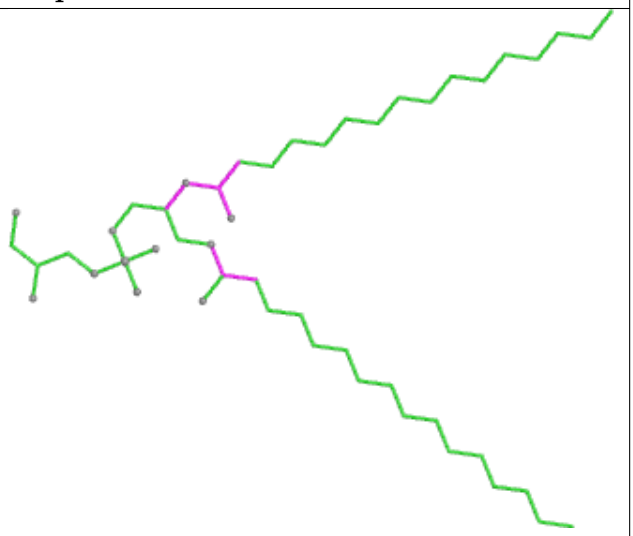


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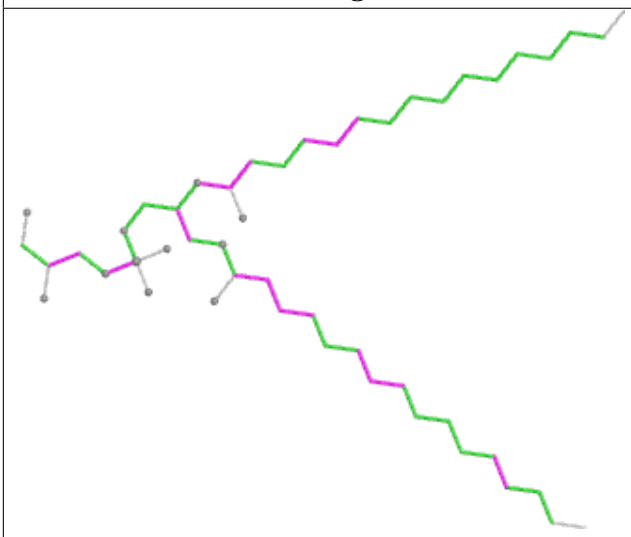
Ligand LHG q 2630



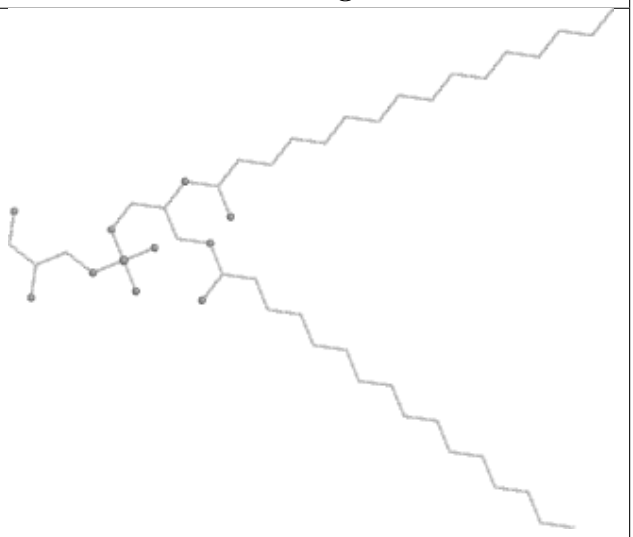
Bond lengths



Bond angles

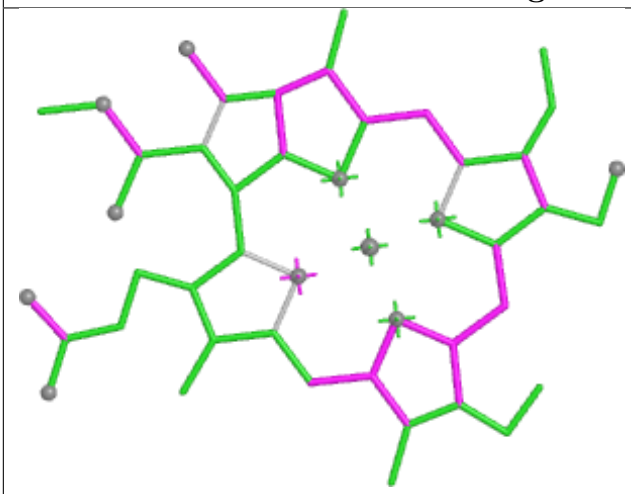


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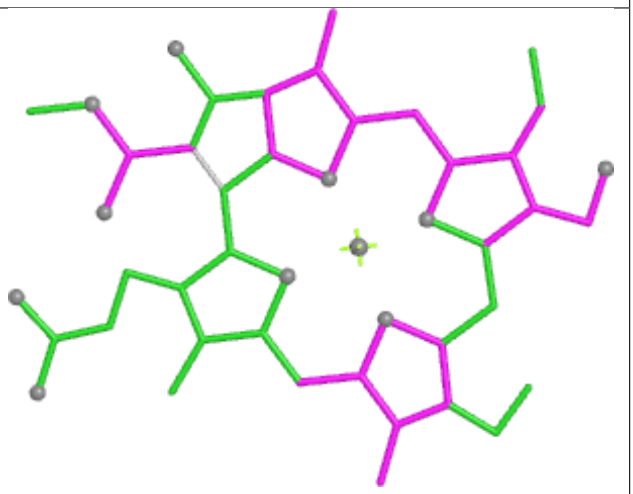


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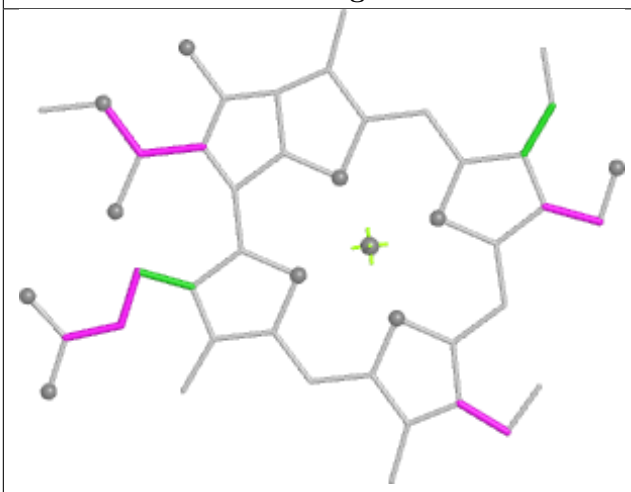
Ligand CHL 1 605



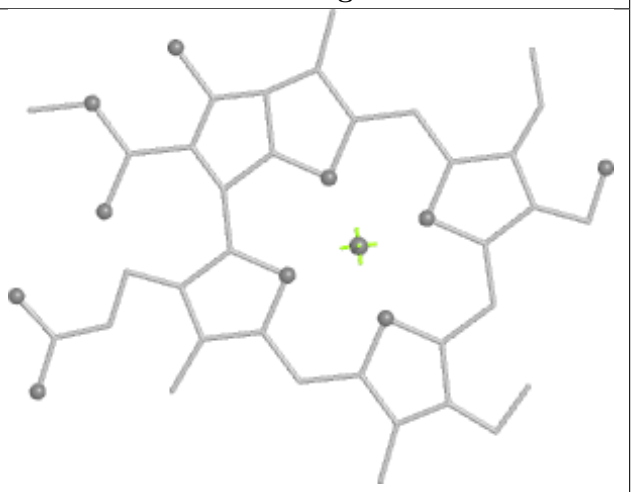
Bond lengths



Bond angles

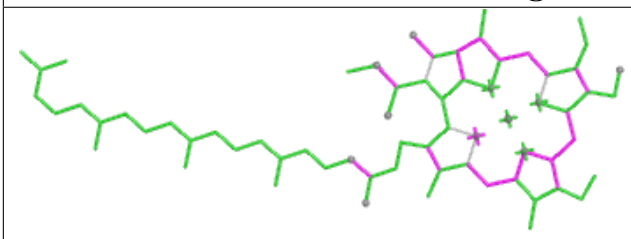


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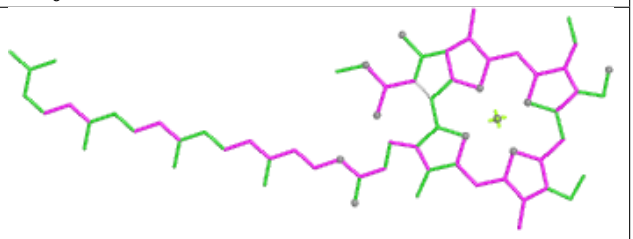


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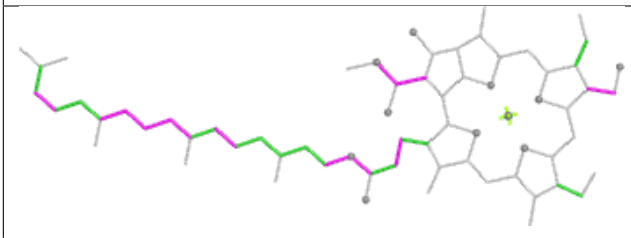
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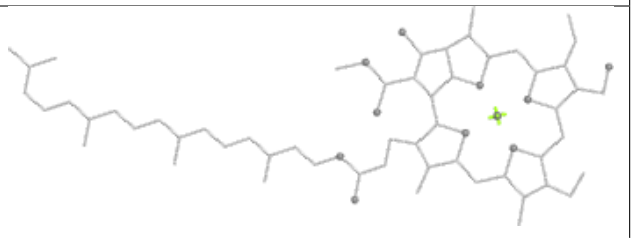
Bond lengths



Bond angles

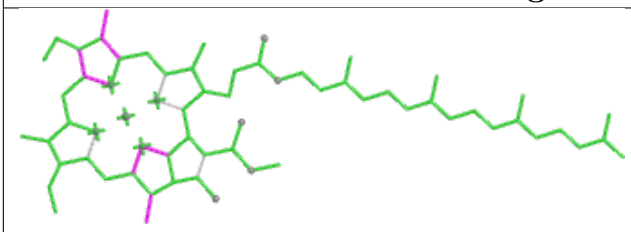


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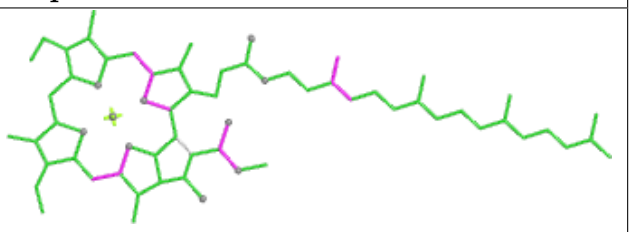


Rings

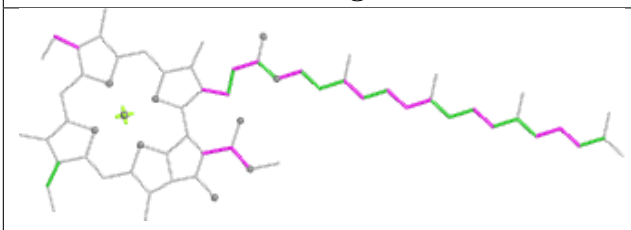
Ligand CLA p 604



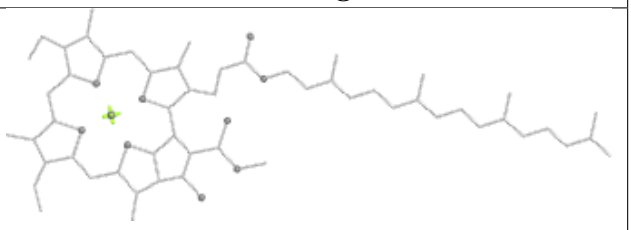
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Bond angles

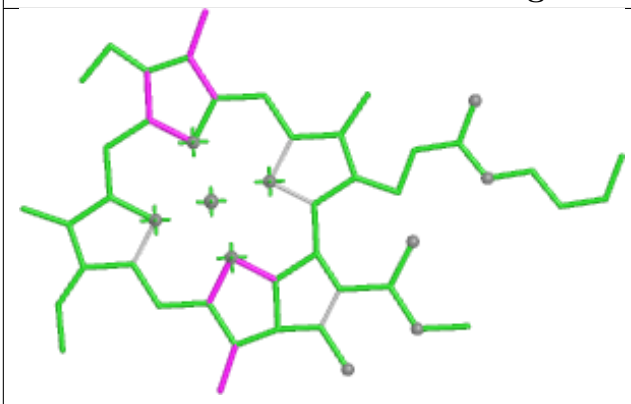


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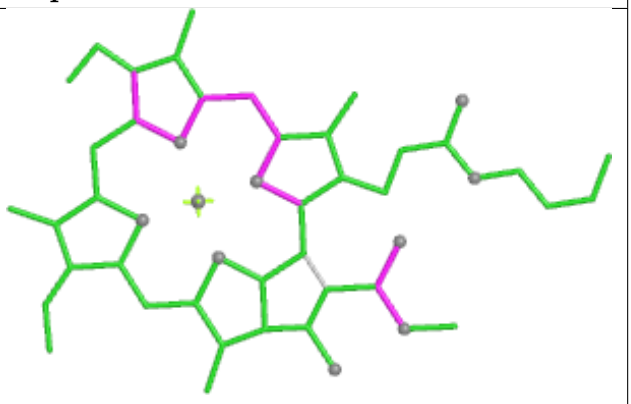


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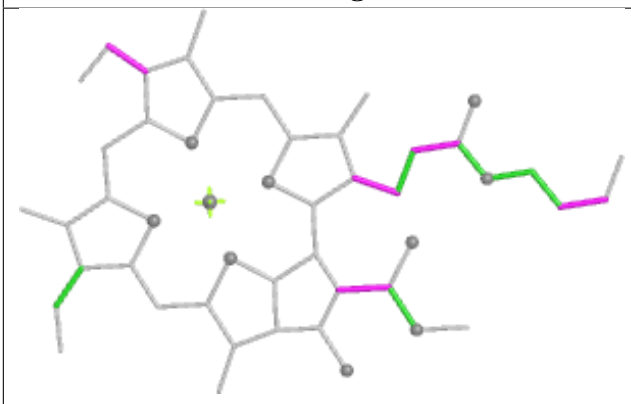
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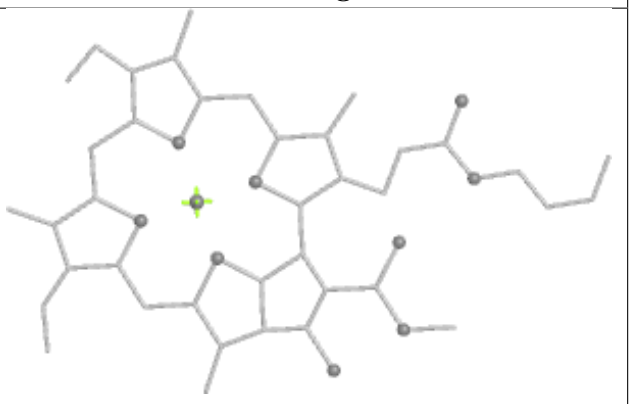
Bond lengths



Bond angles

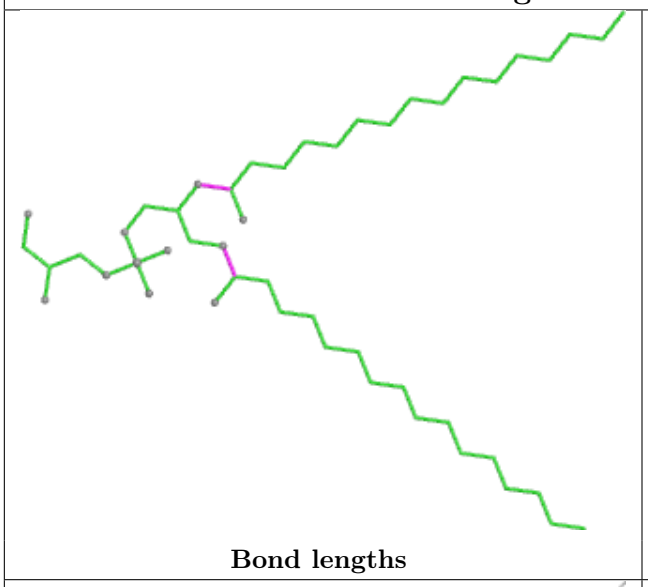


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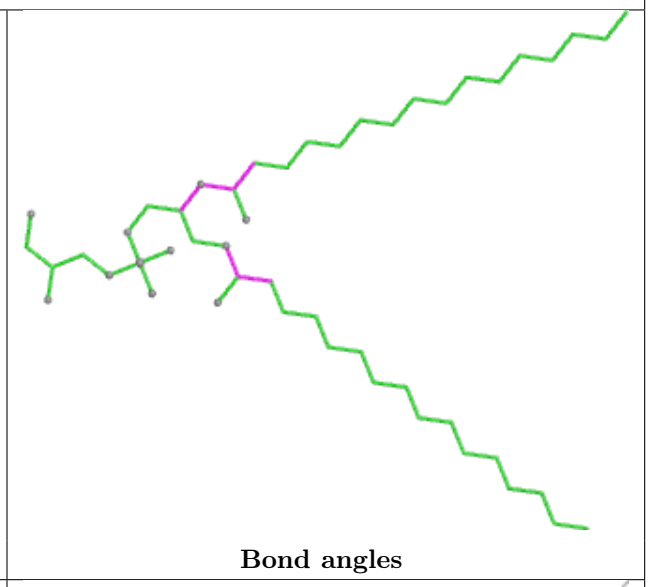


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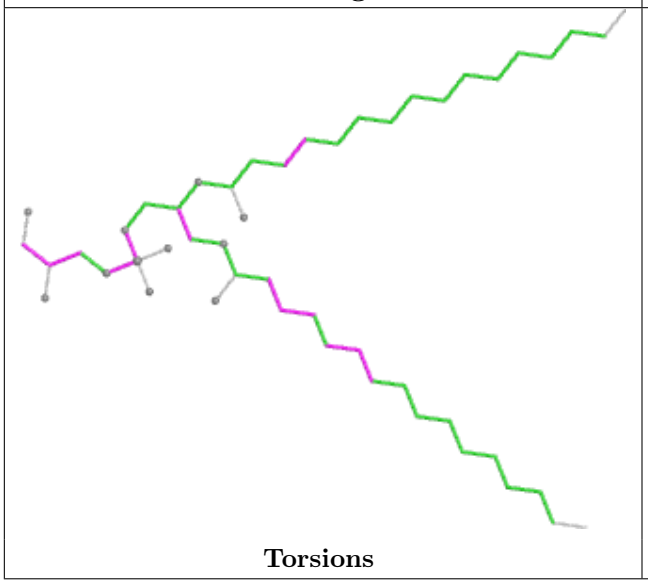
Ligand LHG N 2630



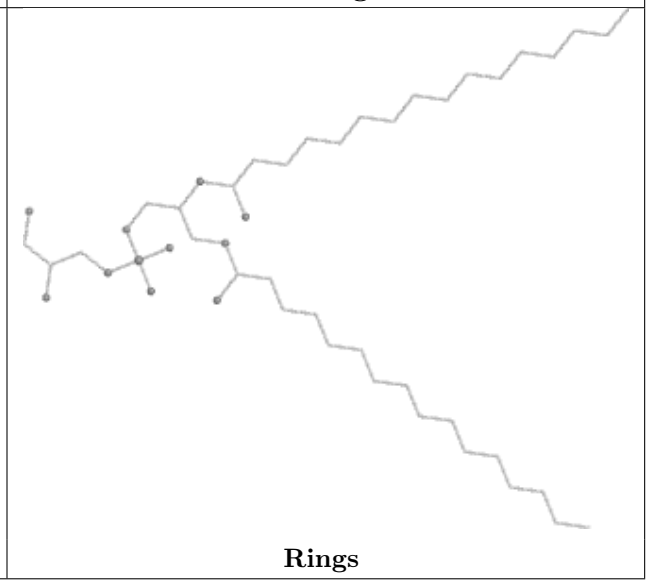
Bond lengths



Bond angles

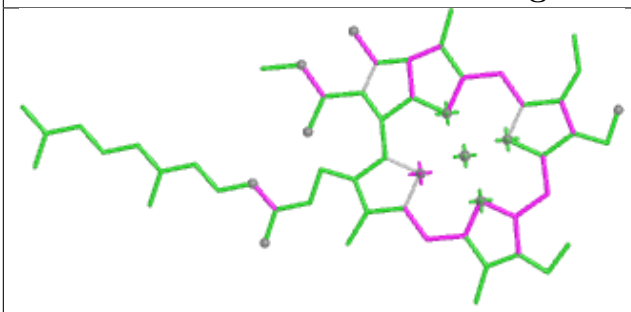


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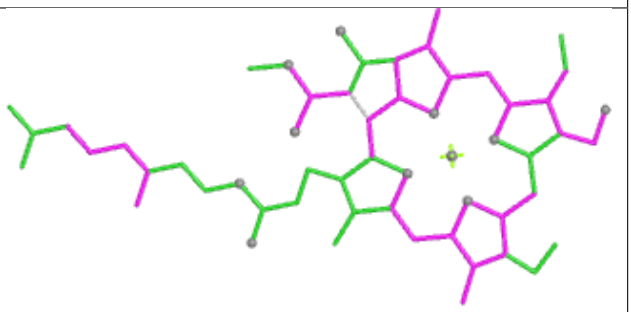


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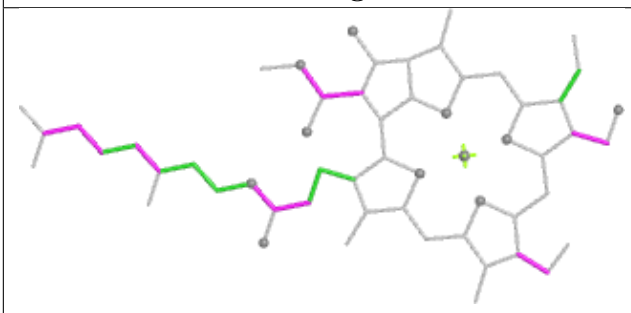
Ligand CHL r 607



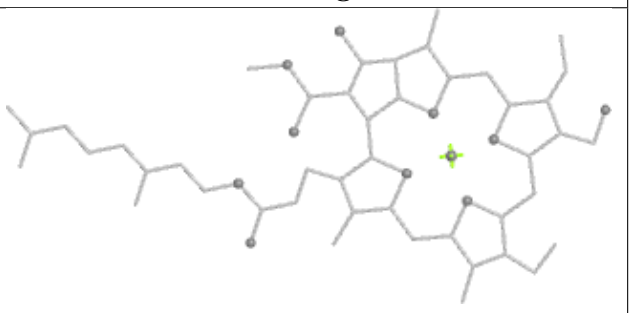
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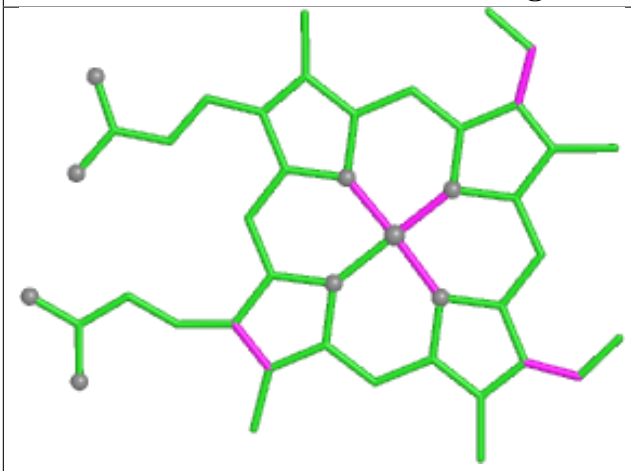


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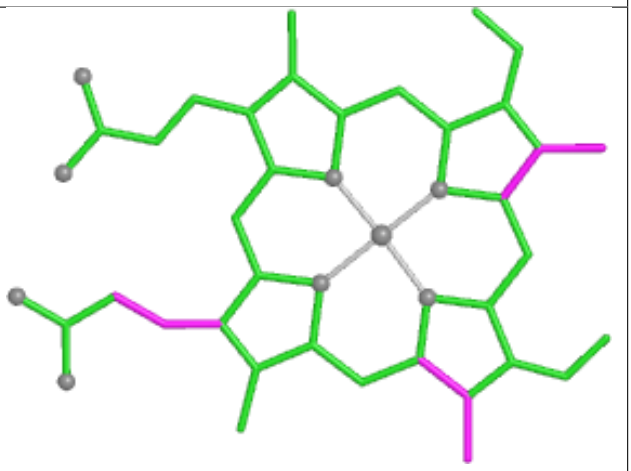


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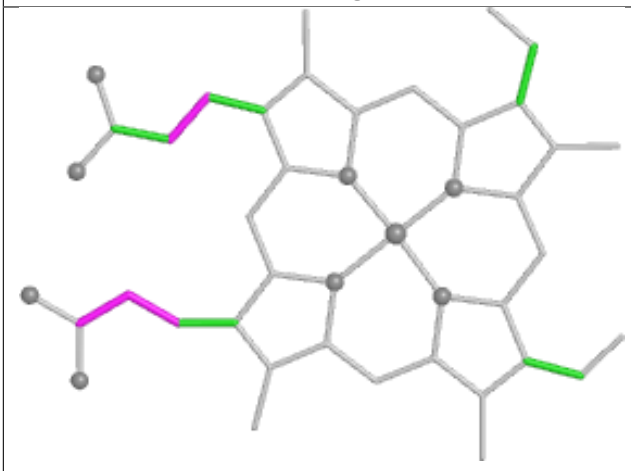
Ligand HEM f 101



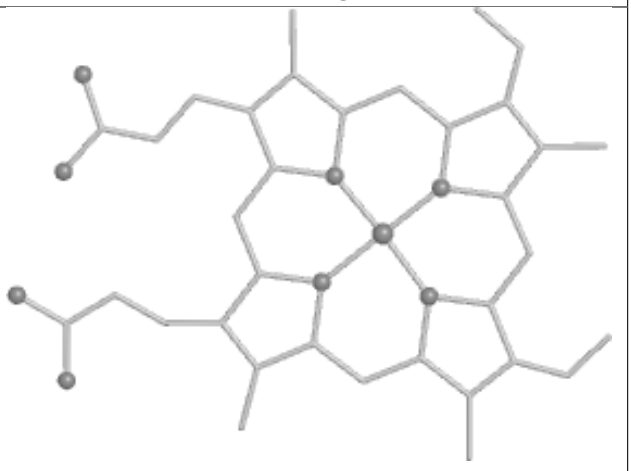
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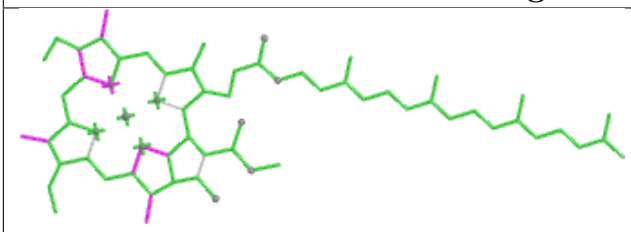


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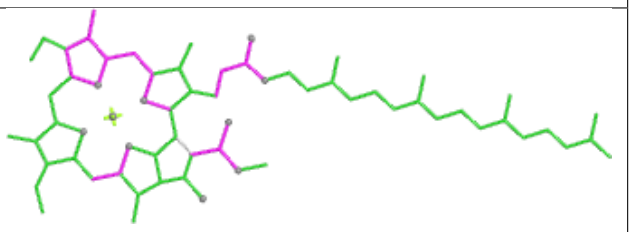


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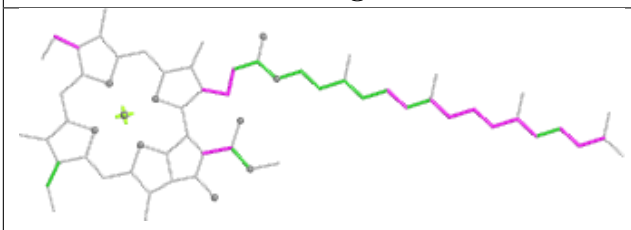
Ligand CLA b 607



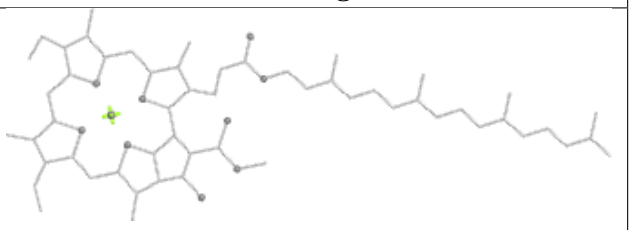
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Bond angles

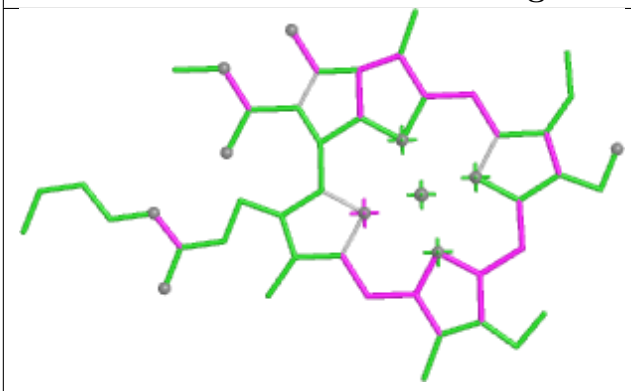


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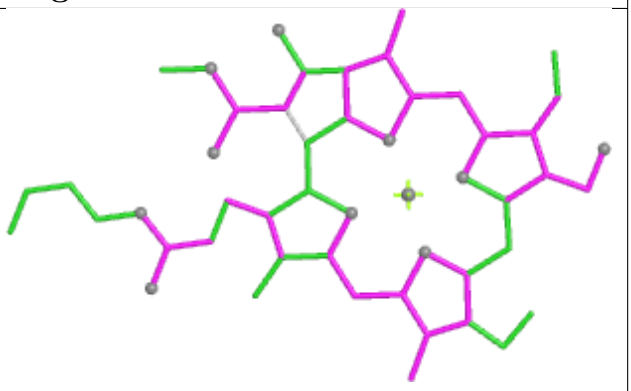


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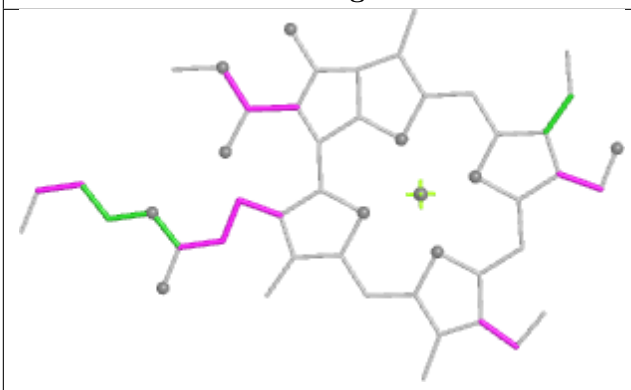
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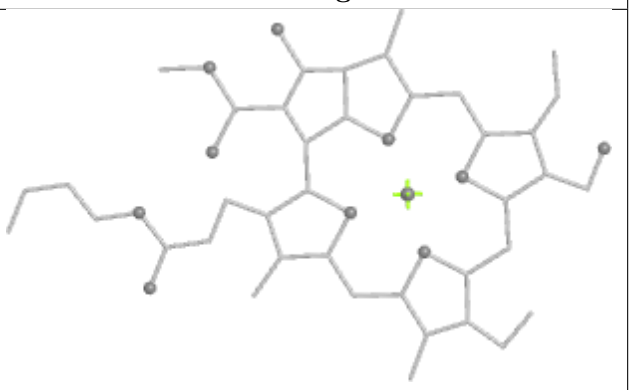
Bond lengths



Bond angles

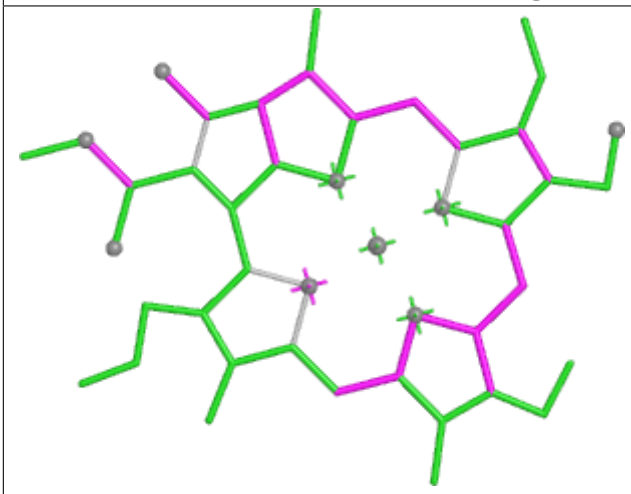


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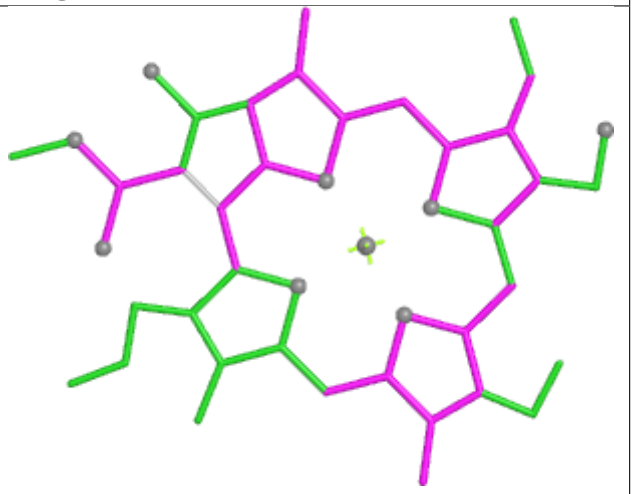


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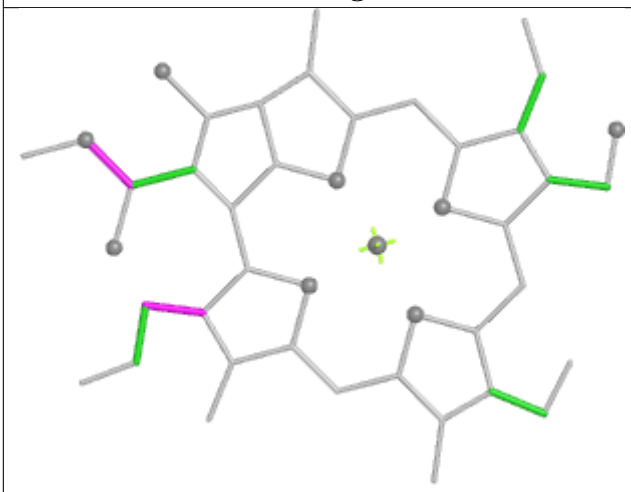
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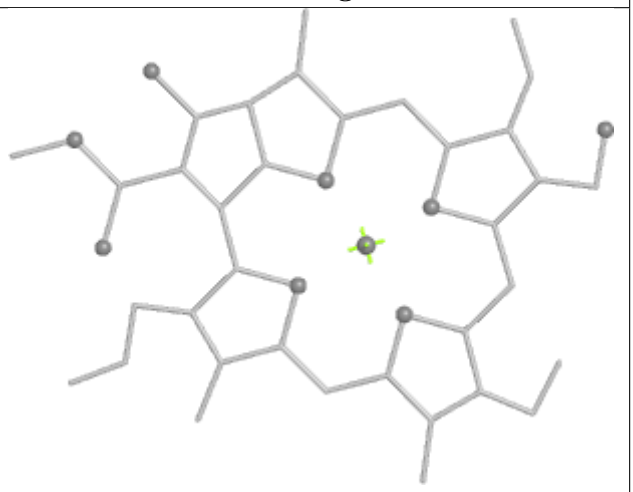
Bond lengths



Bond angles

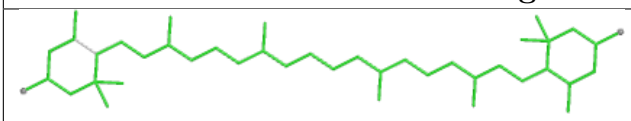


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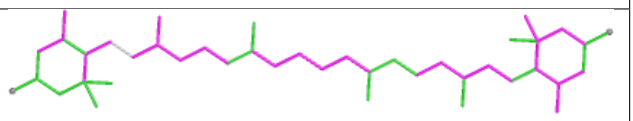


Rings

Ligand LUT S 1621



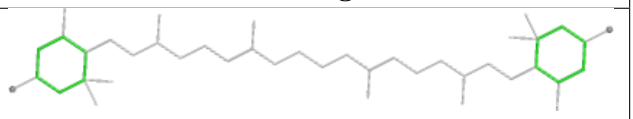
Bond lengths



Bond angles

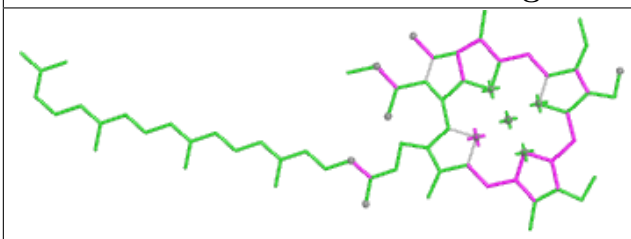


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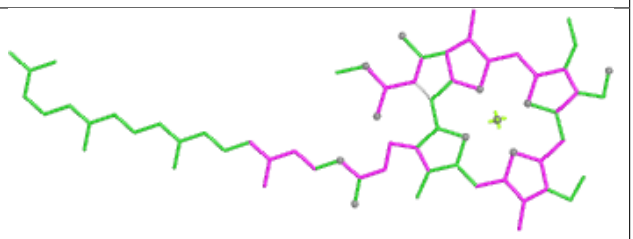


Rings

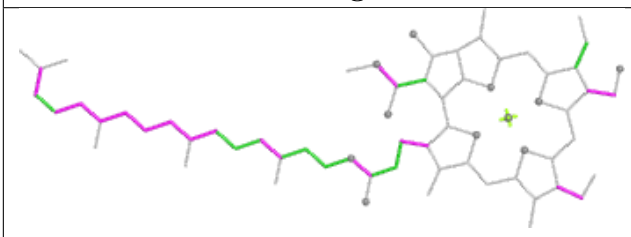
Ligand CHL N 605



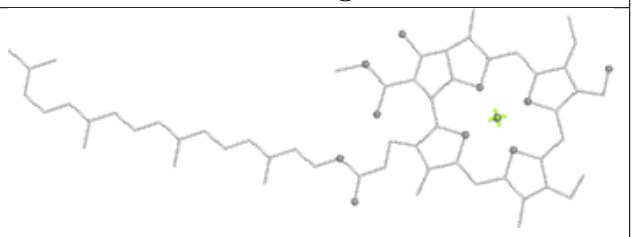
Bond lengths



Bond angles

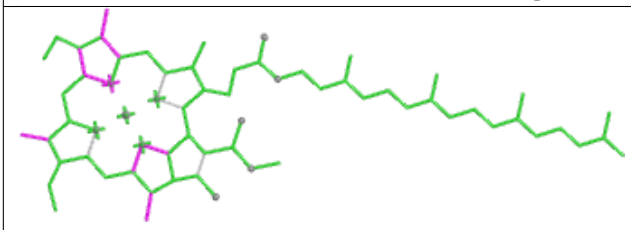


Torsions

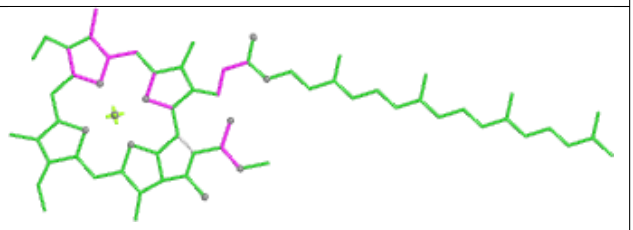


Rings

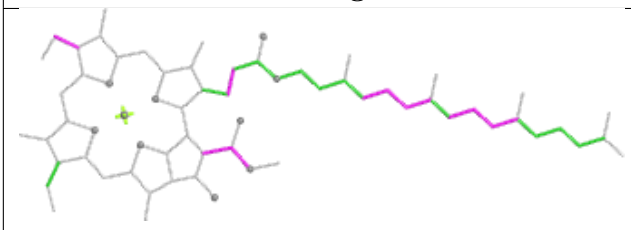
Ligand CLA 6 602



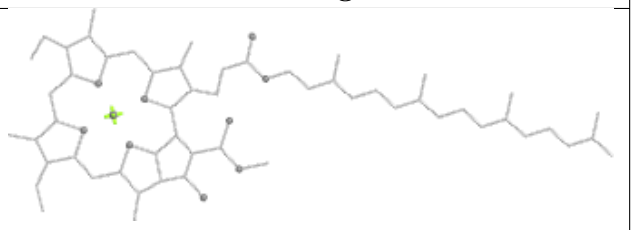
Bond lengths



Bond angles

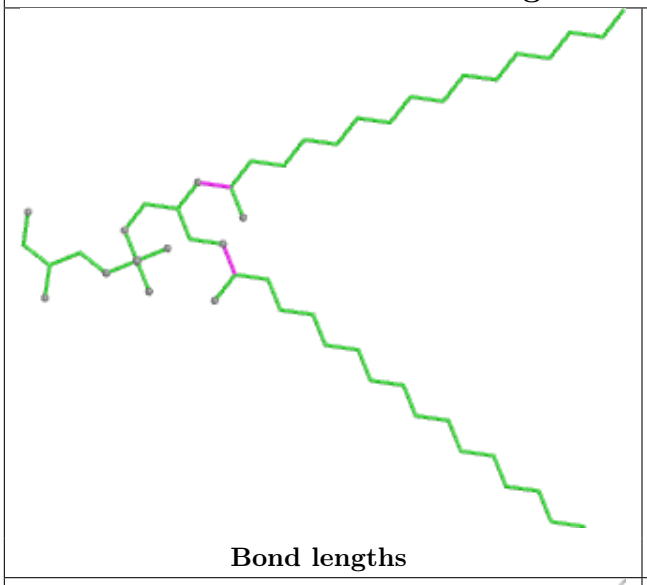


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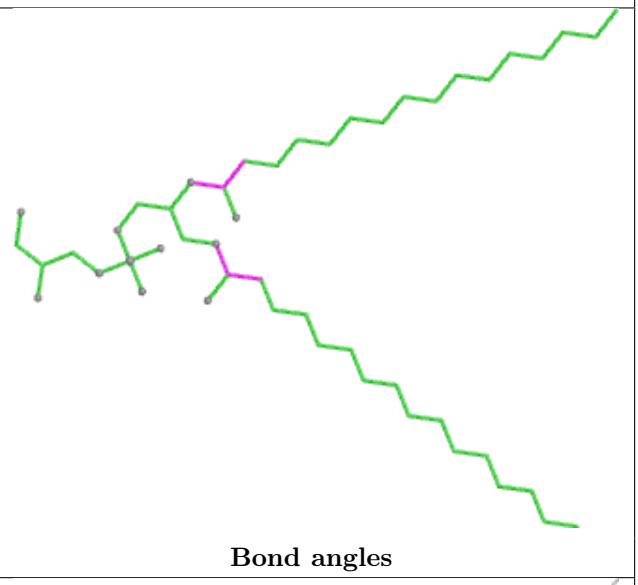


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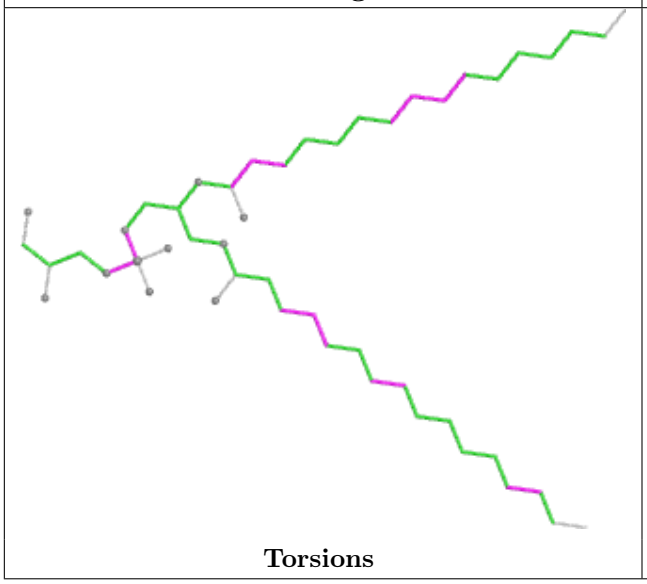
Ligand LHG D 409



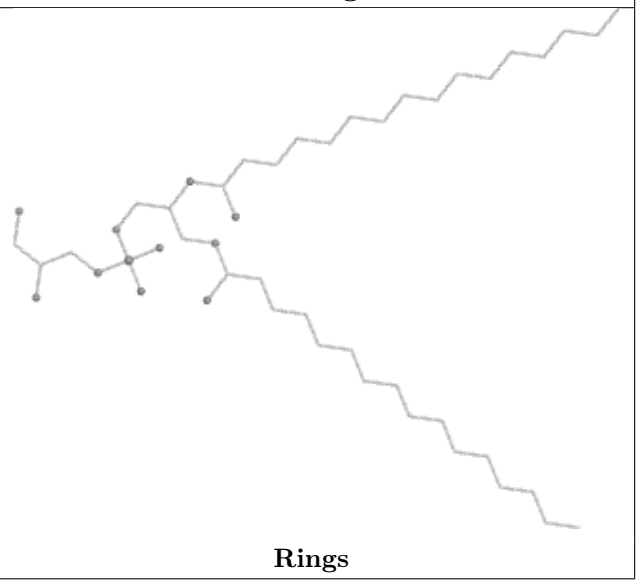
Bond lengths



Bond angles



Torsions

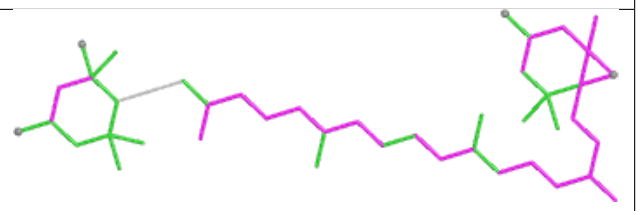


Rings

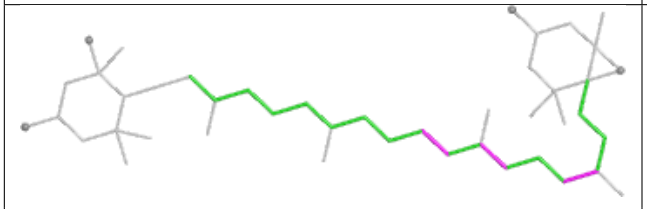
Ligand NEX Y 1623



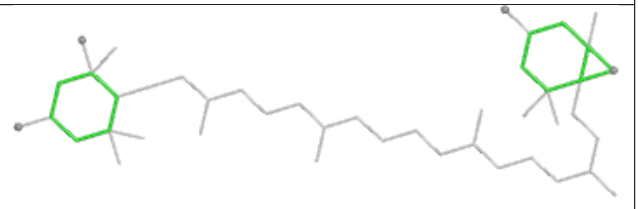
Bond lengths



Bond angles

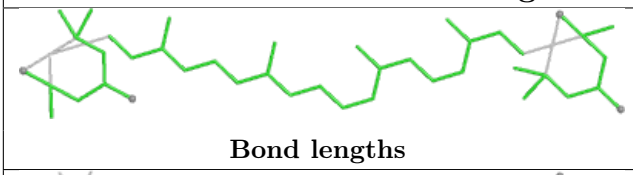


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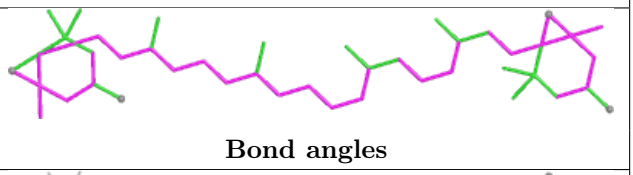


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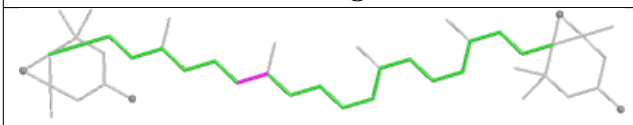
Ligand XAT 8 1622



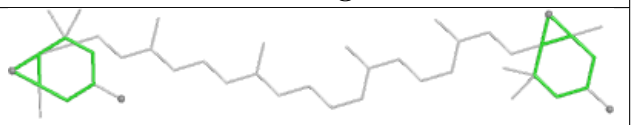
Bond lengths



Bond angles

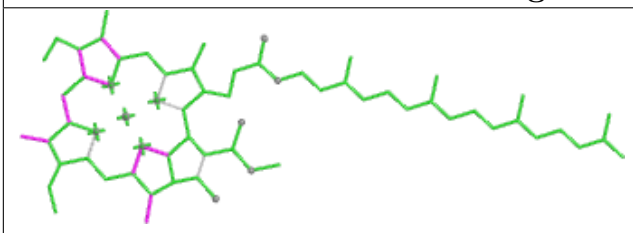


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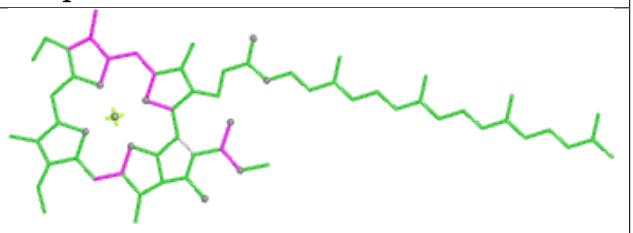


Rings

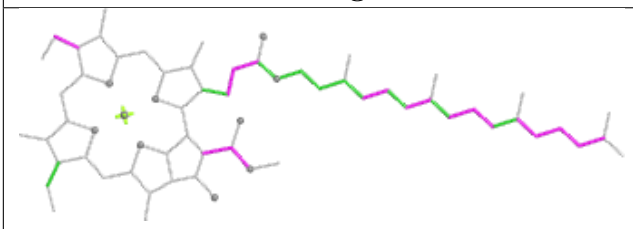
Ligand CLA q 602



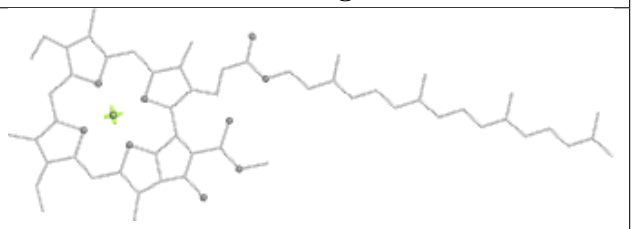
Bond lengths



Bond angles

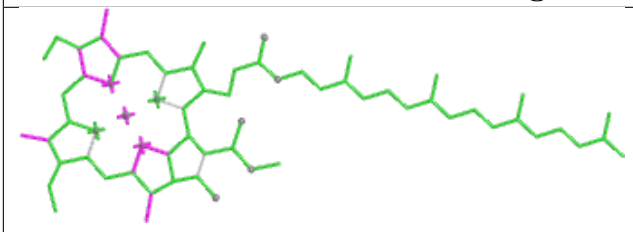


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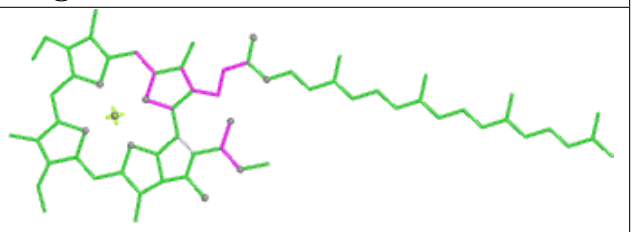


Rings

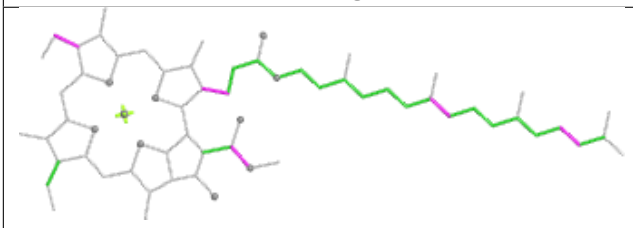
Ligand CLA g 603



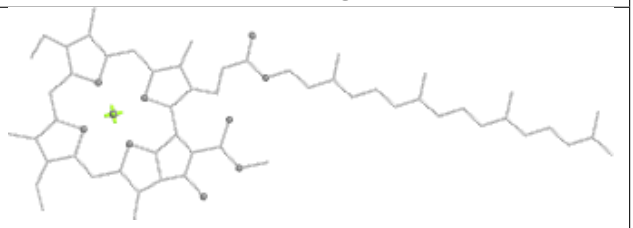
Bond lengths



Bond angles

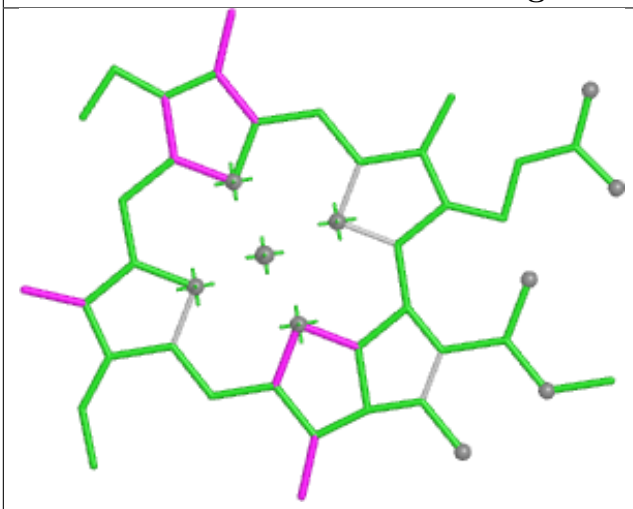


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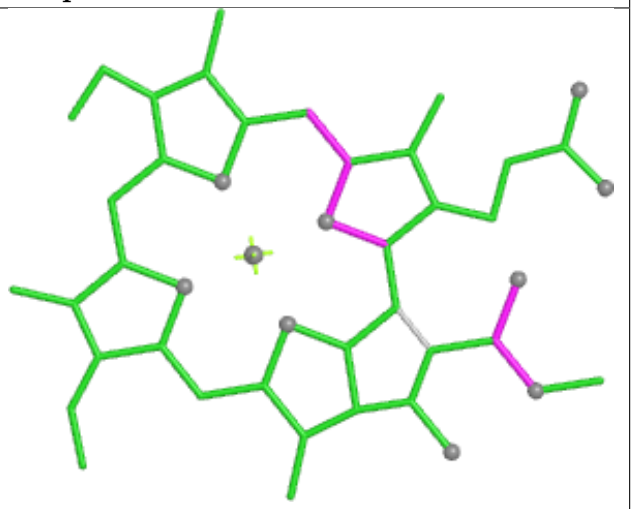


Rings

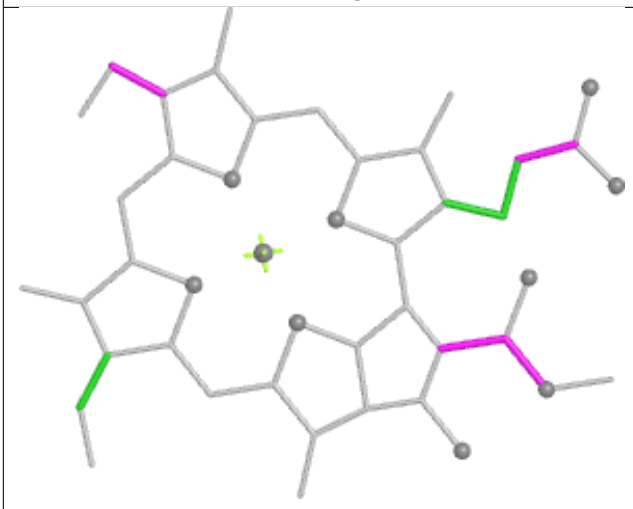
Ligand CLA q 611



Bond lengths



Bond angles

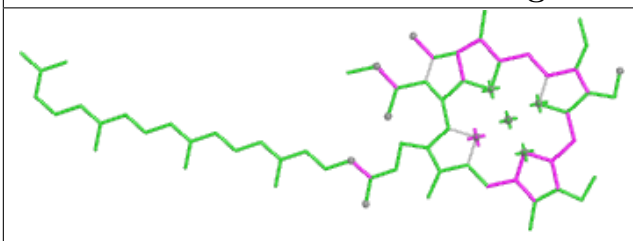


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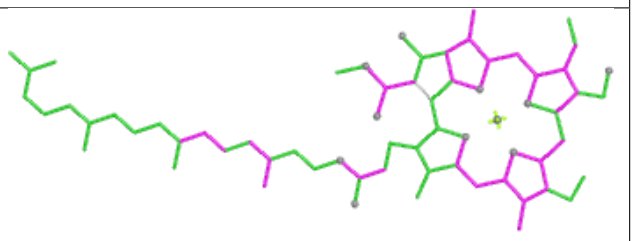


Rings

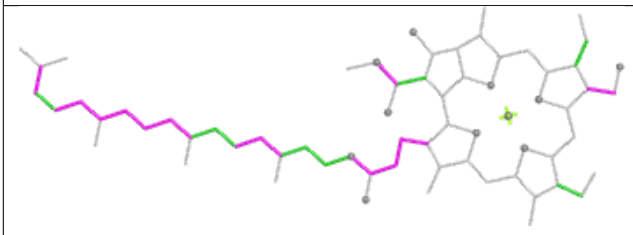
Ligand CHL 6 606



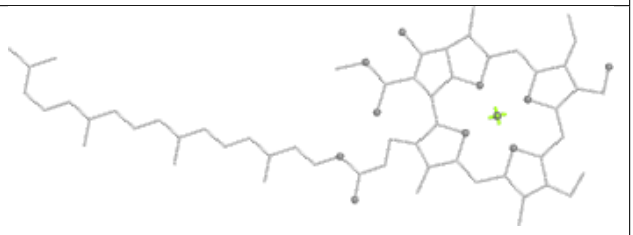
Bond lengths



Bond angles

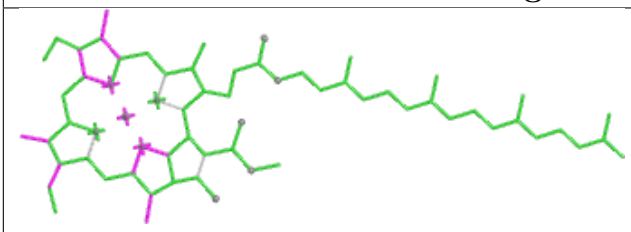


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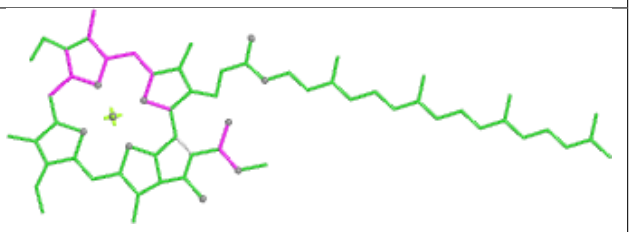


Rings

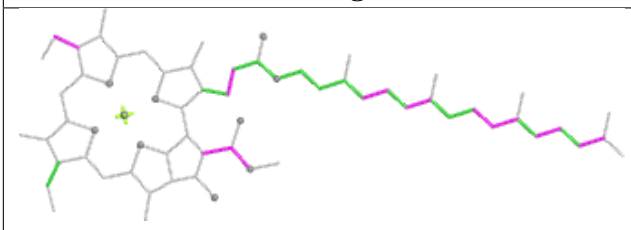
Ligand CLA B 615



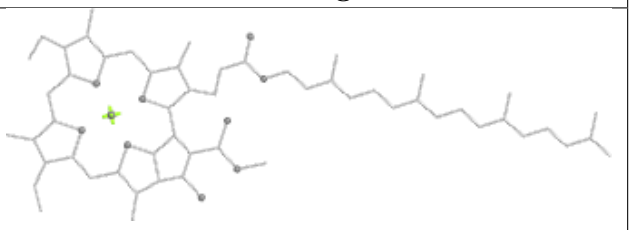
Bond lengths



Bond angles

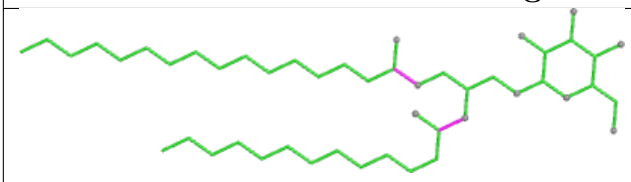


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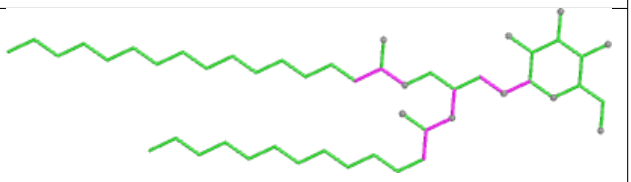


Rings

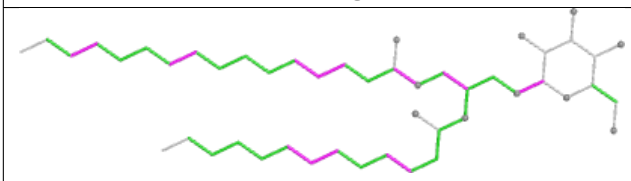
Ligand LMG a 413



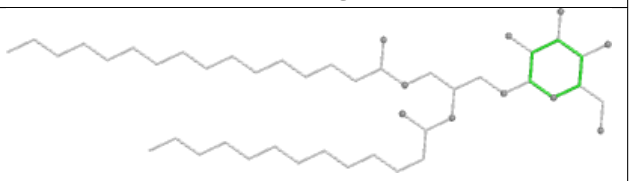
Bond lengths



Bond angles

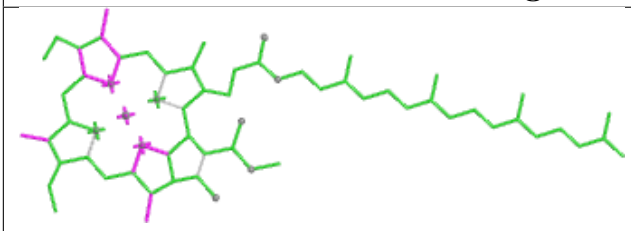


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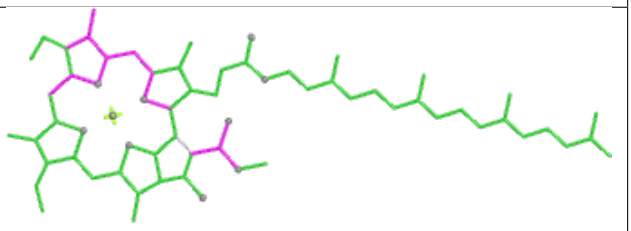


Rings

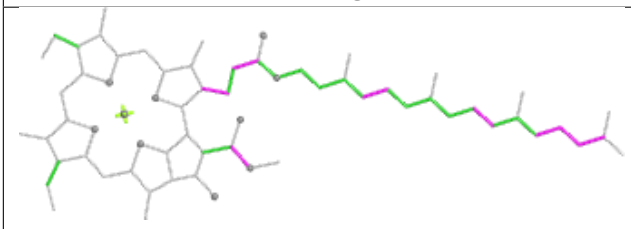
Ligand CLA B 609



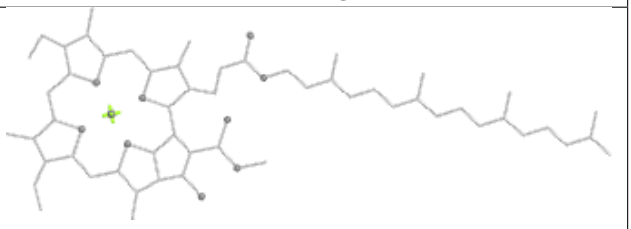
Bond lengths



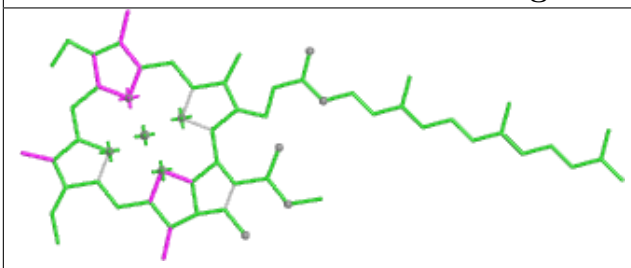
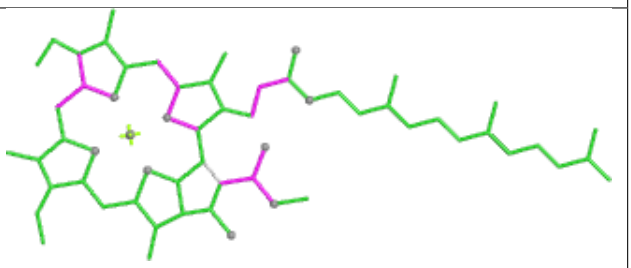
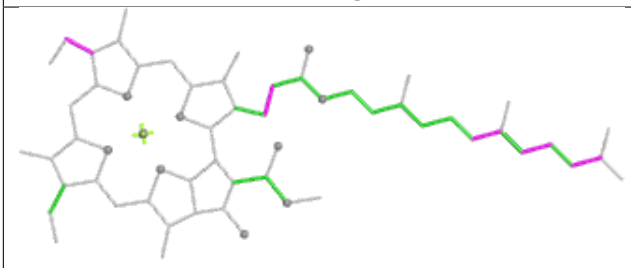
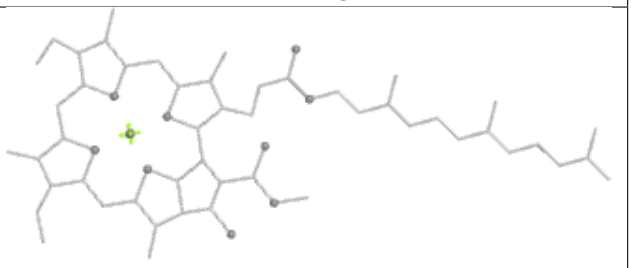
Bond angles

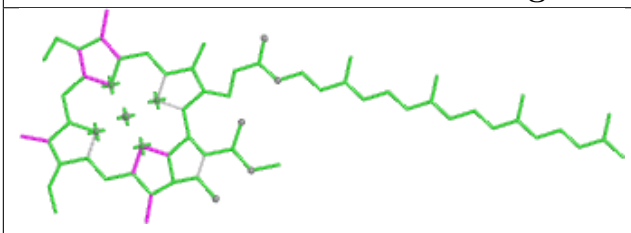
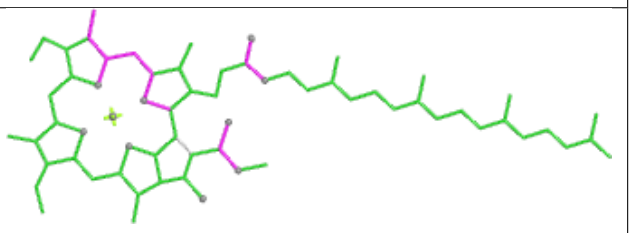
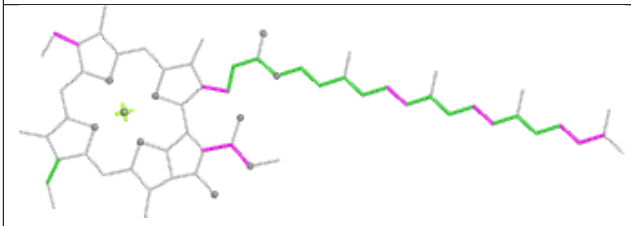
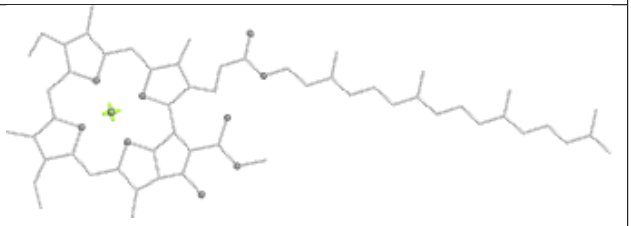


Torsions



Rings

Ligand CLA r 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 610	
 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.

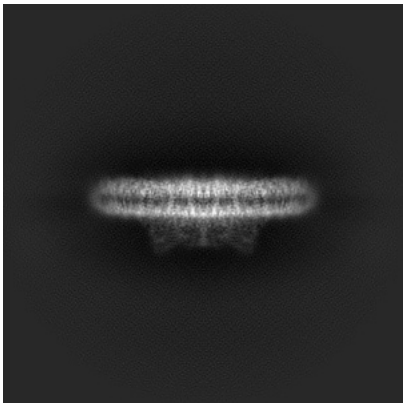
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9956. These allow visual inspection of the internal detail of the map and identification of artifacts.

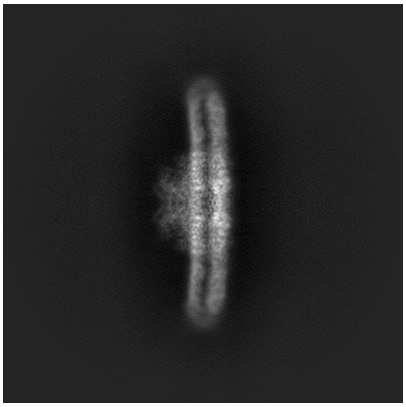
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

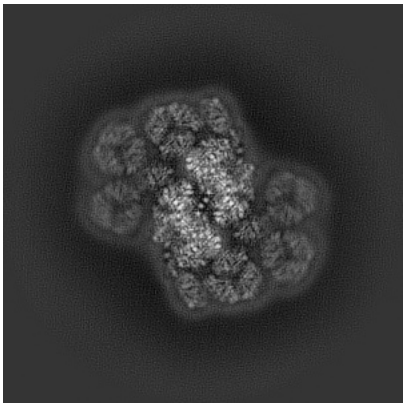
6.1.1 Primary map



X



Y

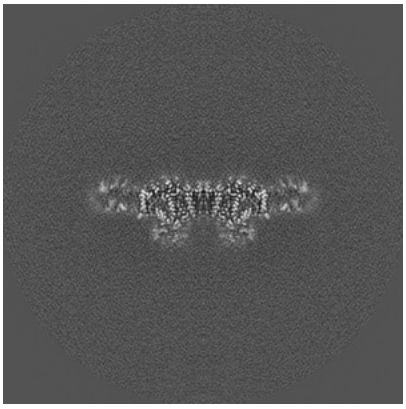


Z

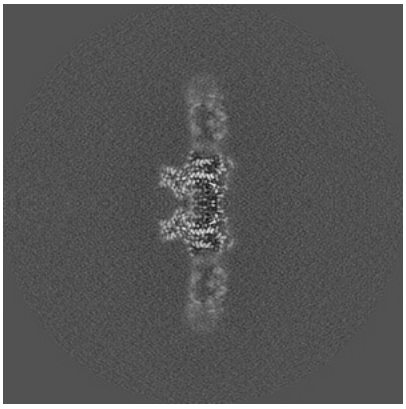
The images above show the map projected in three orthogonal directions.

6.2 Central slices

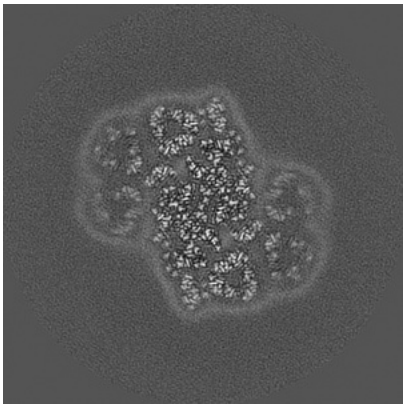
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

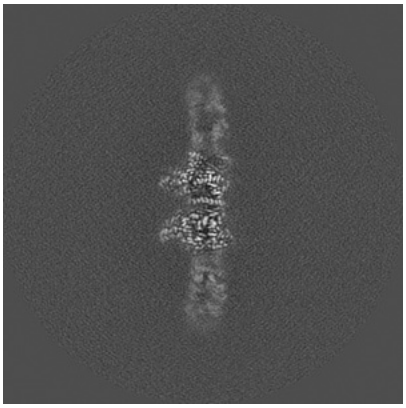
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

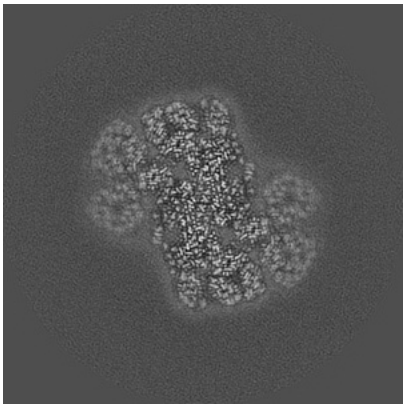
6.3.1 Primary map



X Index: 207



Y Index: 196

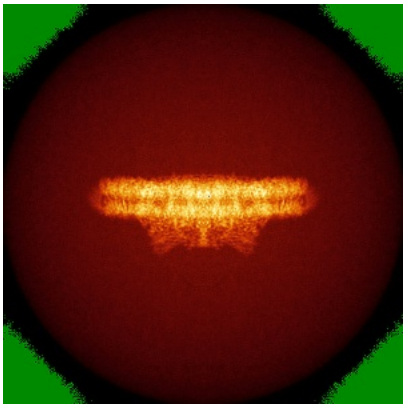


Z Index: 204

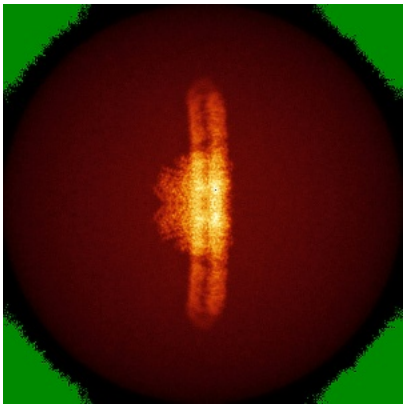
The images above show the largest variance slices of the map in three orthogonal directions.

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

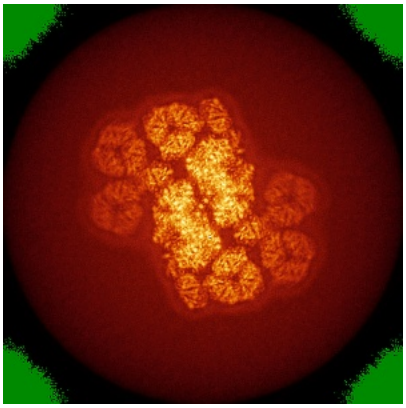
6.4.1 Primary map



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

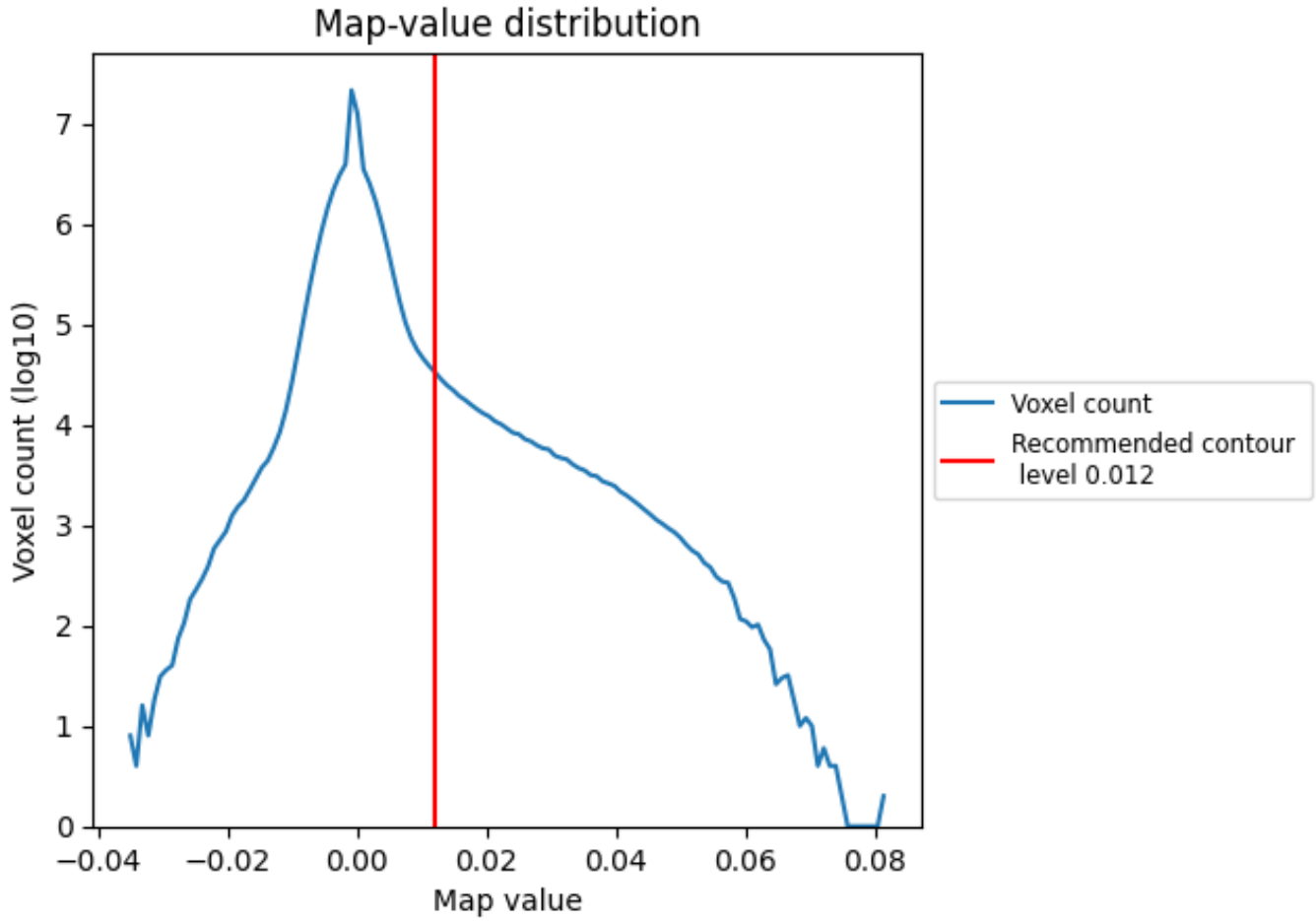
6.6 Mask visualisation (i)

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

7 Map analysis

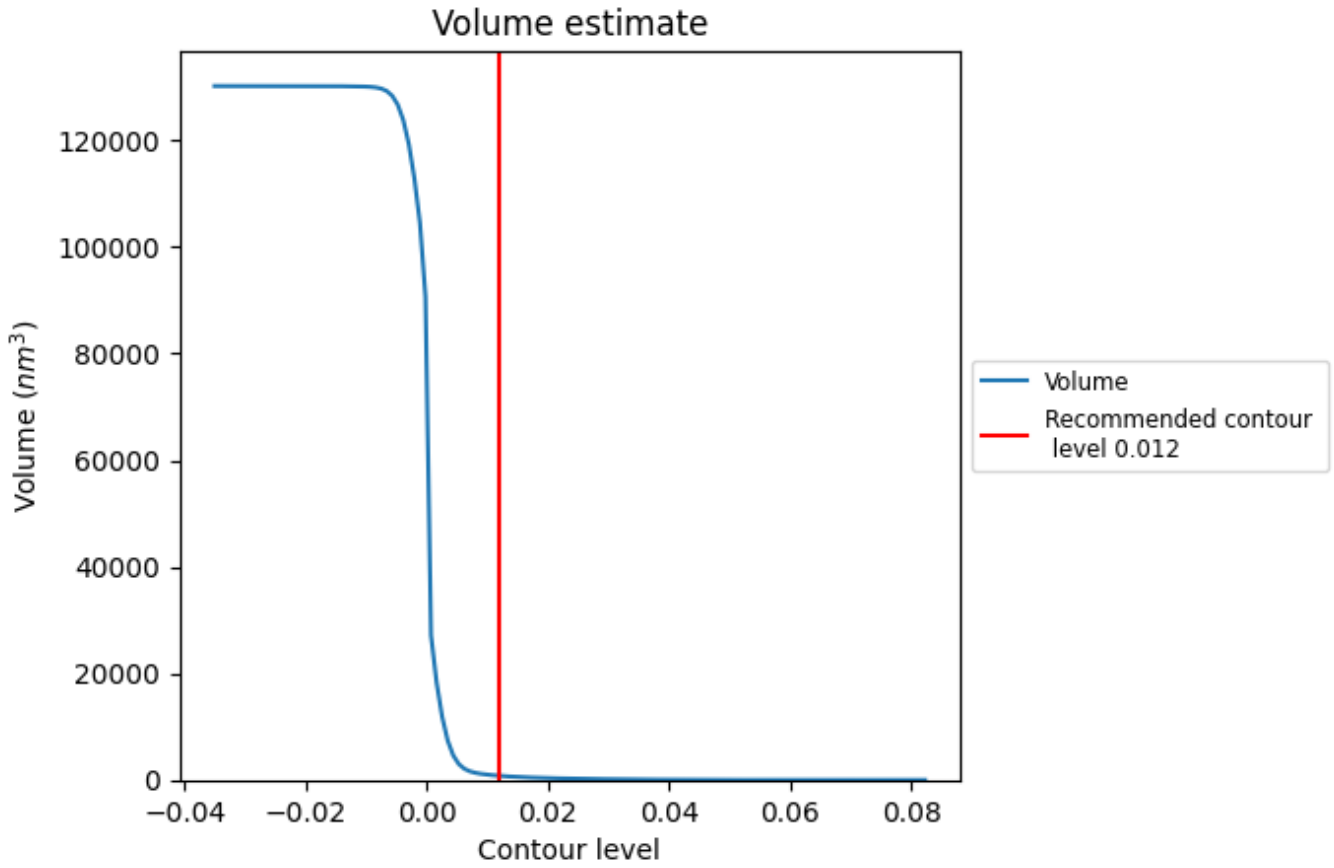
This section contains the results of statistical analysis of the map.

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.

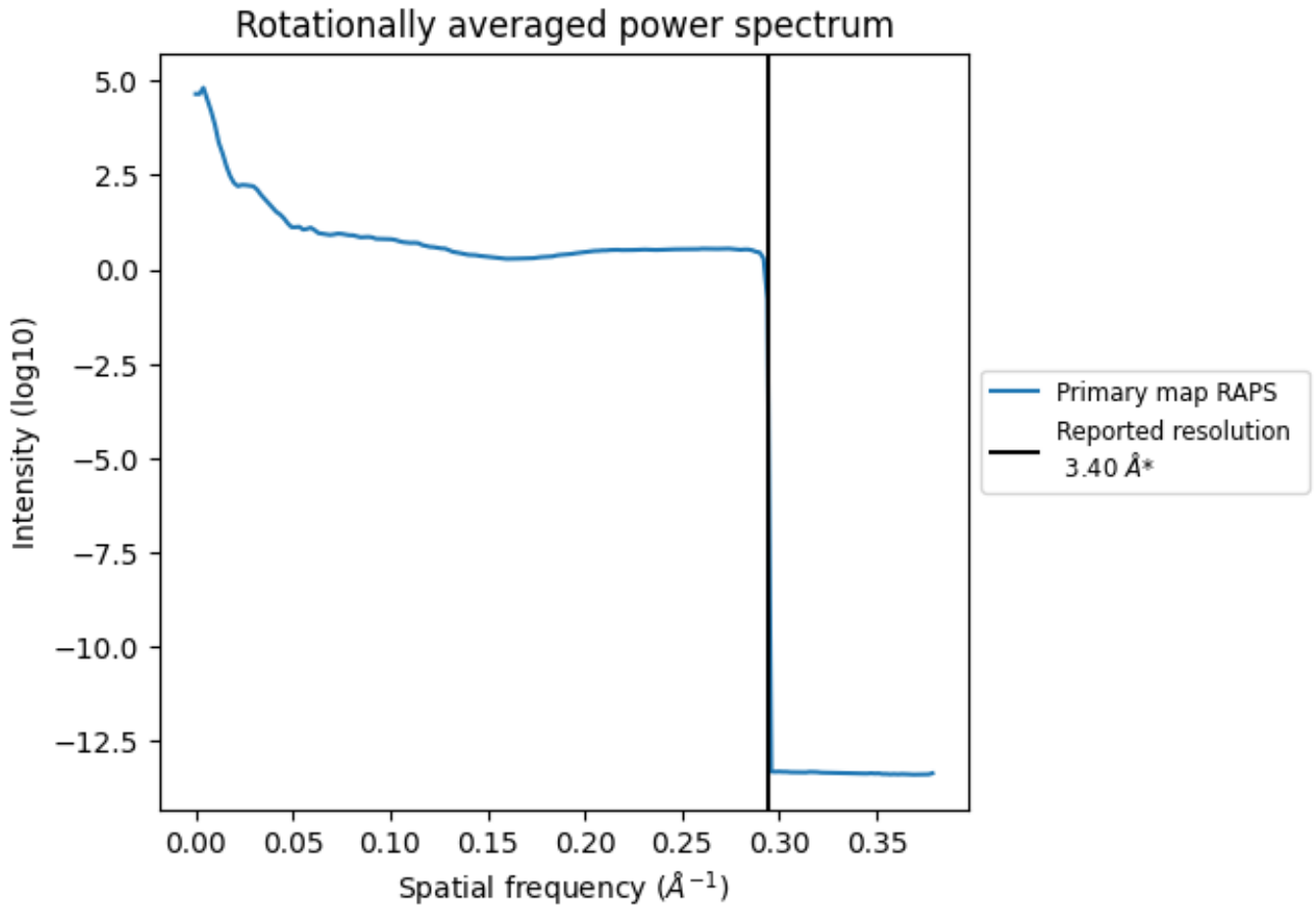
7.2 Volume estimate



The volume at the recommended contour level is 778 nm^3; this corresponds to an approximate mass of 703 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)

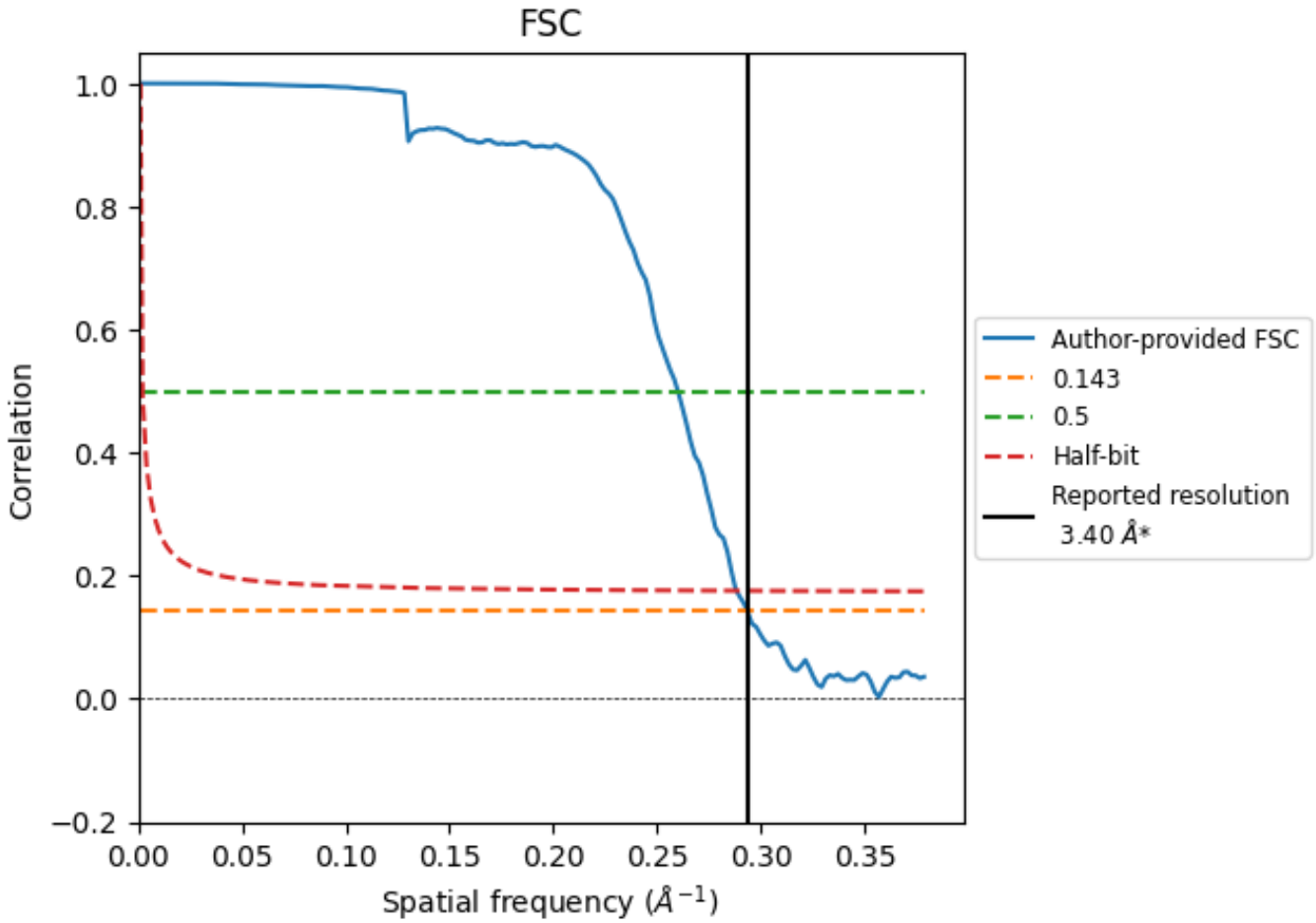


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

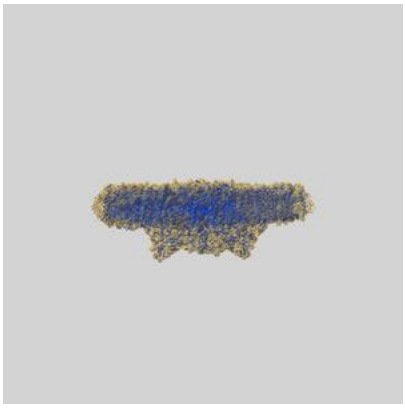
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.84	3.47
Unmasked-calculated*	-	-	-

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

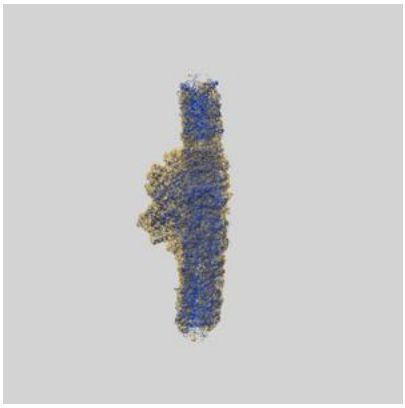
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9956 and PDB model 6KAD. Per-residue inclusion information can be found in section 3 on page 46.

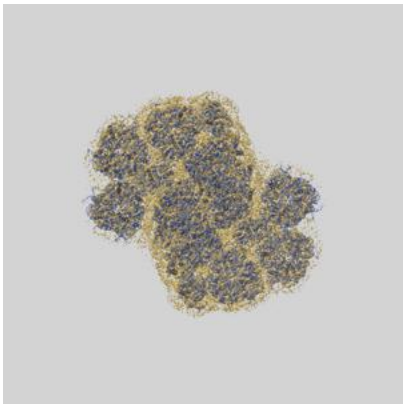
9.1 Map-model overlay



X



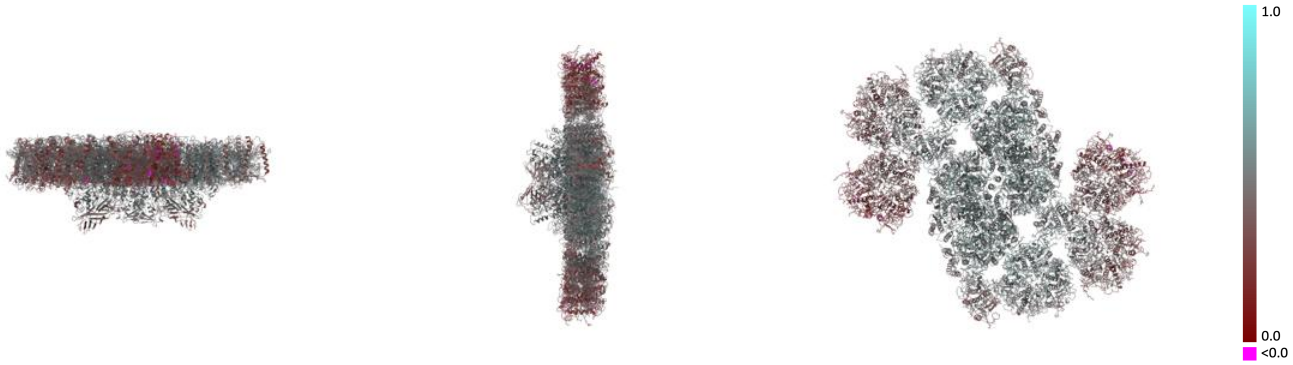
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

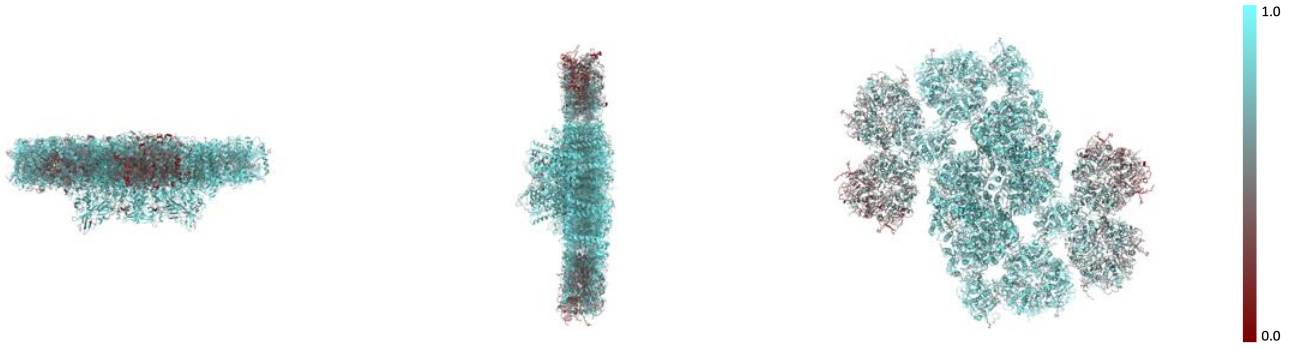
9.2 Q-score mapped to coordinate model (i)



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.

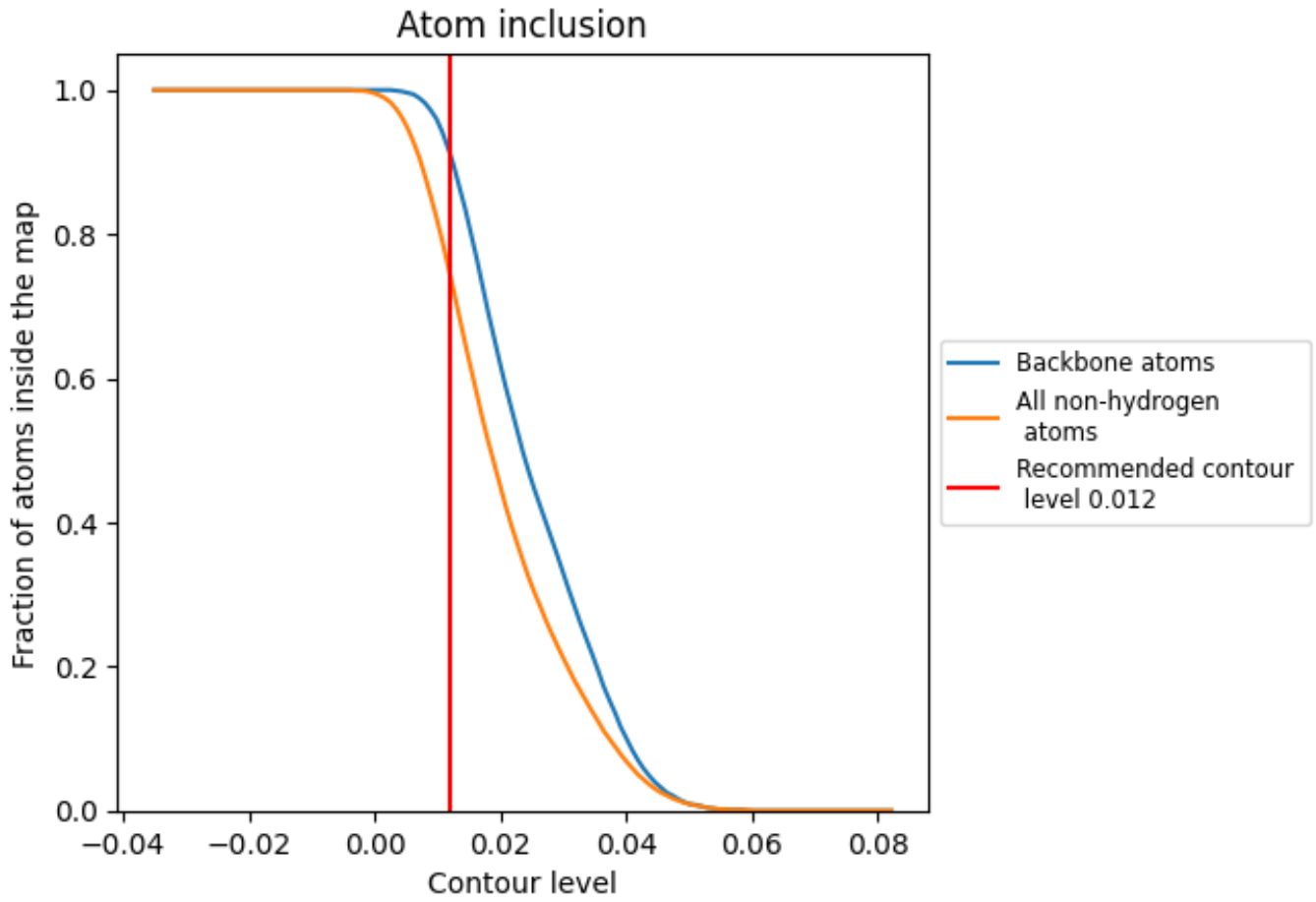
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 74% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.4470
0	0.5850	0.3510
1	0.7050	0.4440
2	0.5550	0.3430
3	0.5780	0.3480
4	0.4720	0.2850
5	0.3430	0.2540
6	0.5790	0.3470
7	0.7090	0.4440
8	0.5770	0.3480
9	0.5530	0.3450
A	0.8910	0.5300
B	0.8700	0.5130
C	0.8510	0.5210
D	0.8760	0.5310
E	0.8360	0.4570
F	0.8250	0.4730
G	0.8140	0.4810
H	0.8670	0.5040
I	0.9180	0.5410
J	0.8200	0.4730
K	0.8190	0.4820
L	0.8620	0.5240
M	0.8250	0.4920
N	0.8130	0.4780
O	0.7010	0.4070
R	0.8070	0.4930
S	0.7660	0.4230
T	0.8260	0.5120
V	0.7170	0.4120
W	0.8640	0.5140
X	0.8460	0.4760
Y	0.8580	0.5270
Z	0.7480	0.4270
a	0.8920	0.5310



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Chain	Atom inclusion	Q-score
b	0.8710	0.5120
c	0.8510	0.5200
d	0.8730	0.5330
e	0.8330	0.4510
f	0.8210	0.4720
g	0.8150	0.4810
h	0.8460	0.5020
i	0.9110	0.5400
j	0.8160	0.4750
k	0.8230	0.4810
l	0.8620	0.5230
m	0.8250	0.4950
n	0.8150	0.4800
o	0.7020	0.4060
p	0.3400	0.2440
q	0.4670	0.2820
r	0.8080	0.4940
s	0.7690	0.4240
t	0.8260	0.5120
v	0.7170	0.4140
w	0.8670	0.5090
x	0.8410	0.4710
y	0.8590	0.5250
z	0.7330	0.4220